Computational Science and Engineering: Challenges and Opportunities

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Contributions Towards a Centre for Computational Science and Engineering at NTNU and SINTEF

NTNU – Trondheim
Norwegian University of
Science and Technology

SINTEF

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The CSE Committee

Appointed by Rector at NTNU and CEO of SINTEF

Preface

Computational Science and Engineering (CSE) has become an inevitable research area focusing on the development and usage of computational methods to solve problems in science and engineering. NTNU and SINTEF have initiated a process to investigate gains from establishing a virtual and multi-disciplinary CSE centre that will foster excellence in the development and usage of computational methods within core research areas at the two institutions.

The initiative is based on the vision that CSE is an indispensable discipline for sustained development and welfare in the Norwegian society. The objective for a possible CSE centre is to be a driving force to move the frontiers in CSE and be a focal point at NTNU and SINTEF for technology transfer of advances in mathematics and informatics to applications in science and technology.

The (virtual) CSE centre is envisioned as a true collaboration between NTNU and SINTEF to achieve synergies between the two institutions' core activities. Joint development activities can give added value in terms of volume and quality, and make us more interesting to cooperate with for academic and industrial partners.

NTNU and SINTEF will include the ideas in the report in our strategic considerations. Initiation of strategic actions will be dependent on a good alignment of the proposed generic development areas in CSE and the key application areas that depend on their development.

Torbjørn Digernes
Rector NTNU

Unni Steinsmo
President – CEO SINTEF

A multidisciplinary research and innovation centre for solving advanced scientific and engineering problems by numerical simulations.

Contents

Executive summary

You have to run as fast as you can just to stay where you are. If you want to get anywhere, you'll have to run much faster.

Lewis Carroll

Computational science and engineering (CSE):
Computer simulations have become an essential methodology in science and engineering during the last decades, and in a wide variety of business fields, innovations are increasingly being based upon simulations. Advanced computer simulations are indispensable in our quest to understand the mechanisms behind climate changes. Likewise, there is a host of upcoming technologies that we cannot hope to utilize, develop, and understand without computer simulations. This is particularly evident at the crossroads to a new era where humans, for the first time, start creating structures and technologies at the scale of single atoms and molecules. Six decades after the invention of the digital computer, advanced simulations are used to enhance and leapfrog theoretical and experimental progress, but can also provide a powerful alternative when phenomena are not observable or when measurements are dangerous, impractical, or simply too expensive.

CSE Committee:
In 2008, NTNU and SINTEF decided to make a study of CSE and established a working group (CSE Committee) with a mandate to review the area, make a situation analysis, and establish a common understanding of the possibilities offered by CSE and the challenges faced by the two institutions in this area. During the autumn of 2008, the CSE Committee visited ten faculties/divisions and distributed a detailed questionnaire to relevant departments at NTNU/SINTEF. The responses from all the meetings and the answers to the questionnaire can generally be summarized as positive and enthusiastic. Based on this first phase, the CSE Committee recommended that a next step should be to produce an expanded "CSE Technology Strategy Report", including a technology review with contributions from internal and external experts. In addition, the report should contain an overview of relevant activities at departments and research centres at NTNU and SINTEF, focusing on research challenges and anticipated collaboration with a potential CSE centre. Invitations to contribute were sent to all faculties at NTNU and institutes in SINTEF; all contributions received by the committee appear in the second half of this report.

National and international trends:
Over the past decade, there have been a number of strategic reports discussing the importance of CSE for society at large, as well as many of the challenges. These reports give a backdrop for what kind of competition NTNU and SINTEF may expect in the future from other universities and research institutes, nationally and internationally. The main findings can be summarized as follows: CSE is indispensable for future progress in science and engineering. Formidable challenges remain to be solved, such as open problems related to multiscale and multiphysics modeling, real-time integration of simulation methods with measurement systems, model validation and verification, handling large data, and visualization. Significant investments in hardware and software are necessary to meet future demands in CSE, but should also be complemented by research on the computational methods that are required to meet the current and future needs to solve complex and coupled problems. Progress in CSE will require the creation of interdisciplinary teams that work together on leading-edge simulation problems. The organization of CSE activities may be realized in different ways and should be carefully assessed in each case. Last, but not least:

Proactive facilitation is needed to foster fruitful multidisciplinary CSE collaboration.

External experts:
Ten short position papers written by national and international experts review enabling technologies within CSE, discuss CSE as a means for scientific discovery, and demonstrate how CSE can be used to understand and improve products, processes, and workflows within industry and health care.

In the future, advanced CSE will be used to improve surgical procedures and develop patient-specific models that enable predictive treatment of cardiovascular diseases. High-performing simulators capable of handling a billion degrees of freedom will open new vistas in simulation-based science and engineering and multiscale modelling will improve the design of multiphase chemical reactors and high-voltage systems. Likewise, advanced computer science such as multiagent systems, semantic web, and cloud computing will be used to develop real-time and decision-support systems for the oil and gas industry and reduced-order models validated through high-performance computing will be used to optimize hydrocarbon production. These are just a few examples of how CSE will have a fundamental impact on tomorrow's society.

A common theme for many of the experts is the emphasis on development of models and computational algorithms, as well as use of high-performance computing facilities. In particular, the experts mention the need for high-performance linear algebra. This applies to the whole spectre of applications, i.e., from atomistic to large-scale mechanics and broad classes of solid, fluid, and heat problems. Here, development of open-source software is shown to be a productive way to engage the entire world of mathematicians and computer and application-oriented scientists.

Altogether, the external experts demonstrate how CSE and advanced computing facilities are indispensable enabling technologies to push frontiers in research and technology development.

Internal experts:
Eight short papers written by leading scientists at NTNU and SINTEF showcase the use of advanced CSE methods and highlight some of the research challenges.

Many areas face challenges in handling large amounts of data. Within seismics, molecular biology, and medical research, there is a need to store and process terabytes of data. Real-time processing of data and information is required to provide automatic control and monitoring of process plants, e.g., in the oil and gas industry. Similarly, in many applications there is a strong need for high-performance computing facilities, from bioinformatics and molecular dynamics to seismic imaging. Here, he rapid and dramatic change in computer architectures witnessed in recent years – moving from single-core to multi-core and many-core system – poses new challenges for algorithms and software. New heterogeneous hardware offers unprecedented computing capabilities, but much research is needed to develop efficient programming models and achieve good resource utilisation.

Similarly, scientists developing predictive models are often faced with problems crossing multiple spatial and temporal scales, e.g., within molecular dynamics and subsurface flow. Here, new multiscale approaches are shown to provide models that are more reliable and significantly more computationally efficient. As an example, one paper demonstrates clever use of multiscale methods to develop highly efficient reduced-order models for subsurface flow.

The presentations by the internal experts both illustrate the potential achieved today by clever use of computational methods as well as the significant challenges ahead of us.

Departments and research centres at NTNU and SINTEF:

A wide variety of scientific and engineering applications is reflected in the descriptions provided by eleven departments at NTNU, ten departments and two divisions at SINTEF, and three research centres. In broad terms, we may characterize most of the applications to be related to solid and fluid mechanics, spanning from atomistic to continuum scale. It may be noticed that many departments now are starting to take a multiscale viewpoint towards their problems. Thus, they ask for multidisciplinary collaboration on physical/chemical theories and computational methods handling different temporal and spatial scales.

The need to strengthen the collaboration between experimental testing and numerical simulation is highlighted by many departments. This was also one of the first observations made by the CSE Committee. Indeed, NTNU and SINTEF have a great opportunity to make such collaborations a competitive edge, if this is stimulated.

The interaction between departments focusing on enabling technology (mathematics and computer science, including cybernetics) and those focusing on application technologies is fragmented and decoupled. There seems to be a lot to gain by making this more institutional and binding. The historical lack of institutionalised collaboration is reflected in the lack of firm views upon the anticipated relationship with a future CSE centre.

The responses obtained from the departments at NTNU and SINTEF indicate an unexploited potential in strengthening collaboration between experimental testing and numerical simulation, as well as more structured interactions between departments of mathematics and computer science and the various departments in science and engineering.

Concluding remarks:

Advanced computation and simulation in science and engineering constitute an important area in rapid growth in many leading industrial nations. The background for this is the continued development of efficient numerical methods and computer hardware that has been seen over the past decades. The consequence is that new vistas have been opened for realistic computer simulations and use of mathematical models in engineering and science.

However, more skills and efforts have to be put into developing advanced computational methodologies and capabilities to be able to take full advantage of the rapid progress, nationally and internationally. This will require the creation of interdisciplinary CSE-teams that work together (with a long-term perspective) on leading-edge simulation problems. National and international experience shows that proactive facilitation is needed to foster fruitful multidisciplinary CSE collaboration.

The international experts demonstrate computational capabilities that are about 10–100 times higher than what is demonstrated internally at NTNU and SINTEF. This leap in computational capabilities is reflected in their ability to push the frontiers in science and technology with a much stronger force than researchers at NTNU and SINTEF.

The only way NTNU and SINTEF may take full advantage of the new opportunities presented by the rapid developments of computational methods and computer hardware is through multidisciplinary collaboration – a CSE centre will facilitate such collaboration.

Introduction

The purpose of computing is insight, not numbers!

R. W. Hamming

Background

Computational science and engineering (CSE) represents a means of scientific discovery that employs a computer system to study physical or man-made systems, as described by mathematical models that incorporate the laws derived from theory and experiments. The development of this field has drawn from a deep pool of scientific, mathematical, computational, and engineering knowledge and methodologies. Six decades after the invention of the digital computer, computational science has attained peer status with theory and experiments in many areas. However, computer simulation should not be mistaken as a magical wand. Simulations must be verified against the laws of the natural (or social) sciences and validated against experiments. Nevertheless, simulations can in certain cases provide a powerful alternative to the techniques of experimental science when the phenomenon of interest is not observable or when measurements are impossible, dangerous, impractical, or too expensive.

Over the past decade, there have been a number of strategic reports discussing the importance of CSE for society at large, as well as many of the challenges. The main findings can be summarized as follows: CSE is indispensable for future progress in science and engineering. Formidable challenges remain to be solved, such as open problems related to multiscale and multiphysics modelling, real-time integration of simulation methods with measurement systems, model validation and verification, handling large data, and visualization. Significant investments in hardware and software are necessary to meet future demands in CSE. Research in computational methods is needed to meet the current and future needs to solve complex and coupled problems. Progress in CSE will require the creation of interdisciplinary teams that work together on leading-edge simulation problems. Proactive facilitation is needed to foster fruitful multidisciplinary CSE collaboration. The organization of CSE activities may be realized in different ways and should be carefully assessed in each case.

In 2008 NTNU and SINTEF decided, working against this background, to make a study of CSE and established a CSE Committee with a mandate to review the area, make a situation analysis, and establish a common understanding of the possibilities offered by CSE and the challenges faced by the two institutions in this area. Implicitly, the mandate also asked the CSE Committee to make recommendations about how NTNU and SINTEF could become more proactive in this area, and if being proactive will be important in the coming years.

During the autumn of 2008, the CSE Committee visited ten faculties/divisions at NTNU/SINTEF. Following these meetings, each departmental head/research director was assigned the task to appoint members to be responsible for answering a web-based CSE questionnaire. The responses from all the meetings and the answers to the questionnaire can generally be summarized as positive and enthusiastic. All the units mentioned ongoing or future research activities that were interdisciplinary in nature and could greatly benefit from collaboration between experts in mathematics, computer science, and the specific applications. The CSE Committee explicitly stated its goal to establish a CSE centre, but tried to not advocate a specific model about how such a centre should be organized. In turn, this was rewarded, sometimes after inspiring discussions, by great openness and a receptive attitude towards the establishment of a formal CSE Centre at NTNU/SINTEF.

Based on this first phase, the CSE Committee recommended that a next step should be to produce an expanded "CSE Technology Strategy Report". Such a report should include a technology review with contributions from internal as well as external experts. Furthermore, it was emphasised that departments and research centres at NTNU and SINTEF should be invited to write a short overview of their activities, focusing on research challenges and anticipated collaboration relevant for a potential CSE centre. This way, the CSE Committee wanted to give examples of recent development in the CSE field – locally, nationally, and internationally – and implicitly also say something about state-of-the-art at NTNU and SINTEF. However, the main purpose for this report would be to serve as a platform for internal decisions and priorities toward establishing a CSE centre at NTNU/SINTEF. Furthermore, it was also anticipated that the report later could be used by NTNU and SINTEF, to showcase our research results and combined expertise towards internal and external academic partners, industry partners, and the Norwegian Research Council.

Structure of the report

The CSE Committee initiated the process of producing the "CSE Technology Strategic Report" medio 2009 by inviting contributors both internally and externally. All the received contributions have been carefully reviewed by the CSE Committee and there have been a number of iterations to attain the current level of quality.

The report consists of the following chapters:

1. National and international trends in CSE;
2. Scientific contributions invited externally (nationally and internationally);
3. Scientific contributions invited internally (NTNU/SINTEF);
4. Overview of research from departments and centres at NTNU/SINTEF.

The contributions within each chapter are presented in alphabetical order.

The first chapter gives a short overview of the national and international state-of-the-art in CSE, thereby giving a backdrop for what kind of competition NTNU and SINTEF may expect in the future from national and international universities and research institutes. The chapter also has a short discussion of how CSE initiatives are organized elsewhere.

The second chapter is meant to give insight into the challenges and potential of multidisciplinary research within CSE. Ten short position papers written by invited national and international experts give examples of the state-of-the-art within certain aspects of mathematics, computer science, and selected applications. The selection of topics is undoubtedly biased and non-inclusive, but we (the CSE Committee) still hope that the variety in topics and approaches serves its purpose and displays what can be achieve by increased focus on high-quality CSE research.

The third chapter gives a taste of ongoing research within NTNU and SINTEF on selected topics that are relevant for CSE. Beyond showcasing high-quality research performed at the two institutions, the intention of the chapter is to indicate the two institutions' ability and potential within the CSE field.

The fourth chapter tries to give insight into what research challenges selected departments and research centres at NTNU and SINTEF are facing that are relevant to the establishment of a CSE centre. Here, we have asked the departments to describe their research challenges and relevant activities and then share with us their anticipated wishes and relation to a potential future CSE centre.

Summary of the contributions from the external experts

Through ten short position papers written by national and international experts, we try to give the reader a taste of the state-of-the-art in CSE and what one can expect to achieve by blending excellence in mathematics and computer science and applying it to challenging real-life problems. In particular, the papers

show how leading-edge computational methods and access to high-performance computing facilities are indispensable to push research frontiers within areas such as quantum and molecular chemistry, material science, and transport phenomena.

Six of the papers demonstrate the use of CSE to understand and improve processes, products, and work processes in industry and medicine. **Fritz** and **Ritums** discuss how multiscale methods are applied within computational material science at ABB to improve insulation of high voltages in AC and DC transmission systems. **Boek** presents four examples of how he uses particulate computer simulations to study complex fluids and micro-scale flow in porous media for oilfield applications. Moving to a very different spatial scale, **Durlofsky** gives an introduction to simulation and optimization of flow processes in petroleum reservoirs and demonstrates how the use of reduced-order models "trained" by full-resolution, full-physics simulations can speed up the optimization of hydrocarbon recovery by a factor 400. **Hughes** gives a fascinating account of how CSE can be utilized to enable "predictive medicine" through the use of patient-specific models to improve the treatment of cardiovascular diseases. **Wlodarczyk et al.** discuss the use of multi-agent systems, semantic web, and cloud computing as a means to develop real-time alarm and decision-support systems for the oil and gas industry. Finally, **Deen et al.** describe the use of front-tracking, immersed-boundary methods, and multiscale methods for quantitative description of transport phenomena and chemical transformations in multiphase chemical reactors.

Likewise, two of the papers discuss how advanced computations are used as a means for scientific discovery. **Hjorth-Jensen** shows how high-performance computing can be used to understand nuclear many-body problems through large-scale ab inition calculations. **Ruud's** contribution gives an overview of computational quantum chemistry where the aim is to understand how the building blocks of atoms, the nuclei and the electrons, interact with each other to create molecules.

Finally, two of the papers discuss enabling computational technologies. **Keyes** presents the TOPS project that is researching, developing, deploying, and disseminating a toolkit of open-source solvers to be used for *petascale* computing of scientific and engineering applications. The development of the TOPS software is shown to be a productive way to engage the entire world of computational mathematicians, computer scientists, and application-oriented scientists. **Fischer** discusses how high-order spectral methods combined with high-performance computing can be used to study transport phenomena in a wide range of applications. The contribution demonstrates highly operable software handling *a billion* degrees of freedom, which opens up new vistas regarding simulation-based science and engineering.

A common theme for all the contributions is the emphasis on both development of mathematical/numerical algorithms and access to high-performance computing facilities. In particular, many of the external experts mention the need for high-performance numerical linear algebra. This applies for the whole spectre of applications, i.e., from atomistic to large-scale mechanics and broad classes of solid, fluid, and heat problems.

Summary of the contributions from the internal experts

Eight short papers written by leading scientist at NTNU and SINTEF were selected to showcase the variety in research approaches and some of the methodological and application expertise and that exist at the two institutions.

Four of the papers discuss scientific and engineering problems relevant to petroleum production, which is a major strategic research area at NTNU/SINTEF. Starting at the micro-scale, **Hansen** presents fundamental research on how oil and water compete in individual pores in subsurface rocks. Moving up several length scales, **Lie** argues that multiscale approaches can be fruitful to model subsurface flows in a more reliable and efficient way and demonstrates clever use

of multiscale methods to develop highly efficient reduced-order models for use in optimization and data integration. **Arntsen** discusses research challenges in seismic imaging, modelling, and inversion and points, in particular, to challenges associated with handling *hundreds of terabytes* of data. **Johansen** shows optimization of oil and gas production as an example of engineering cybernetics: the field that deals with real-time processing of data and information for the purpose of automatic control and monitoring.

The paper by **Drabløs** is representative of another strategic research area: bioinformatics is a computer-based discipline in which approaches from computer science (and mathematics) are used to analyse complex data from molecular biology and medicine. Molecular dynamics, as presented by **Kjelstrup**, is another area in which advanced computations and multiscale approaches have made a tremendous impact.

The last two papers focus on generic computational technologies. **Rønquist** discusses higher-order methods for incompressible flow and challenges and approaches for problems with moving boundaries. **Natvig** discusses the rapid change in hardware architecture we are facing today and presents the P6-model (Parallel Processing challenges: Performance, Portability, Programmability and Power efficiency) that summarises the conflicting aspects that have to be balanced for optimal utilization of current and future hardware generations.

International and national trends

Over the past decade there have been a number of reports discussing the importance of CSE for the society at large, but also pointing to many of the challenges. In some of the reports, CSE goes under the name simulation-based science and engineering (SBES). Given the leading role the USA has played in the development of this area, it is not surprising that many of these reports have come from there; see [1-5]. We mention three reports in particular:

- The WTEC report [1] is a community-driven report written by experts from academia, government agencies, and industry in the USA. The report gives a thorough international assessment of research and development in simulation-based science and engineering.
- The SBES Report [3] is a report of the National Science Foundation from 2006, with contributions from many leading scientists and engineers (the NSF Blue Ribbon Panel on Simulation-Based Engineering Science).
- The ScaLeS Report [4] is a two-volume report made for the Office of Science, U.S. Department of Energy in 2003. More than 300 active scientists from leading universities, national laboratories, and industry contributed to this report.

All three reports have had a significant influence and are often cited. Even though the emphasis is on US interests, many of the findings and recommendations are, in our opinion, quite universal and relevant for other nations as well. Given the intellectual resources expended to produce these reports, it is worthwhile recalling some of the main findings:

Computer simulation is more pervasive today and having more impact than ever before – hardly a field is untouched, and many are (completely) transformed by the possibility of performing realistic simulations.

CSE is indispensable to future progress in science and engineering.

Formidable challenges remain to be solved in many areas, including mathematical modelling, algorithm development, software development, efficient use of new hardware, and education and training of the next generation engineers and scientists.

The main recommendations given in these reports all emphasize the importance of interdisciplinary research, a proactive role to address the educational aspect, and sufficient investment in, and challenges related to, hardware and software development. The reports also point to important tipping points: computers are now affordable and accessible to researchers in every country around the world. The entry-cost for performing computer simulations is almost zero, meaning that anyone in principle can practise CSE from anywhere. Furthemore, next generation massively multicore computer chip architectures promise unprecedented accuracy and resolution, as well as the ability to solve the highly complex problems that face society today. Finally, and perhaps most importantly, the toughest scientific and technological problems facing society today are grand challenge problems, whose solution requires a partnership between experiment, theory, and simulation, and between industry, academia, and government, working across disciplines.

Among the more local surveys of simulation-based science, we mention the Nordic survey on grand-challenge problem [6], the scientific progress report from Notur [7] that gives an overview of high-performance simulation in Norway, and the report leading up to the eVITA program [8], which discusses the need for a large research program in eScience, which has a significant overlap with CSE.

Computational methods

Most people are aware of the tremendous development that has happened in computer hardware the last decades. However, it is important to realize that there have also been enormous developments in basic theory and algorithms over the first six decades of scientific computing, and that these improvements have contributed as much to increases in compu-

tational simulation capability as improvements in hardware and software; e.g., see [4]. Significant progress has been made in modelling approaches: multiphysics approaches enable us to couple models from multiple scientific disciplines, multiscale approaches enable us to model phenomena that involve the interaction of different physical processes acting on multiple scales, etc. Modern discretization methods preserve important physical principles, are adaptive, and can offer high-order approximations, possibly with goal-oriented error control. Iterative methods in linear algebra scale (almost) linearly with the number of unknowns to be solved for (as opposed to classical elimination methods that scale with power 2-3). Advanced gridding and visualization techniques enable us to build models with high realism and present models and data in an intuitive manner. Likewise, statistical methods can be used to analyse large data sets, assimilate and integrate measured data, and quantify uncertainty in models and their predicted outcome. Finally, algorithms for concurrent computing enable the use of high-performance parallel computers, whereas hardware-aware methods can be used to auto-tune the performance to the underlying architecture of a particular computer.

Despite the enormous wealth of impressive computational methods, further research is necessary to meet the ever increasing demand for more complex, realistic, and predictive simulations; see [1–4, 9–13]. In particular, new methods are needed to perform uncertainty quantification, to model stochastic problems, and to improve integration of simulation with observations and real-time measurement etc.

Computational infrastructure

Modern simulation models are often very sophisticated and computationally intensive and usually consist of subtasks that have quite different computational characteristics; this is discussed extensively in the recent Berkeley report [14]. One example is multiscale methods that integrate discrete particle and continuum submodels.

A key prerequisite to employing such simulation models is the efficient utilization of computational resources. Traditionally, these have come in two flavours: serial simulation on PCs and workstations, and parallel simulations on clusters and other specialized high-performance hardware. This situation, however, has changed dramatically in recent years: simplified solutions for building computer clusters based on commodity hardware enable virtually anybody to set up their own small-scale high-performance facility. Likewise, parallel processors have recently entered the mass marked; today, multicore processors with 2-8 cores are found in all new PCs and are often accompanied by a many-core hardware accelerator for computer graphics (so-called GPUs) that may contain up to 1600 cores. This development has a simple physical reason: the microprocessor industry is no longer able to increase frequency and performance of single-core processors because this leads to higher power consumption than what is economically feasible. The solution is to use multiple cores, and multicore processors are now emerging in all markets from embedded systems to supercomputers.

As researchers and programmers have come to realize that serial performance has reached its zenith, there has been an increased focus on new algorithms that can benefit from parallel and heterogeneous architectures. Further insight into different architectures, and their implications on algorithm performance, is essential in algorithm design and for application developers to bridge the gap between peak performance and experienced performance. Most applications consist of a mixture of serial and parallel tasks, and will ultimately perform best on heterogeneous architectures. The optimal type and composition of processors, however, will vary from one application to another; see [14]. Heterogeneous computing [15] refers to the use of heterogeneous (or asymmetric) processing cores with different compute characteristics to maximize performance.

In particular, the combination of multi-core CPUs and

many-core accelerators (GPUs) offers unprecedented floating-point processing power and energy efficiency. Hardware accelerators, like GPUs, are special-purpose hardware designed to maximize the performance of a restricted set of operations, and will hence deliver a much higher number of floating point operations per second or per watt than traditional CPUs. Complex functionality is also sacrificed, disabling their ability to run operating systems. Instead, accelerator cores are managed by traditional cores and are used mainly to offload resource intensive operations. Such heterogeneous systems, consisting of traditional multicore architectures in combination with accelerator cores, have got increasingly popular in recent years even though they break with the traditional evolutionary processor design path. The most recent Top500 list [16], which ranks the most powerful supercomputers in the world, illustrates how GPU technology is at the forefront: the fastest system worldwide in theoretical performance is the Chinese Nebulae, based on GPU technology with 2.98 petaflops. Furthermore, current generation GPU solutions for computation boost up to 2.5teraflops double-precision performance in a standard 1U server chassis, and twice that in single precision. This trend is expected to continue and there seems to be an increasing community of researchers believing that future high-performance computing will be heterogeneous. This means increased challenges on the programming side, but also increased rewards at the performance side.

Software development

Software development has generally been a major challenge within high-performance computing. Special attention and skills were required to exploit the early vector machines, while parallel programming has been a challenge for many research groups in recent years. Software development does not seem to get easier with the presence of multicore technology and special many-core hardware accelerators. The number of available processors in a supercomputer has also been steadily increasing, making it challenging to achieve scalability across all aspects of a simulation process (e.g., scalability in the communication between processors, scalability in the numerical algorithms, scalability in handling larger and larger data sets, etc.).

However, over the last couple of decades we have seen significant progress in certain areas of software development. First, we now have a standardized interface for communicating between processors across a large set of processors (MPI – Message Passing Interface). Likewise, there are vendor-driven initiatives like OpenCL that aim to develop a framework for writing programs that execute across heterogeneous platforms consisting of CPUs, GPUs, and other processors.

Second, we have witnessed the successful development of very efficient and robust libraries for basic linear algebra operations (e.g., BLAS, LAPACK, ATLAS, etc) that may be auto-tuned for optimal utilization of underlying hardware. Much effort has also been devoted to the development of higher level libraries (e.g., PETSc, TOPs). Despite this progress, software development is a challenge for many research groups.

An important aspects related to software development is maintenance and continuity of larger simulation codes used by a number of researchers or a whole research community. This is an important, but costly, task that is not always rewarded in a similar way as traditional academic research. This can be a particular challenge for many smaller research groups. However, for larger community codes (e.g., molecular dynamics codes), this type of effort may be coordinated by a research laboratory (e.g., Sandia National Laboratory), with contributions from many institutions around the world. It may also be coordinated in a CSE centre, as for example in Julich where they have developed a “numerical laboratory” for a specific class of application (e.g., plasma physics). Two other trends are supporting this development: open-

source software has a strong position in academic circles. Likewise, there is an increasing awareness about the lack of reproducibility and replicability in many simulation-based publications. Imposing this fundamental scientific principle in CSE will inevitably lead to a significantly more pronounced focus on open and sustainable software development.

One of the major challenges over the next few years will be to develop numerical infrastructure that can exploit the huge number of processors becoming available (e.g., hundreds of thousands). With this aspect in mind, it will be a significant advantage to be using a community-based code versus having to develop and maintain a local research code only used my a few researchers. We speculate that there is a possibility that we will get a new "class society", separating those who are able to exploit the new hardware becoming available and those who are not.

2.4. The interdisciplinary challenge – CSE Centres

CSE is a highly interdisciplinary activity and this has been recognized for many years. Nonetheless, it has proven nontrivial to realize a successful concept in practice. Different universities and research laboratories have addressed this issue in various ways. A number of CSE centres have been established around the world, each having their own unique feature, which seems to suggest that there is no predetermined "template" or "formula" for how to organize such a centre.

The main discriminating factors seem to be: (i) whether a centre has its own building(s) or whether the centre is virtual; (ii) the type of impact of the centre, i.e., whether it plays an important role on a local, national, or international level; (iii) the scientific focus of the centre, i.e., whether this represents a balanced emphasis on mathematics, computer science, and applications (MAC), or on only one or two of these areas; (iv) the type of groups and collaborations that are promoted by the centre.

Examples of CSE centres are *Institute for Computational Engineering and Sciences (ICES)* at University of Texas at Austin, U.S.A., and *Institute for Advanced Simulation (IAS)* in Julich, Germany. Both of these centres possess the combined interdisciplinary expertise necessary to solve challenging problems in science and engineering. New institutions are also embracing the idea of interdisciplinary research and development. An example of this is *King Abdullah University of Science and Technology (KAUST)* in Saudia Arabia. The closest one gets to a CSE centre in Norway is probably SIMULA Research Laboratory, where a large number of experts in mathematics and computer science are co-located with applications expertise in medicine and geosciences. Their focus on the development of a sustainable numerical infrastructure as a prerequisite for scientific discovery in other fields is at the core of the CSE idea.

We also remark that addressing challenging problems in science and engineering through simulation has been emphasized in the USA at a level that go beyond a single institution like a university or research laboratory. For example, the US Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program is a multi-institutional effort to address important scientific problems requiring unprecedented computing resources.

National trends

Norway is quite fragmented when it comes to CSE. All the major universities have strong research groups in mathematics and computer science that potentially could and should interact with application scientists. However, such interactions are typically based on collaborations involving a few persons rather than the supporting institutions. During the last decade there has been a trend towards forming research centres based upon the SFF, SFI, and FME funding schemes from the Research Council of Norway. With the exception of Centre of Mathematics for Applications at the University of Oslo, all these centres are applica-

tion driven and have limited focus on generic activities in CSE to support a wide range of applications within science and engineering. Likewise, most of the large programmes at the Research Council of Norway focus on specific application areas (Climit, Fuge, Nanomat, Petromaks, Renergi, etc) and development of advanced simulation capabilities is at most a side activity with limited coordination.

Norway has been involved in supercomputing since the mid 1980s when the first Cray computer was purchased and the Supercomputing programme (or "Tungregneprogrammet") was established. The main focus of the Supercomputing programme was the computational infrastructure, in particular, maintaining and upgrading the high-end computers. The supercomputers were used by the national universities and the Meteorological Institute (currently called met.no). Around 2000, the NOTUR project was established with the aim to better coordinate the investment in national infrastructure for supercomputing, with the main focus still on hardware. Some funding was also channelled towards helping research groups acquire better competence in CSE (primarily the Technology Transfer Programmes). Still, a large number of the users of the national supercomputing infrastructure are using old legacy codes based on computational methods that long ago were bypassed by more recent developments.

Around 2000, the BeMatA programme was established with a focus on providing funding for research in computational methods. Funding for basic research was balanced with funding for more applied research, in particular, research in computational methods with relevance to marine applications. The following eVITA programme was established in 2005 as an initiative to coordinate the funding for high-performance computing facilities and computational methods. Quoting the website of the Research Council of Norway:

> *"eVITA is a research and infrastructure programme designed to address computing and data-intensive challenges in science, technology and medicine. By promoting research on methodologies, competence development and investment in new eInfrastructure, eVITA will work to ensure that Norwegian research in the eSciences achieves a high international standing, and seek to address important national challenges in the national priority areas of energy and the environment, oceans, food, and health."*

Unfortunately, the allocated budget has so far been too limited to allow the program to seriously address the need for methodological development and national coordination within CSE in particular and eScience in general.

Altogether, this lack of long-term investment in computational methods and a sustainable numerical infrastructure means that Norwegian academic institutions and industry is lagging behind in the use of advanced simulations and is missing out on a lot of the opportunities that such simulations create in applications of national importance.

Education

Computational science and engineering (CSE) offers a computational approach to solve problems in science and engineering that complements a pure theoretical and/or experimental approach. CSE has emerged because of the rapid advances in computational methods and computational infrastructure. The field naturally combines skills from many different fields. This interdisciplinary nature will also impact future education [17]. We already see the emergence of specific CSE programmes in universities, at least at a graduate level, perhaps not so much at the undergraduate level. (A noteworthy exception is the "Computers in Science Education" initiative at the University of Oslo, see [20].) The introduction of "Computational X" classes is fairly common. As a

recent example from Norway, we have the Computational Neuroscience programme at UMB; see [18].

What seems clear is that the strict borders between different departments are starting to become blurred. As an example, we mention the MSc program in Computation for Design and Optimization at MIT which started in 2006 [19]. However, it is also clear that many current university programmes are not sensitive enough to this development; it is not always easy for today's students to mix classes from different departments in order to gain a sufficiently broad set of interdisciplinary skills.

We have seen a trend over the past few years towards using more computation and simulation in various classes. For example, it is now fairly common to use commercial software packages like Matlab and Maple in undergraduate education in order to complement and illustrate theoretical results. Students are also more and more expected to be able to use computational tools for project work. However, most students have insufficient skills in numerical methods, software development, and how to exploit modern computer architecture to solve problems in their own domain-specific fields.

One thing is certain: computational science is here to stay.

Finally: *It is of the utmost importance for the future credibility of computational science to educate students with a critical mindset towards the use of modelling and computation.*

1.7. Conclusions

CSE is indispensable to future progress in science and engineering.

CSE has attained peer status with theory and experiments in many areas.

Formidable challenges remain to be solved, such as open problems related to multiscale and multiphysics modelling, real-time integration of simulation methods with measurement systems, model validation and verification, handling large data, and visualization.

Significant investments in hardware and software are necessary in order to meet future demands within CSE.

Research in computational methods is necessary to meet the current and future needs to solve more and more complex and coupled problems.

Progress in CSE will require the creation of interdisciplinary teams that work together on leading-edge simulation problems.

The organization of CSE activities may be realized in different ways and should be carefully assessed in each case.

Proactive facilitation is needed to foster fruitful multidisciplinary CSE collaboration

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Simulation of complex fluids and flow in porous media

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POROUS MEDIA

My research is aimed at the flow of complex fluids in porous media. Whilst at Schlumberger Cambridge Research, my work has been aimed mainly at various applications in the oilfield, including the design of drilling fluids, hydraulic fracturing operations, reservoir fluids and Enhanced Oil Recovery. I use particulate computer simulations to study how the complex flow behaviour emerges from the properties of both the underlying fluid and the porous medium. For this purpose, I have developed a range of statistical mechanical simulation techniques, across length and time scales. These include (Ab Initio) Molecular Dynamics (MD), Dissipative Particle Dynamics (DPD), Brownian Dynamics (BD), Multi-Particle Collision Dynamics (MPCD or SRD) and lattice-Boltzmann (LB) simulations. In the following, I will elaborate a few cases in more detail.

Clay swelling

During oil exploration, drilling through shale beds often causes serious problems, caused by the uptake of water from the drilling fluid by swelling clay minerals. To elucidate the molecular mechanisms underlying clay swelling, I have used Monte Carlo (MC) simulations [1] followed by Ab Initio Molecular Dynamics (AIMD) simulations [2]. These simulations have revealed the differences between the hydration and adsorption of Na+ and K+ cations in the clay interlayer spacing. The main computational challenge in this field is the upscaling of the swelling behaviour from the molecular to the continuum scale [3].

Wormlike micelles

Certain surfactants self-assemble into wormlike micelles in an aqueous environment and disassemble into spherical micelles when they see oil. This type of surfactant, forming visco-elastic gels, is ideally suited for hydraulic fracturing operations to stimulate reservoir production. The design of surfactants which form stable, viscous, wormlike micellar solutions at high temperature is a topic of major research interest. I have developed a multi-scale simulation methodology to design these surfactant fluids from first principles, using a number of coarse-graining steps. [4] In the first step, MD simulations are used to calculate the mechanical properties for a small segment of a wormlike micelle. These properties are used in subsequent Brownian Dynamics (BD) simulations to obtain the rheological properties of an ensemble of wormlike micelles. I have carried out rheological measurements and found excellent agreement between experiment and simulation [5]. The rheology can be modified if non-uniform shear rates within the rock pores cause migration and non-uniform concentration of micelles, as shown in subsequent BD simulations in a contraction-expansion capillary [6,7], see Figs.1 and 2. The big challenge in this field is to coarse-grain from the mesoscopic to the continuum (Darcy) level.

Asphaltenes

Controlling the deposition of asphaltenes in oil reservoirs is a major problem in recovery of hydrocarbons. I have developed a colloidal dynamics simulation technique, called Multi Particle Collision Dynamics

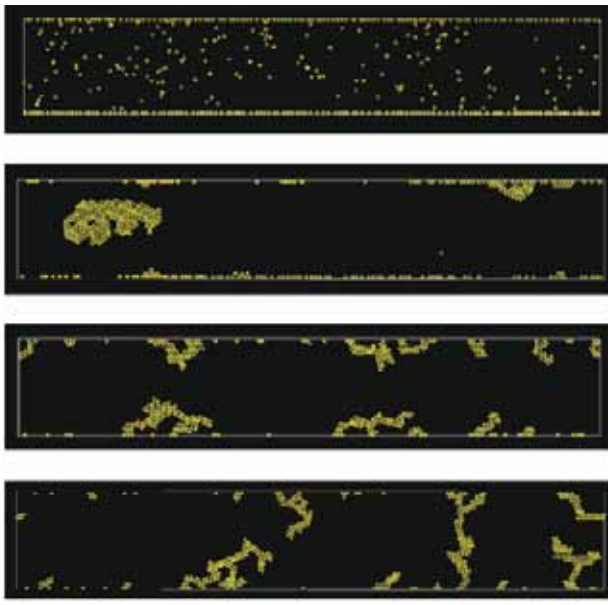

Figure 1: Example of a simulated contraction-expansion pore space containing a long wormlike micelle [7].

(MPCD) to investigate the aggregation and deposition of colloidal asphaltenes in capillary flow [8], see Figure 3. Capillary flow experiments show excellent agreement with the simulation results for the dimensionless conductivity. At the molecular scale, I have developed a methodology to determine Quantitative Molecular Structures (QMR) of asphaltenes, based on experimental data, such as molecular weight and elemental analysis [9]. It turns out that only a small number of structures is required to describe the experimental properties of asphaltenes. Recently, we have upscaled the molecular representation to the nano-aggregate level [10]. The big challenge in this area is to coarse-grain the behaviour of asphaltenes from the molecular to the continuum level.

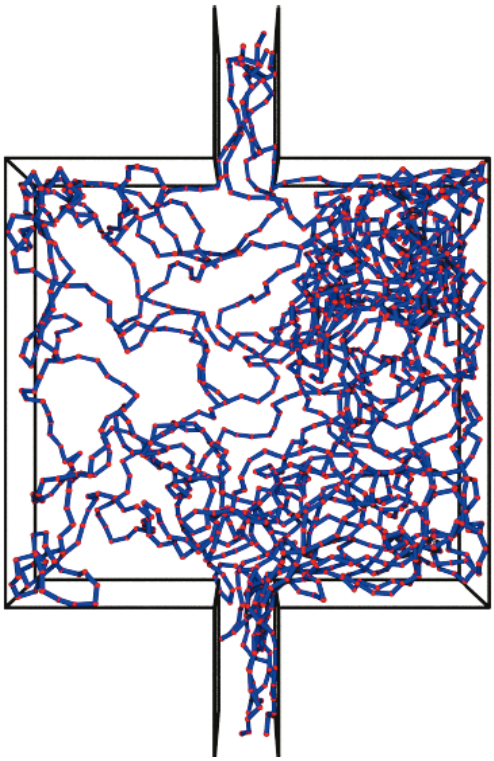

Figure 2: Computed concentrations of viscoelastic surfactant solution (VES) flowing (top to bottom) through an expansion- contraction [7].

FLOW OF COMPLEX FLUIDS IN POROUS MEDIA

It is of great fundamental and practical interest to investigate the flow of complex multi-phase fluids, as they flow through porous media. I focus on the development of lattice-Boltzmann (LB) simulation methods to study flow at the pore scale. In particular, I have developed LB models to study immiscible

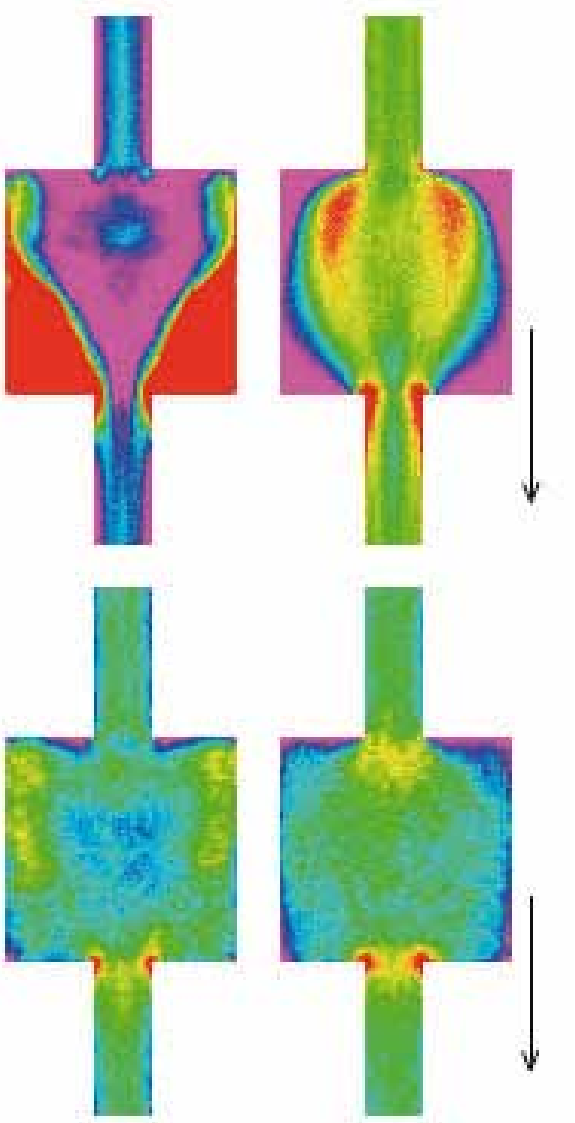

Figure 3: Simulation snapshots for asphaltene deposition steady-state behaviour as a function of increasing colloid – colloid potential well depths [8]: from top to bottom 2, 5, 10 and 20 kT.

fluid flow in porous media [11]. This model was extended to study the flow of non-Newtonian fluids [12]. A powerful simplification can be made through replacing the 3D flow by an equivalent 2D flow, using an effective viscous drag force, based on lubrication theory. In this fashion I have studied viscous fingering in a Hele-Shaw cell [13], both for immiscible and chemically reactive fluids. I have conducted simulations to compare the flow field in a 2D micro-model of a Berea sandstone. Using the LB flow field, a particle tracking algorithm is used to calculate the dispersion of tracer particles in the Berea geometry [14]. Using XMT data of Bentheimer sandstone, I have calculated single phase and immiscible (oil-water) displacement in 3D rock geometries [14]. It turns out that the relative permeability can be reliably calculated from the LB simulations. This is an important contribution in the field of Enhanced Oil Recovery (EOR) processes. The big challenge in this area is the calculation of relative permeability curves for representative rock samples from first principles.

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Fundamentals of chemical reaction engineering

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The research group Fundamentals of Chemical Reaction Engineering (FCRE) focuses on fundamentals of the discipline of chemical reaction engineering. Our main area of interest is the quantitative description of transport phenomena (including fluid flow) and the interplay with chemical transformations in multiphase chemical reactors. The generation of new knowledge and the development of new reactor models with improved predictive capability for this industrially important class of chemical reactors constitute an important goal for our research activities. Through the planned cooperation with other (application oriented) research groups, both fundamental aspects and those closely related to applications are studied by our concerted action.

The fundamental study of multiphase chemical reactors is closely linked to the topic of this report, i.e. Computational Science and Engineering. Our work in this field is illustrated by two examples of computational results obtained through different computational fluid dynamics (CFD) techniques. Figure 1 shows the capabilities of a hybrid front tracking-immersed boundary model to study the effect of particle properties on bubble-induced drift (Deen et al. 2009). Figure 2 shows an example of a discrete particle model (DPM) where the simulation of a spout fluidized bed involving dispersed particles and droplets that are brought into motion by a fluidizing gas. The influence of the restitution coefficient is investigated in this example. This parameter depends on the stiffness of the particle material, as well as the physical properties of the liquid layer around the particles (van Buijtenen et al. 2009).

FUTURE OUTLOOK

Dense dispersed multiphase flows have been the subject of intense research over the past few decades owing to its wealth of scientifically interesting phenomena as well as its direct relevance for innumerable industrial applications. For instance, large-scale dense gas-solid flows are notoriously complex and its phenomena difficult to predict. This finds its origin in the large separation of relevant scales: particle-particle and particle-gas interactions at the microscale (< 1 mm) dictate the phenomena that occur at the macroscale (> 1 metre), the fundamental understanding of which poses a huge challenge for both the scientific and technological community. This is exemplified most clearly by the fact that state-of-the-art reactor design of multibillion dollar industries is still mainly

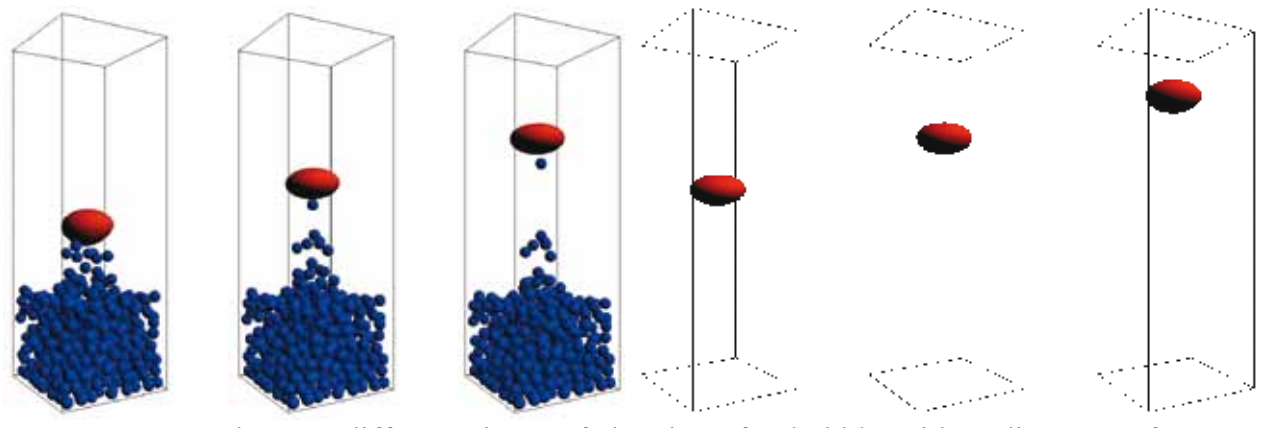

Figure 1: Snapshots at different times of the rise of a bubble with a diameter of 0.02 m through a suspension of 512 spherical particles (left) and liquid without particles (right).

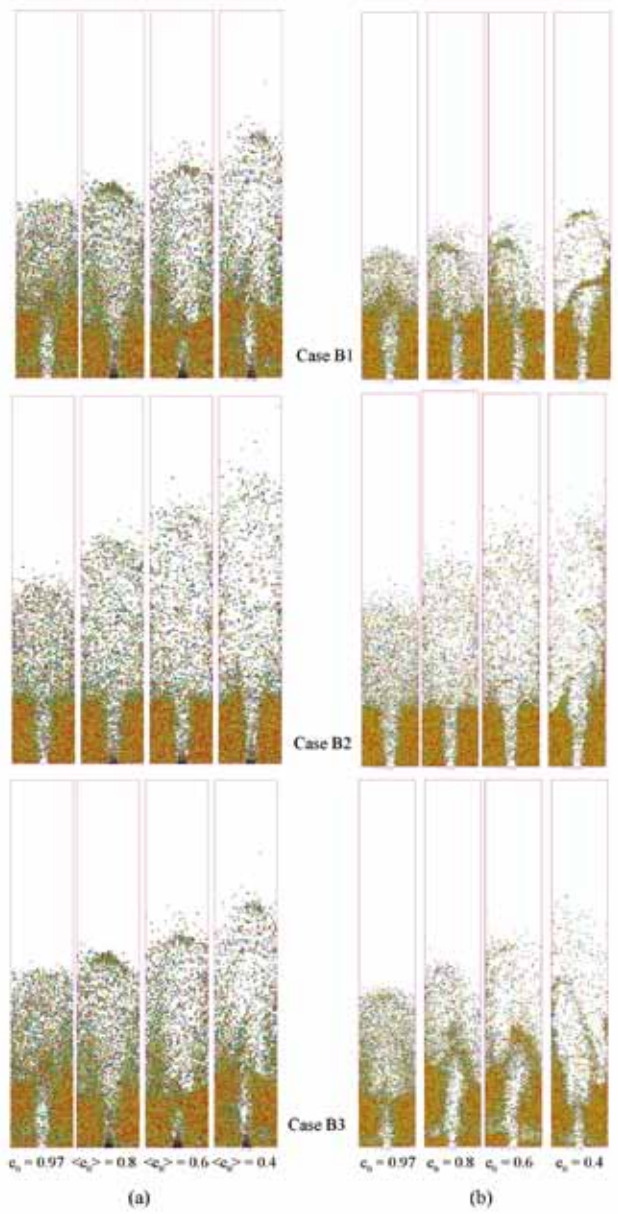

Figure 2: Discrete particle simulation snapshots of the instantaneous particle positions in a spout fluidized for different variable restitution coefficients (a) and different constant restitution coefficients (b) for case B1 (intermediate / spout - fluidization regime), B2 (spouting-with-aeration regime) and B3 (jet-in-fluidized-bed regime).

an empirical process, which relies heavily on extensive experimentation conducted at laboratory scale and subsequently at pilot-scale.

In future research we want to take up this challenge and work towards a fundamental understanding of large-scale mass and heat transfer, based on the physical processes that take place at the most detailed level, namely the exchange of mass and heat at the scale of the particle surface. We will employ a multi-scale approach where the gas-solid flow is described by three different models (see Figure 3): one where the flow between the particles is fully resolved (detailed scale),

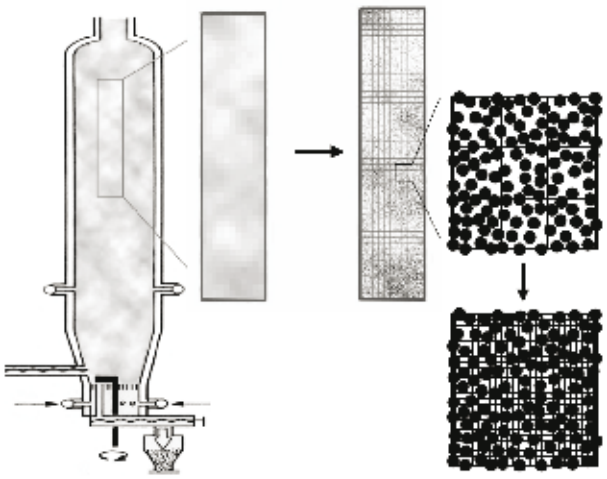

Figure 3: Graphic representation of the multi-level modelling scheme. The arrows represent a change of model. On the left there is a fluidized bed on a life-size scale that can be modelled with the aid of phenomenological models, a section of which is modelled by the two-fluid model (see enlargement), where the shade of grey in a cell indicates the solid phase volume fraction. On the right, the same section is modelled using discrete particles. The gas phase is solved on the same grid as in the two-fluid model. The bottom graph shows the most detailed level, where the gas phase is solved on a grid that is much smaller than the size of the particles, (after van der Hoef et al. 2006).

one where the flow is unresolved (intermediate scale), and one where the particle and gas phase are considered as interpenetrating continua (large scale). Such an approach is by widely recognized now as the most rigorous and viable pathway to obtain a full understanding of dense gas-solid flow, and has become very topical in chemical engineering science. The unique aspect of this approach is the scale and the comprehensiveness of the research. We intend to study the exchange of heat, momentum and energy, and the effects of polydispersity and heterogeneity, at all three levels of modelling. All of this needs to be validated by one-to-one experiments. The generated insight and models will be extremely relevant for the design and scale-up of industrial equipment involving dispersed particulate flow, and could in the future replace the expensive and time-consuming trial-and-error experimentation process.

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Simulation and optimization of subsurface flow processes

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Subsurface flow simulations are a key component in the design and optimization of oil and gas production operations. Such simulations will have an analogous role in the planning and management of geological carbon sequestration. The equations appearing in these formulations describe the movement of one or more components (such as methane, octane, water, and carbon dioxide) flowing within one or more phases (aqueous, oleic, vapour) through porous formations such as oil reservoirs or aquifers. The governing partial differential equations are derived by writing mass conservation equations for each component. These equations are then combined with appropriate constitutive relations, in this case Darcy's law for multiphase flow, as well as thermodynamic models for phase behaviour. Darcy's law is widely used in subsurface flow modelling – it relates phase flow rates to pressure gradients in terms of rock properties (absolute permeability), fluid properties (viscosities) and rock-fluid interactions (relative permeability functions). In some cases, additional physics must be incorporated – examples include chemical reactions, thermal effects and geomechanical effects – which lead to additional equations and couplings.

The numerical solution of the subsurface flow equations requires discretization on a computational grid. The most commonly used discretization procedures are based on finite volume approaches, though finite elements are used in some cases. The generation of a suitable grid can be a challenge, as geometrically complex geological features such as faults, fractures and layering can strongly impact flow and may therefore need to be resolved. Wells can also lead to gridding challenges, as they can be quite general geometrically (e.g., multibranched) and can intersect geological features at arbitrary angles.

There are a number of key complications associated with practical subsurface flow modelling. These include the multiphysics and multi-scale aspects of many problems, the computational requirements associated with optimization, and the need to handle geological uncertainty. We now consider two examples of subsurface flow problems that illustrate some of these challenges.

IN-SITU UPGRADING

Increasing demand for oil is expected to result in a shift away from light, easy-to-produce crude oils toward heavy oils and possibly to other unconventional resources such as oil shales. Shell's in-situ conversion process, which is still in the pilot testing stage, is one of the approaches being studied for oil shale production. In this process, heat is introduced into the reservoir through high-temperature (~375 °C) downhole heaters. This facilitates a sequence of chemical reactions, which convert the in-situ high-carbon-number resource into more desirable products (lighter components). Simulating this process is difficult, however, as it entails chemical reaction modelling coupled to multiphase fluid flow, thermal and geomechanical effects, and porosity/permeability evolution. Flow simulations of this and related processes will be essential, however, if these operations are to be fully understood and optimized.

Our group has recently developed a prototype capability for modelling the in-situ upgrading of oil shales. These simulations include components in the solid, oleic and vapor phases, solution of the energy equation to determine the temperature field, and the modeling of temperature-dependent chemical reactions which describe the transformation of solid kerogen (an oil precursor present in the oil shale) to light oil and gas components.

Simulation results for this problem are presented in Figure 1, where we show a top view of reservoir temperature and oil saturation at different times. The locations of the six downhole electrical heaters are evident in the early-time temperature plots; the production well is at the centre. Oil is generated first near the heaters and then throughout the reservoir, and is essentially all produced by 500 days. The tim-

ing for oil and gas production, as well as the relative amounts of oil and gas produced, depend on the heater temperature and spacing. Thus, this type of model can be used to optimize in-situ upgrading processes. Although these simulations are highly demanding computationally, there are still many effects that are simplified (e.g., the chemical reaction system) or neglected entirely (geomechanics, porosity/permeability evolution, reservoir heterogeneity) in our model. The development of more comprehensive formulations will therefore be very useful.

OPTIMIZATION OF SUBSURFACE FLOW PROCESSES

Simulation models are increasingly being used to optimize subsurface operations. Examples include determining the optimal placement of new wells and finding optimal settings (rates, well pressures) for existing wells in order to maximize an objective function such as net present value. Optimizations of this type can be very demanding computationally as they typically require many simulations. Both gradient-based and gradient-free techniques are being investigated and applied for these optimizations. Gradient-based procedures can be very efficient, though they converge to local optima. Some gradient-free procedures, by contrast, explore the global search space though they may require many more simulations. The incorporation of geological uncertainty into these optimizations, which can be achieved by optimizing over many geological realizations, adds substantially to computational demands.

The large computational requirements associated with optimization are a concern in many application areas, and researchers have devised a number of reduced-order modelling (ROM) procedures to accelerate the function evaluations (simulations) required for optimization. The idea in ROM procedures is to establish a simplified representation for the model that is valid over a certain range. Construction of the ROM requires some number of 'training' simulations, which are full-resolution, full-physics simulations. Training simulation results are then used to generate very fast surrogate models that can be applied in optimizations.

Here we present an example of this approach for subsurface flow modelling. The particular ROM in this case was constructed using a 'trajectory piecewise

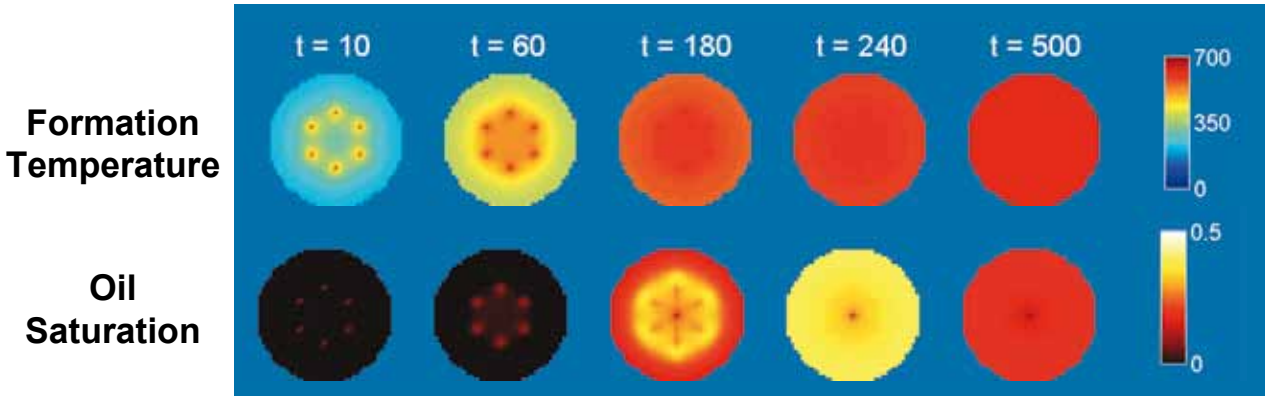

Figure 1: Top view of oil shale reservoir simulation results showing temperature (top row) and oil saturation (bottom row) at different times (from Fan, Durlofsky and Tchelepi, SPE 118958, 2009)

linearization' (TPWL) in which the simulation model is linearized and then represented in a reduced form using a special projection matrix. The optimization here is bi-objective – it seeks to determine well pressures that maximize the cumulative oil production while minimizing cumulative water injection. This requires a total of about 14,000 simulation runs. The result, shown in Figure 2, is a Pareto front, which defines the set of optimal solutions. In this figure, the ×s (TPWL) designate the optimization results using the ROM surrogate, while the solid circles and triangles represent optimized solutions that use the fully-resolved model. It is evident that the ROM surrogate provides a reasonable level of accuracy for this optimization. The overall speedup using the ROM is quite dramatic here, about a factor of 400 relative to the full-resolution model. This is, however, a fairly simple oil-water simulation containing relatively few (24,000) grid blocks and a limited range of well settings. An outstanding challenge is to extend and generalize ROM procedures to more complicated cases such as the in-situ upgrading example discussed above.

There are of course many other interesting issues in subsurface flow modelling that are not considered here. These include multi-scale treatments, history matching (inverse problem) procedures, closed-loop reservoir modelling, uncertainty quantification, and the inclusion of additional physics in simulation models

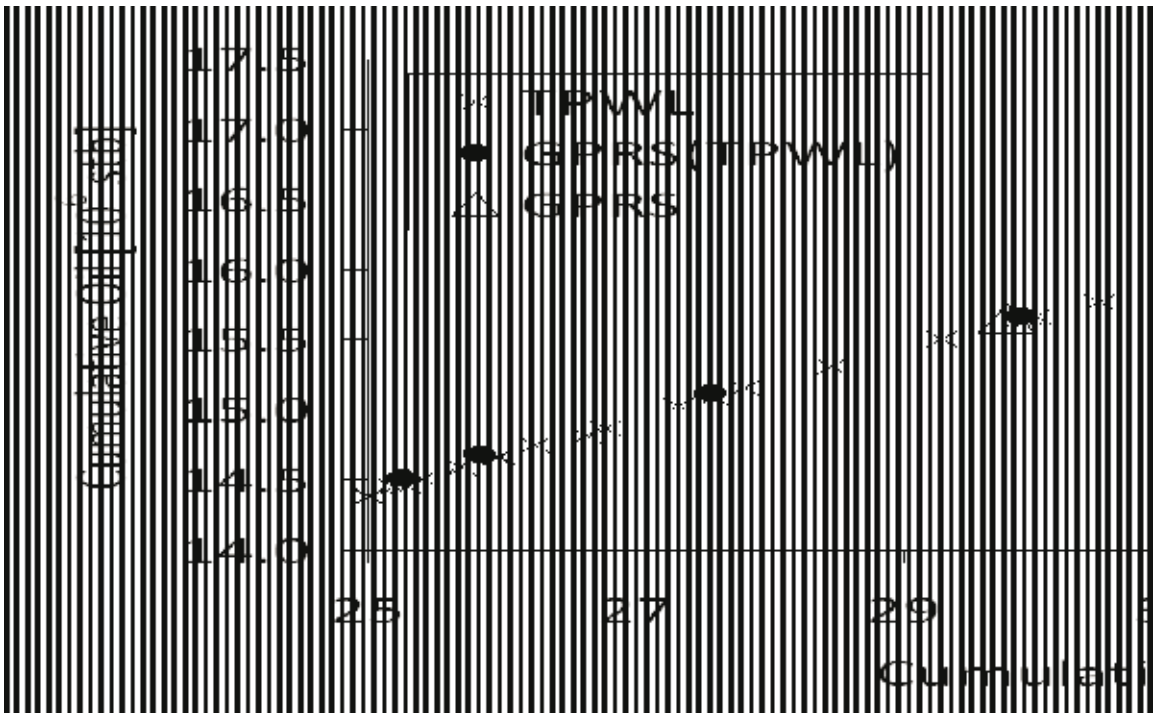

Figure 2: Optimized cumulative oil produced versus cumulative water injected. TPWL denotes ROM results while GPRS and GPRS(TPWL) designate full-resolution simulations performed using Stanford's General Purpose Research Simulator (from Cardoso and Durlofsky, J. Comp. Phys. 229, 2010).

Simulation of transport phenomena

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Simulation-based science is a major research thrust at Argonne, ranging from nanophotonics to accelerator design, reactor design, astrophysics, biofluids, and ab initio calculations of nuclear properties. Argonne researchers also address algorithmic, software, and computer science questions arising at the petascale and beyond. Cutting-edge research is facilitated by access to the IBM Blue Gene/P – one of the world's fastest computers – in the Argonne Leadership Computing Facility.

Our group develops numerical algorithms and software for simulating transport phenomena. A principal driver is the need to simulate feature interaction over a broad range of scales. For example, current accelerator designs call for picosecond wave packets propagated over tens of meters. Meaningful predictions over such distances require highly accurate numerical discretizations to minimize cumulative errors. Our codes are based on the high-order spectral element method, which provides rapid convergence and geometric flexibility. We have developed fast multilevel solvers having iteration counts that are bounded independent of problem size that are capable of scaling beyond a million processors. These developments have enabled the study of challenging problems, including high-Reynolds number flows in reactor cores, turbulence in vascular flows, onset of magnetorotational instabilities in MHD flow, influence of bottom topography on density-driven ocean currents, and interaction of light with nanoscale particles. We discuss two of these in detail.

Nuclear power is a promising approach to carbon-free energy. One element of a comprehensive reactor programme calls for fast recycling reactors that transmute minor actinides produced by light water reactors and thus reduce load demands in geological repositories. Our group uses Argonne's BG/P to study thermal hydraulics within the core and upper plenum

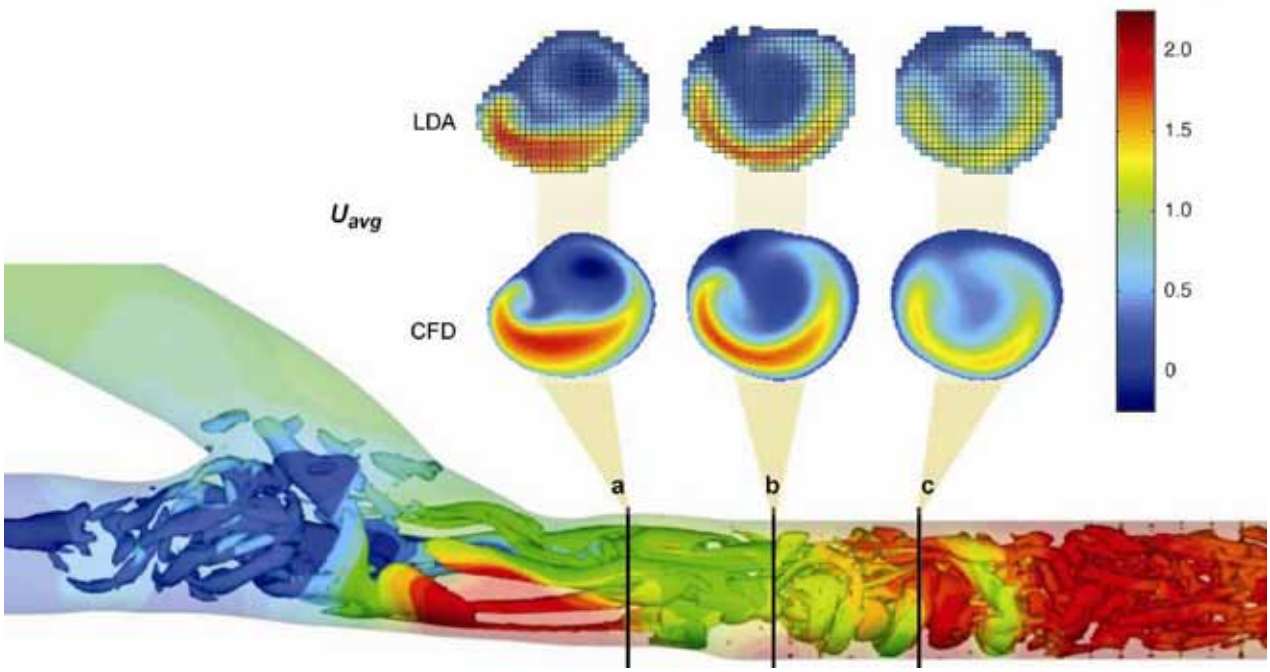

Figure 1: Experimental (LDA) and simulation (CFD) predictions of turbulent flow in an arteriovenous graph. Cross sections show time-average velocity distributions (m/s) while the lower figure shows turbulent vortices, coloured by pressure.

region – among the least understood elements of the design. We employ a hierarchy of simulation fidelities, including direct numerical simulation for simple geometries, large eddy simulation (LES) and Reynolds-averaged based models for more complex geometries, and subchannel codes for the full reactor. The fluid-thermal codes are being coupled to neutronics and structural mechanics codes to simulate feedback effects. The validated codes will guide design analysis, previously possible only through experiments, thus dramatically cutting costs.

The reactor project is pushing the envelope for complex-domain Navier-Stokes simulations. The attached figure shows the pressure distribution computed using LES for a fuel subassembly with 217 wire-wrapped fuel pins over a single wire pitch (length H). Simulations of wire-induced mixing are being compared with experiments. The discretization comprises 3 million spectral elements of order N=7, for a total of 1 billion gridpoints. The calculation sustains 80% parallel efficiency on 130 000 processors. Reactor designs call for hundreds of subassemblies of length ~10H. Macroscopic effects will require simulating all the subassemblies, increasing the problem size by three orders of magnitude. LES will be used to validate Reynolds-averaged models for coarser-resolution simulations, which will then be scaled to the full reactor problem.

Biomedicine is another promising area for simulation. With the biofluids group of Frank Loth (U. Akron) and the surgical team of Hisham Bassiouny (U. Chicago), we use simulation to understand how turbulence influences the failure of arteriovenous (AV) grafts, which provide dialysis ports for patients with kidney disease. AV grafts are synthetic tubes that are surgically implanted to provide a round-the-clock short circuit from an artery to a vein. By connecting high-pressure vessels to low-pressure ones, high flow rates are established that result in efficient dialysis. Unfortunately, the flow is accompanied by transition to a weakly turbulent state, manifested as a 200–300 Hz vibration at the vein wall. This excitation overstimulates smooth muscle cell growth interior to the vein, which can lead to complete vein occlusion and to graft failure within six months of implant.

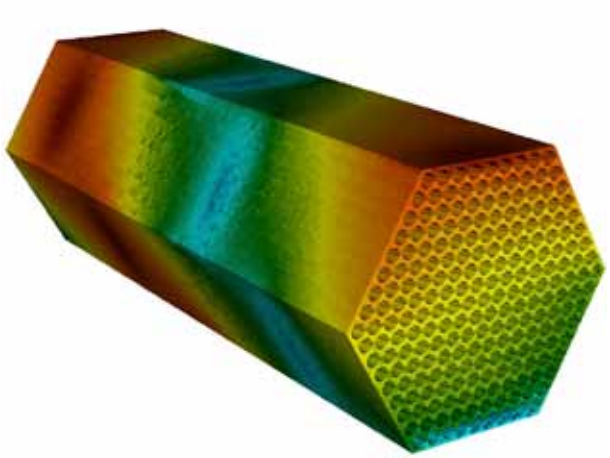

Figure 2: Pressure distribution for turbulent flow in a reactor fuel bundle.

Because such flows are not fully turbulent, they lack an inertial subrange amenable to subgrid-scale modelling required for LES or Reynolds-averaged Navier-Stokes simulations. Currently, one must directly resolve all scales of motion; and since the physical dissipation is small, high-order methods are essential for efficiency. Weakly turbulent blood flow exhibits a much broader range of scales than its healthy counterpart and thus requires an order of magnitude increase in spatial and temporal resolution, making fast iterative solvers and parallel computing essential. We focus on subject-specific modelling in which we compare in vivo data, in vitro LDA measurements, and spectral element simulations for a given geometry. The accompanying figure attests to the reliability of the spectral element predictions. To date, we have identified what are and are not sources of turbulence in AV grafts, with the relative size of the inlet and outlet ports identified as a major factor in triggering transition.

Computational material science at ABB

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Computational Material Science and Engineering has a long tradition in ABB, not only in our global corporate research organization, but also in many of our product-development units. Our ambition to offer leading technology for power distribution and automation, optimal control and efficient, sustainable use of energy in the industrial environment of our customers requires a high degree of research in various methods of computational science.

Obvious fields of activity are calculations and simulations of electro-magnetic fields, semiconductor technology, coupled electric and thermal transport, fluid dynamics, plasma physics and structural mechanics. In general, finite element and finite volume methods for the solution of partial differential equations are in widespread use. In this contribution, we rather wish to highlight on some aspects of our increased interest in computational material science.

Insulation of high voltages in AC and DC transmission systems is a challenge for a variety of reasons. This is particularly for the increasingly popular transmission of high voltages through DC cables. Here a more microscopic picture of electric transport and other dynamic processes is needed. Therefore, to a clearly larger extent than before, we will investigate the predictive power of multi-scale methods used in computational chemistry and materials science. Two examples:

From density functional theory ("ab initio" quantum mechanical calculations) we expect a clearer picture of the particular mechanisms of electron transport in cross-linker polyethylene. Earlier work [1] was recently revisited and the massively increased computational power of today was used to come to more precise and quantitative analysis. An increased understanding of electron transport in polymeric insulators by applying molecular modelling techniques to estimate the trapping ability of likely physical and chemical traps present in polyethylene is highly beneficial when trying to optimize and control the amount of additives, the selection of catalysts in a production process, as well as when estimating dielectric strength for dimensioning whole systems. Computational mapping of the full electron levels of embedded defects allows a microscopic calculation of hopping-based electron and other charge transport models. Figure 1 shows a realization of a tridecane ensemble with identified chemically active points.

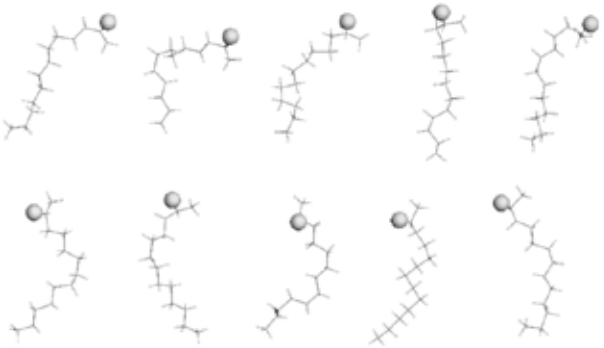

Figure 1: Tridecane chain ensembles from recent new simulations are presented (unpublished). The ball indicates the highest electrostatic potential of a defect which serves as a basis for estimating electron trapping depth.

A second example from polymeric insulation materials is about diffusion processes of light-weight molecules through a larger-weight matrix. Such diffusion processes may depend on a number of characteristic quantities that need to be calculated with molecular dynamics methods. Force fields used for calculating realizations of the amorphous state of Silicone Rubber (PDMS, Polymethylhydrosiloxane) are the basis for a whole research project on molecular diffusion processes under the influence of high electric fields. A high-performance computing environment and massively parallel algorithms allow for large enough ensembles of molecules in order to avoid typical shortcomings of finite size or incorrect ground-state description of amorphous systems (Figure 2). Both long chains of PDMS as well as cross-linked molecules

of a much smaller weight can be simulated together in one system. One of the specific goals of this project is a quantitative evaluation of surface-directed diffusion of lighter molecules in order to understand certain surface properties of outdoor insulation materials.

In general, dielectric strength and the microscopic understanding of breakdown are and will increasingly be fields of computation-based research. For gases, insulating liquids and solid insulation a common picture of discharge mechanisms may emerge through the combination of analytical theories with precise simulations. A microscopically sound description of the charge carriers involved and their molecular properties will allow for the better development of efficient insulation technologies for the future demand of high-voltage transmission equipment. Also, the inclusion of chemical reactions and aspects of degradation and ageing are of increasing interest.

When looking far into the future, detailed knowledge of material states, properties, and dynamics are a condition for designing material-intrinsic diagnostics. Contemplating the role of "smart materials" and their relation to the now ever-present discussion of the "smart transmission and distribution grid", there is considerable fascination in using embedded, material-adapted diagnostic functionality based on a microscopic understanding, simulation and measurement of degradation processes in insulator materials. Clear knowledge of the health-state of high voltage transmission components will be a future requirement in a lifetime-cost driven business environment.

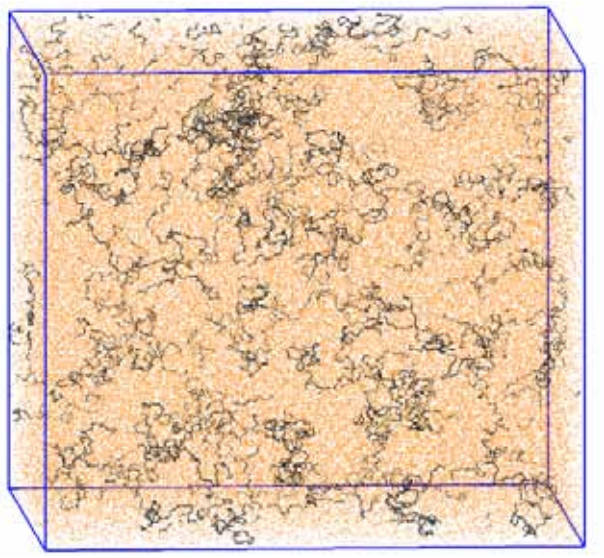

Figure 2: Shown are PDMS plus crosslinker molecules before reaction. About one million atoms are contained in box of 20x20x20 nm3. The dark chains represent about 200 crosslinker molecules. Molecular dynamics simulations of this size require high-performance computers and highly parallel algorithms.

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Ab initio approaches to quantum mechanical many-body problems in nuclear physics

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Nuclei comprise 99.9% of all baryonic matter in the universe and are the fuel that burns in stars. The rather complex nature of the nuclear forces among protons and neutrons generates a broad range and diversity in the nuclear phenomena that we observe. Furthermore, these rare nuclei lie at the heart of nucleosynthesis processes in the universe and are therefore an important component in the puzzle of matter generation in the universe. Experiments indicate that developing a comprehensive description of all nuclei and their reactions requires theoretical and experimental investigations of rare isotopes with unusual neutron-to-proton ratios that are very different from their stable counterparts. These rare nuclei are difficult to produce and study experimentally since they can have extremely short lifetimes. Theoretical approaches to these nuclei involve solving the nuclear quantum many-body problem.

The many-body problem spans nuclei from A=2 (the deuteron) to the superheavy region, and different theoretical techniques are pursued in different regions of the chart of nuclei. This is depicted in Fig. 1 where the current reach of various theoretical methods is interposed in the chart of nuclei.

Many-body quantum mechanics deals with the development of stable algorithms and numerical methods for solving Schrödinger's or Dirac's equations for many interacting particles in order to gain information about a given system. Typical examples of popular many-body methods are coupled-cluster methods, various types of Monte Carlo methods, perturbative expansions, Green's function methods, the density-matrix renormalization group, density-functional theory and large-scale diagonalization methods just to mention some of the more popular ones. The numerical algorithms cover a broad range of mathematical methods, from linear algebra problems to Monte Carlo simulations. Furthermore, high-performance computing topics such as efficient parallelization are central to any serious study of many-body problems.

The nuclear many-body problem is particularly difficult to solve due to the complex character of the nucleon-nucleon and three-nucleon interactions. The numerical problems are compounded for rare isotopes with an unusual ratio of proton to neutron number, and for nuclei along the drip lines. These nuclei are the focus of current experimental programs in low-energy nuclear physics. This means that one needs to account for the fact that many of the nuclei close to the stability line can be weakly bound and therefore the nuclear interactions will couple bound, continuum, and resonant states. This leads to a further increase in dimensionality compared with stable nuclei. The current worldwide experimental programmes address topics which are of great relevance for our understanding of the stability of matter itself, with applications and relevance to many other fields, including astrophysics (synthesis of elements in the universe and stellar evolution), particle physics (using nuclei to discover physics beyond the Standard Model), and societal applications.

In the context of the various algorithms and approaches referenced above, the challenges for understanding nuclei are to determine the nuclear interaction and calculate from that interaction nuclear properties. This may involve including any continuum aspects when necessary. In addition, nuclear theorists are working toward determining an appropriate energy density functional for a nuclear Density Functional theory approach which should eventually have connections to the ab initio approaches.

The rapid growth in computational hardware that has spanned the last 40 years has enabled continuous and breathtaking advances in the way we attempt to solve our theoretical problems. Not only do computers allow us to solve larger problems in the same framework as on previous systems, but they also allow for innovation and applications of computing to new classes of problems that could not have been previously considered. In considering algorithms currently applied to the nuclear ab initio problem, other methods, such as

Green's function Monte Carlo approaches and large-scale diagonalization, scale exponentially with particle number for a given accuracy. Coupled-cluster theory (a widely used ab initio method in quantum chemistry), on the other hand, scales as a polynomial with the number of particles and the number of single-particle basis states.

Using the coupled-cluster method, we have recently been able to perform, see Refs.~[1-3], the large-scale

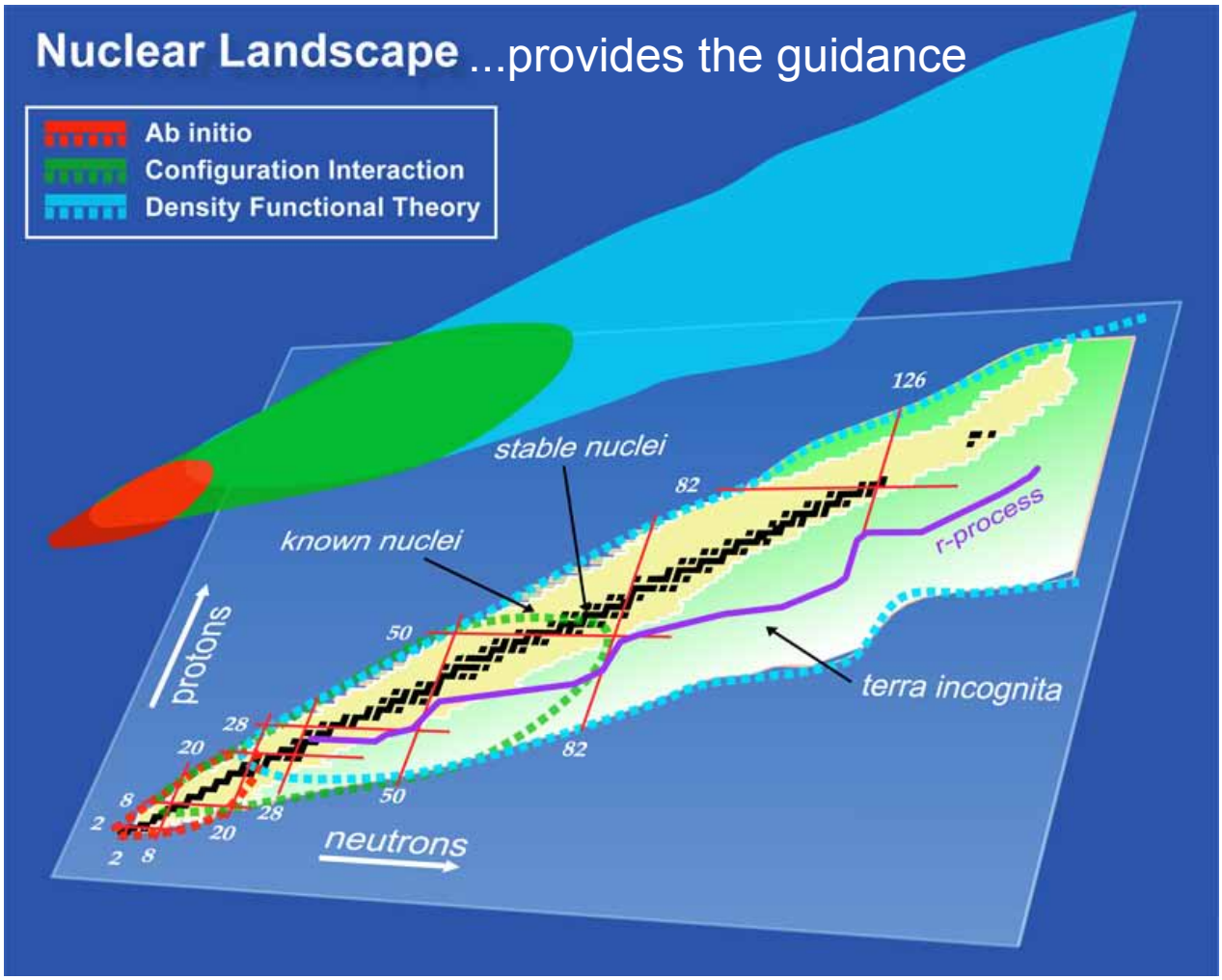

Figure 1: The theoretical methods and computational techniques used to solve the nuclear many-body problem. The red vertical and horizontal lines show the magic numbers, reflecting regions where nuclei are expected to be more tightly bound and have longer half-lives. The anticipated path of the astrophysical r-process responsible for nucleosynthesis of heavy elements is also shown (purple line). The thick dotted lines indicate domains of major theoretical approaches to the nuclear many-body problem. For the lightest nuclei, ab initio calculations (Green's function Monte Carlo, no-core shell model, coupled cluster method), based on the bare nucleon-nucleon interaction, are possible (red). Medium-mass nuclei can be treated by configuration interaction techniques [interacting shell model (green)]. For heavy nuclei, the density functional theory, based on self-consistent/mean-field theory (blue), is the tool of choice. By investigating the intersections between these theoretical strategies, the aim is to develop a unified description of the nucleus.

ab initio calculation of nuclei in the mass region of calcium and nickel isotopes, dealing in practice with a number of configurations close to ten to the power of 100 Slater determinants.

The coupled-cluster equations define a non-linear set of coupled equations. The typical very large number of unknowns makes a direct solution of the non-linear equations infeasible, and one has to resort to iterative approaches in order to obtain solutions of the equations. In the largest calculation we have performed to date we solved some ten to the power of nine non-linear equations on 1000 2Gb parallel processors at Oak Ridge National laboratory in the USA. Stable and convergent solutions of such large sets of non-linear equations require implementation of sophisticated mathematical techniques. We have implemented convergence accelerators such as the direct inversion in the iterative subspace and the modified Broyden method. The aim of these iterative methods is to construct an optimal vector which minimizes the non-linear equations at each iterative step.

Our future aims are to perform ab initio calculations of the binding energies and other ground state properties of all so-called closed-shell nuclei, from helium to lead. One of the major goals from these investigations is to be able to understand better nuclear correlations, in particular those which arise from three-body interactions. This may allows us to define better density functionals for nuclei, functionals which in turn can be used to study properties of nuclei beyond the domain of ab initio methods.

Without the access to present-day supercomputing facilities, such an ambitious project is not possible.

I am much indebted to my colleagues David Dean, Gaute Hagen and Thomas Papenbrock at Oak Ridge National Laboratory and the University of Tennessee, Knoxville, for our long-standing collaboration on ab initio methods.

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The predictive paradigm for the treatment of cardiovascular disease

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Engineering has played an increasing role in medicine in my lifetime. That will undoubtedly continue, but I believe it is also about to take on a new and fundamentally different role that will have profound consequences in the future.

Here are some data from the American Heart Association. Cardiovascular disease (CVD) is the leading cause of death of both men and women in the United States and the entire industrialized world. By 2010 it is estimated that it will be the leading cause of death in the developing world as well. In 2002, over 70 million Americans suffered from one or more types of CVD, over 43 million were under the age of 65, approximately 6.4 million were hospitalized, and over 1.4 million died, which amounted to 38% of all causes of death [1]. It is not widely known but CVD is also one of the leading causes of death of children. In 2005 the estimated direct and indirect cost of CVD in the United States alone was approximately $393 billion, making CVD the most costly component of total healthcare spending [1]. Consequently, the understanding and treatment of CVD are subjects of the greatest national and international importance.

The historical and current paradigm in cardiovascular medicine is diagnosis. Physicians use various tests to determine a medical condition and then plan a treatment or intervention based upon experience. There is no attempt to predict an outcome although there may be some statistical data to indicate the success rate of a procedure. Success may be defined in various ways depending on the nature of the treatment. It may be the ability to regain certain bodily functions, or simply to survive. However, statistics alone are not reliable predictors of success for individual patients. There is simply too much variability from case to case, especially for diseased patients. The current situation is far from satisfactory.

It is interesting to compare medical practice with engineering. Both are problem-solving disciplines. However, in engineering there is an attempt to accurately predict the performance of a product or procedure. The entire design process is based upon predicted outcomes. Very often a number of criteria must be satisfied simultaneously. Sophisticated computer and analysis technologies are employed.

Lack of a predictive process is referred to in engineering as the "build them and bust them" approach. It is not satisfactory in engineering, and it should not be satisfactory in medicine. It seems that medicine may be about to change, primarily because of the emergence of medical imaging technology, already the most important tool for diagnosing CVD, but with even greater future potential. Medical imaging promises to do for the practice of medicine what the telescope did for astronomy and the microscope for biology. The fidelity and resolution of medical imaging technology are progressing at a rapid pace. However, the pace has become so rapid that for the newer, high-resolution technologies, such as, for example, the 64-slice CT, there is little statistical basis for treatment planning. In order to correct this situation it appears inevitable that, in the future, the practice of medicine will have to resemble the practice of modern engineering more closely.

An example is illustrative. Until fairly recently, research in the computer simulation of arterial blood flow utilized very simple, idealized models and the relevance to medical practice was very limited. However, a new era in vascular research has begun [2] in which realistic, patient-specific models are employed, not only to simulate pre-operative, diseased configurations, but also to analyse post-operative outcomes. This has evolved into the concept of "predictive medicine" in which patient-specific computer modelling and analysis are performed to evaluate the efficacy of various possible treatments and plan and design the optimal intervention based upon predictions of outcomes. It is clear that with current technology and sufficient effort, the immediate consequences of an intervention can be predicted. For example, the effectiveness of a bypass graft configuration can be

assessed with reference to the redistribution of blood flow. However, the implications of the intervention are important after a certain time has elapsed – a month, three months, six, a year, two, etc.

Patient-specific modelling and analysis technologies for the human cardiovascular system are under development at a number of research laboratories throughout the world. The ultimate goal is to provide cardiologists and cardiovascular surgeons with improved technologies to prevent and treat cardiovascular disease. These technologies will enable clinicians to craft cardiovascular therapies that are optimized for the cardiovascular system of each individual, and to evaluate interventions for efficacy and possible side effects before they are performed. They will also provide design methodologies enabling biomedical engineers and physicians to devise new therapies, while decreasing costs and increasing safety associated with the introduction and clinical testing of new therapies.

The concept of predictive medicine has a long history. As early as the time of Hippocrates (ca. 460 BC – ca. 370 BC), the Cos physicians wanted to reassure their patients by predicting the outcomes of their treatments, but their medical knowledge and technology were too primitive to support their ambitions. Now, almost two and a half millennia later, it appears that the time may be right.

The development and clinical implementation of the predictive paradigm may well represent a milestone in the history of engineering and medicine, and one that may have significant benefit for the health and welfare of humanity.

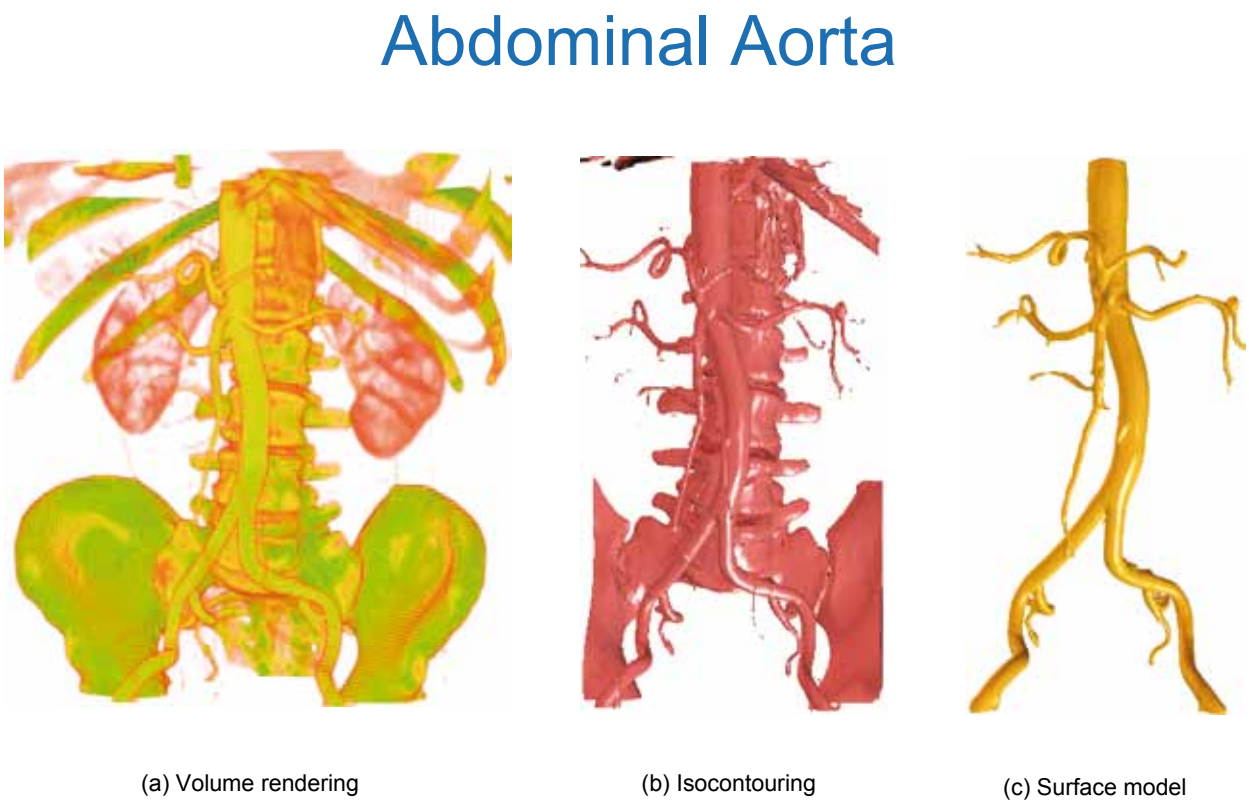

Figure 1: Steps in the construction of a computer model of a patient's abdominal aorta.(a) - volume rendering; (b) - isocontouring; (c) - surface model and its path after removing unnecessary components.

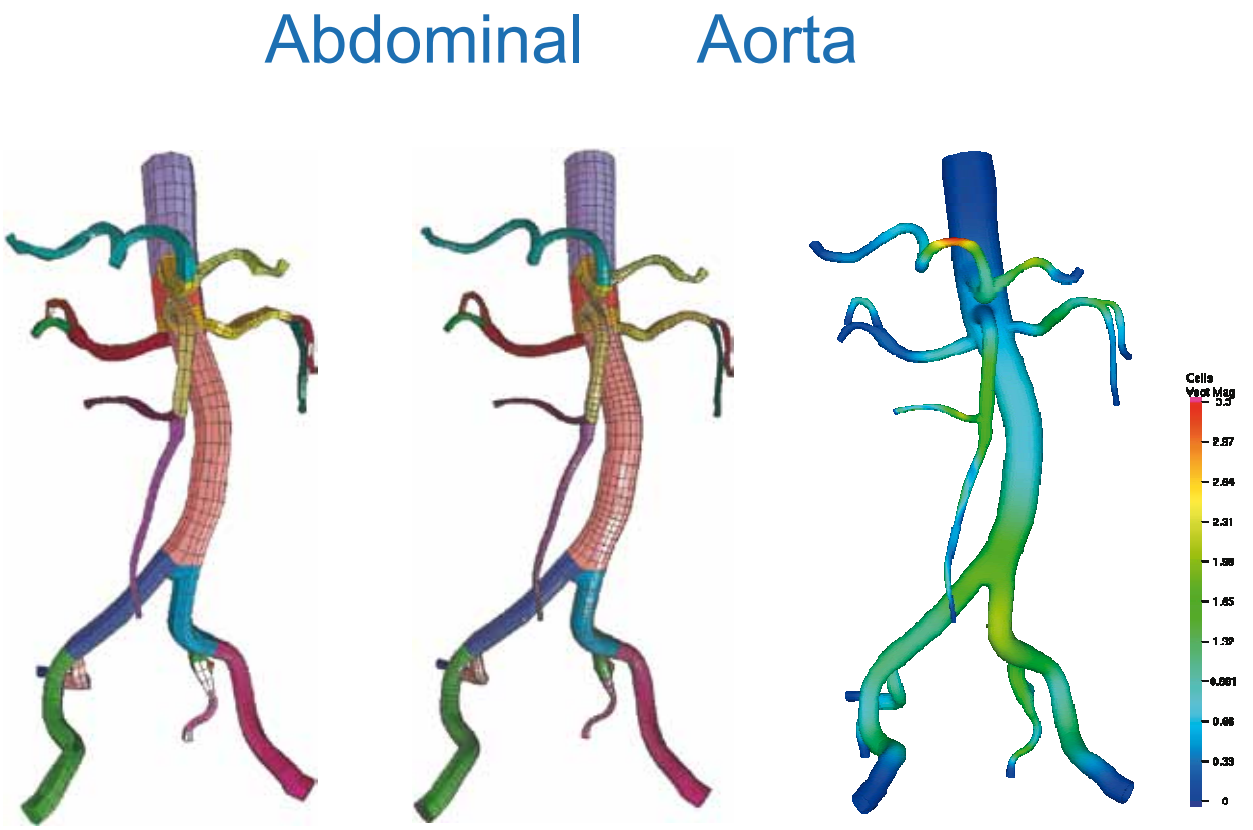

Figure 2: The abdominal aorta model is divided into 26 patches of elements, and each color represents one patch. From left to right are the control mesh, the solid NURBS mesh after refinement (73,314 elements), and fluid-structure interaction simulation results: contours of the arterial wall velocity (cm/s) during late systole plotted on the current configuration. Only major branches are utilized in the calculation.

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Towards optimal petascale simulations (TOPS):

an enabling technology center of the U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) Initiative

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The Towards Optimal Petascale Simulations (TOPS) project is researching, developing, deploying, and disseminating a toolkit of open source solvers for systems that typically arise when scientific and engineering applications such as accelerator design, climate dynamics, combustion, magnetically confined fusion, particle physics, subsurface flows, and the like are modelled via the finite discretization of partial differential equations. Such simulations are increasingly used in parameter identification, process control, uncertainty quantification, and other optimization contexts, which require repeated, related PDE analyses. Optimal and scalable solution algorithms – primarily multilevel methods, wrapped in Krylov, then Newton, and sometimes yet further outer iterations – reduce computational bottlenecks by one or more orders of magnitude on petascale computers, relative to solvers more commonly in use at smaller scales, enabling scientific simulation on scales of resolution and with complexities of models heretofore impossible for most applications. Along with usability, robustness, and algorithmic efficiency, an important goal of TOPS is to attain high computational performance by accommodating to distributed-shared hierarchical memory architectures. (See Figure 1 for weak scaling to the edge of BlueGene.)

The driving philosophy of TOPS is that optimal scalable solvers are required throughout CSE and therefore the cost of their research and development can be amortized through proper interface design. However, their deployment and dissemination to each application generally requires individual expert attention; no two PDE systems are alike, which is why there are *national laboratories* and not simply *numerical libraries*. TOPS solvers possess a combinatorially vast number of custom tunings, to be chosen for each application-architecture combination. In accomplishing a given task, there exist numerous alternatives with different tradeoffs between overall flops and bytes, or between instantaneous flop/s and byte/s rates, with communication up and down the memory hierarchy and across the network of distributed processing elements taxed in widely different proportions based upon aggregation and synchronization decisions. At such levels are factors of two to one hundred in performance won or lost.

TOPS scientists often find that applications scientists make too many decisions upstream of calling a solver and hide them. Thus, seeking to integrate a multirate coupled system, a physicist may simplify, linearize, operator split, and run loops around the system to be solved, generating a family of sparse linear systems to be solved in the innermost loop. However, presenting TOPS with a much higher level task, such as computing sensitivities of output functionals at the end of the integration with respect to input uncertainties, can perhaps be done far more efficiently, accurately, and

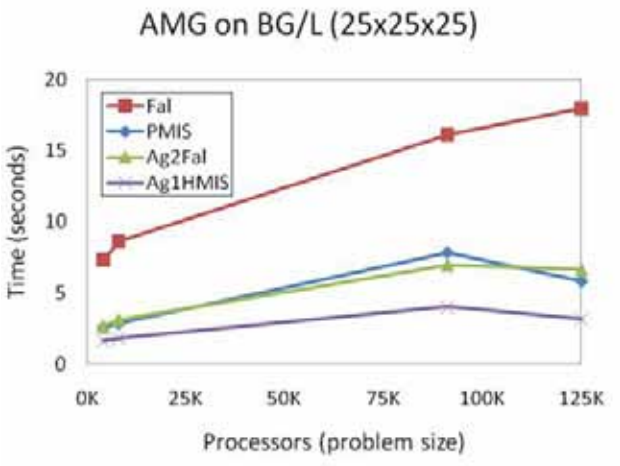

Figure 1: Weak scaling of the Hypre Algebraic Multigrid solver, with four different coarsening strategies, from the default to a custom-tuned setting for Poisson on BlueGene, in which each processor holds a 25^3 chunk of the discretization. Low and flat performance curves are ideal. The problem size is proportional to the number of processors. [c/o Ulrike M. Yang, Lawrence Livermore National Laboratory]

reliably through more advanced mathematical formulations. Hence, TOPS operates by developing a large collection of interoperable tools, and then deploying them in tight collaborations. Such collaborations lead to the most productive research topics for algorithm designers, since they invariably expose new problems whose solutions have high impact.

The convergence rates of solvers traditionally employed in PDE-based codes degrade as the size of the system increases. This creates a double jeopardy for applications – as the cost per iteration grows, so does the number of iterations. Fortunately, the physical origin of PDE problems provides a natural way to generate a hierarchy of approximate models, through which the required solution may be obtained efficiently, by bootstrapping. The most famous examples are multigrid methods, but other types of hierarchical representations are also exploitable, making intermediate use of lower fidelity models, lower order discretizations, and even lower precisions. The philosophy that underlies optimality is to make the majority of progress towards a high quality result through inexpensive intermediates.

Most PDE simulation is ultimately a part of some larger scientific process that can be hosted by the same data structures and carried out with many of the same optimized kernels as the simulation, itself. By adding a convenient software path from PDE analysis to PDE-constrained optimization, for instance, a preconditioner for the PDE solver becomes a block of a preconditioner for the optimization solver– with reuse of efficiently implemented distributed data structures. Similarly, TOPS increases the value of simulations executed in a fully nonlinearly implicit solver framework by providing sensitivity analysis of the solution with respect to parameters and optimization. TOPS has provided users of its Bell prize-winning PETSc toolkit access to the solvers in Hypre, SuperLU, and Trilinos, for example, without change of the user interface. (Figure 2 depicts typical interdependencies of various components of TOPS solvers.)

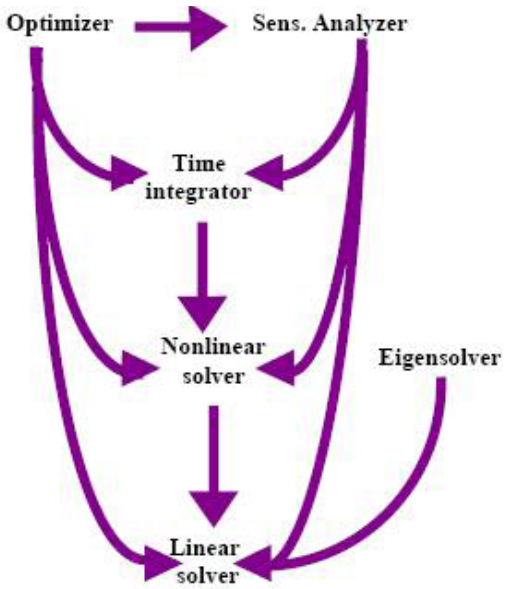

Figure 2: Inter-relationships between TOPS solver components. In a PDE context, all share grid-based data structures and parallel software infrastructure.

TOPS finds that open source availability of code is a productive way to engage the entire world of computational mathematicians, scientists, and computer scientists in the development of debugged, performance-ported, feature-enhanced software. TOPS software is used and enhanced every day, from Berkeley, to Beijing, to Bergen. TOPS provides support for the software packages Hypre, PARPACK, PETSc, SUNDIALS, SuperLU, TAO, and Trilinos, among others. Some of these are in the hands of thousands of users, who have created a valuable experience base on thousands of different computer systems with varied applications.

See **www.scalablesolvers.org** for more information about TOPS.

Quantum chemistry

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Quantum chemistry is concerned with the understanding of how the building blocks of atoms, the nuclei and the electrons, interact with each other to create molecules. These interactions are described by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t)=\hat{H}\Psi(r,t)$$

Although seemingly a very simple equation, the equation contains operators that describe the pairwise attraction between the electrons and the nuclei, the pairwise repulsion of the electrons, and the pairwise repulsion of the nuclei. Even very small molecular systems, such as the water molecule that only contains 13 particles, lead to very complicated interactions, as illustrated in Figure 1. For this reason, quantum chemistry is in general concerned with finding approximate solutions to the Schrödinger equation.

The advent of efficient numerical algorithms for solving the many-body Schrödinger equation, and in particular the advent of density-functional theory, as well as the continued improvements in computer hardware, have made quantum chemistry an integral part of many parts of modern chemical research. Indeed, for many branches of chemistry, experimental spectra are nowadays always used together with quantum-chemical calculations. The calculations can provide valuable insight into non-observable effects in the electronic structure of a molecule that in turn explain experimental observations that would be otherwise difficult to deduce from measured data only.

As an example of the interplay between theory and experiment, consider the determination of the absolute configuration of chiral molecules. A molecule is said to chiral if its mirror image cannot be superimposed on itself. The two mirror images are said to be enantiomers. Almost all physical properties of two chiral molecules are identical, except for their interactions with electromagnetic light, as well as with chiral receptors such as those found in the human body. The biological properties of two enantiomers are thus very different, and a knowledge of which enantiomer is present is very important. Modern experimental techniques such as Raman optical activity can distinguish between two enantiomers (the spectra are the same, but with opposite signs). Only a comparison with theoretical spectra can enable a conclusion be reached regarding which enantiomer is present. An example of such a comparison between theory and experiment is given in Figure 2.

Even though quantum chemical calculations have moved from the specialists to the general chemistry community, there are still large methodological challenges facing quantum chemistry. Modern quantum chemical methods scale at least cubically with the complexity/size of the problem, and for highly accurate methods, the scaling may be even less favourable, being as high as N^6 og N^7. At the same time, we know that the Coulomb operator has a limited range, and that for sufficiently large systems the computational cost should only grow linearly.

Several possibilities are currently pursued nationally and internationally for solving these problems, based

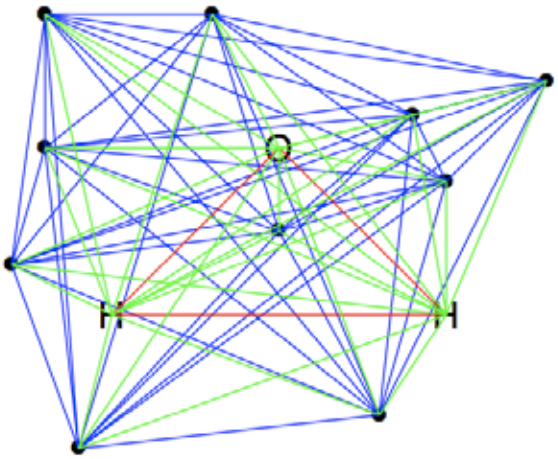

Figure 1: A "virtual snapshot" of the electrostatic interactions in the water molecule. Blue lines represent electron-electron repulsions, red lines nuclear-nuclear repulsions and green lines the electron-nuclear attractions.

on the generic techniques provided for instance in computational sciences. One such approach is the fast multipole moment method. Although originating in the study of galaxies, its introduction into quantum chemistry is based on the observation that the equation to be solved when studying gravitational problems bears many resemblances to the electrostatic interactions of interest in quantum chemistry. The difference is primarily the separation of the interacting particles. Indeed, it has been demonstrated that the fast multipole method can be applied also in the study of charge distributions that are well separated in extended molecular systems, and this constitutes an important ongoing research activity at the Center for Theoretical and Computational Chemistry (CTCC).

An alternative approach, that also borrows elements from generic computational science methods, is the multiscale approach. Here we build for instance the

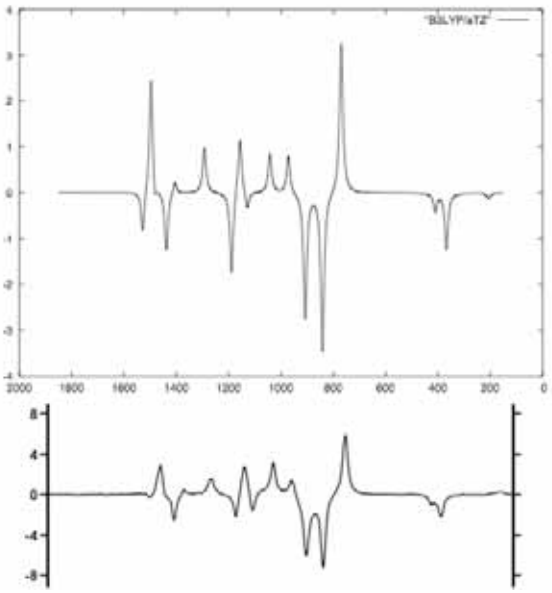

Figure 2: Comparison of a theoretically calculated Raman optical activity spectrum of S-methyloxirane (top) against an experimentally observed spectrum of methyloxirane. The agreement between the two spectra fixes the absolute configuration of the molecule to S-methyloxirane.

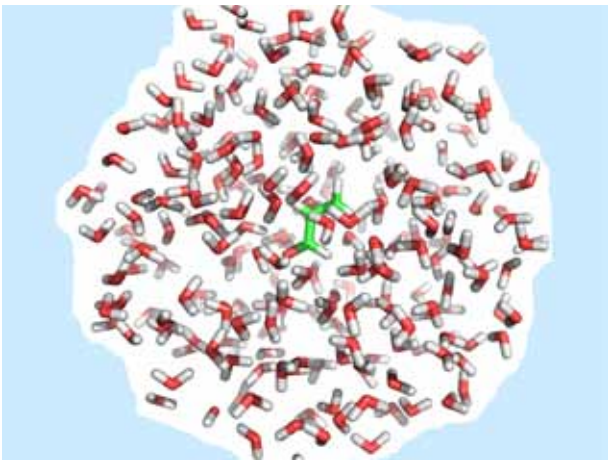

Figure 3: A three-level multiscale model for describing larger chemical systems, including both a quantum mechanical level (QM), a molecular mechanics level (MM) and a dielectric continuum (indicated by the blue surroundings).

model system from different elements that are treated by various computational methods depending on the length scales involved in the different building blocks. An example of such a multiscale model is illustrated in Figure 3, where we treat a chromophore involved in electronic rearrangements at the full quantum-mechanical level, the solvent molecules closest to the chromophore at a molecular mechanics level, and finally the long-range electrostatic interactions by a simple dielectric continuum model.

A recent new development we have been pursuing at the CTCC is the use of multiwavelets as basis functions. Numerical techniques such as these, originating in image compression, are generally not used much in quantum chemistry, but the multiwavelet approach holds the promise of providing highly accurate results at an inherently linear scaling cost.

The accessibility of modern quantum chemistry calculations has to a large extent transformed current practice in chemical research. Through continued interactions with practitioners in the field of computational sciences, new methodological advances can be expected. At the same time, quantum chemistry may contribute important problems (and solutions) to the field of computational sciences.

For more information about the quantum chemistry activities at the CTCC, visit our web pages at www.ctcc.no.

Integrated data processing

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Most industries nowadays are information and knowledge driven. Large amounts of data are collected and need to be shared across different businesses, domains and applications. By combining heterogeneous data from several sources it is possible to derive information that is not available otherwise. However, several challenges remain. First, one has to deal with complexity and overhead increase. Large amounts of data need to be processed and the number of relations between data needs to be handled. Second, data distribution and availability become issues. Data are distributed over various places. This creates efficiency concern, where fetching all the data by the agent is not always possible or effective. Third, cross-industry data integration is needed. Data are shared among many applications or even between several companies, which leads to significantly different nomenclature. Programming paradigms currently spread in industry are not efficient in solving those problems.

The Department of Electrical Engineering and Computer Science at the University of Stavanger is investigating how concepts of multi-agent systems, semantic web and cloud computing can be brought together to solve the above problems in the oil and gas industry. The main research goal is real-time alarm and decision support systems based on semantic data streams (WITSML). Focus is on real-time monitoring of key well behaviour parameters, data for the detection of anomalies or deviations from normal expectations, risk quantification of formation fracturing, lost circulation, wellbore instabilities, stuck pipe, formation damage and automatic prediction of expected well behaviour to complete the current operation. This work is related to several projects: IDP-D&C[1], AutoConRig[2] and IOHN[3] and further research initiatives.

Multi-agent systems have already been investigated for some time and have proven to be a solution for complex distributed processing problems. They constitute an efficient paradigm that helps in reducing the complexity of a problem by its distribution to intelligent, mobile and autonomous agents. Multi-agent systems can also be a way to implement extensive complex event processing systems. In the research on the alarm and decision support system these characteristics are leveraged to demonstrate the usefulness of multi-agent system approach.

In those systems, complex problems can be broken down into a set of smaller, less complex problems. This gives better understanding and minimizes the amount of errors. Using intelligence property of agents, different kind of reasoning algorithms can be implemented in each of them. Algorithms included in the research are mainly rule engines, Bayesian networks and Petri nets. Agents are mobile and can easily communicate, both inside the platform and outside of it. They can be distributed to keep control over system efficiency. One interesting case is to move the agent to the place where data are instead of fetching data to the agent.

The last characteristic is autonomy. It can be utilized in several ways. First of all, failure in some parts of the system does not bring the whole system down. In case of failure, agents can be recreated, or more agents of the same kind can be created as needed. Moreover, each agent might have different goals. This is a useful way of addressing some types of problems and helps domain experts to design new solutions.

Semantic Web is an extension of current web in which the data are given well defined, machine understandable meaning. It enables automatic extraction and merging of data from different sources. Semantic technologies like XML, RDF and OWL enable the description and connection of data and resources in a new and sophisticated manner. Ontologies are used to design models (i.e. interpretations) of the world, and give an understanding of how different things (data, resources etc.) are connected and related. This knowledge can further be distributed, made available to and autonomously interpreted by other units. In case of inconsistencies between already existing solu-

tions Semantic Web techniques can be used to mediate between them. This makes it possible to integrate data across the industry or even across different industries.

Multi-agent systems and Semantic Web used together can be a solution to problems of complexity, distribution and integration. However, it is important to provide a way that would facilitate their practical implementation. Based on cloud computing concepts, industrial cloud[4] (illustrated in Figure 1.) is introduced as a platform for industrial digital information integration and collaboration. Unified data standards and common ontologies are connected with open and shared architecture in order to facilitate data exchange and service composition between several companies. Industrial cloud is created on the base of public and enterprise cloud technologies and solutions. It facilitates integrational tasks like policies, reliability management, security and trust, outsourcing and subcontracting. Furthermore, it adds support for semantic interpretation of data, mapping, data fusion and service discovery and composition.

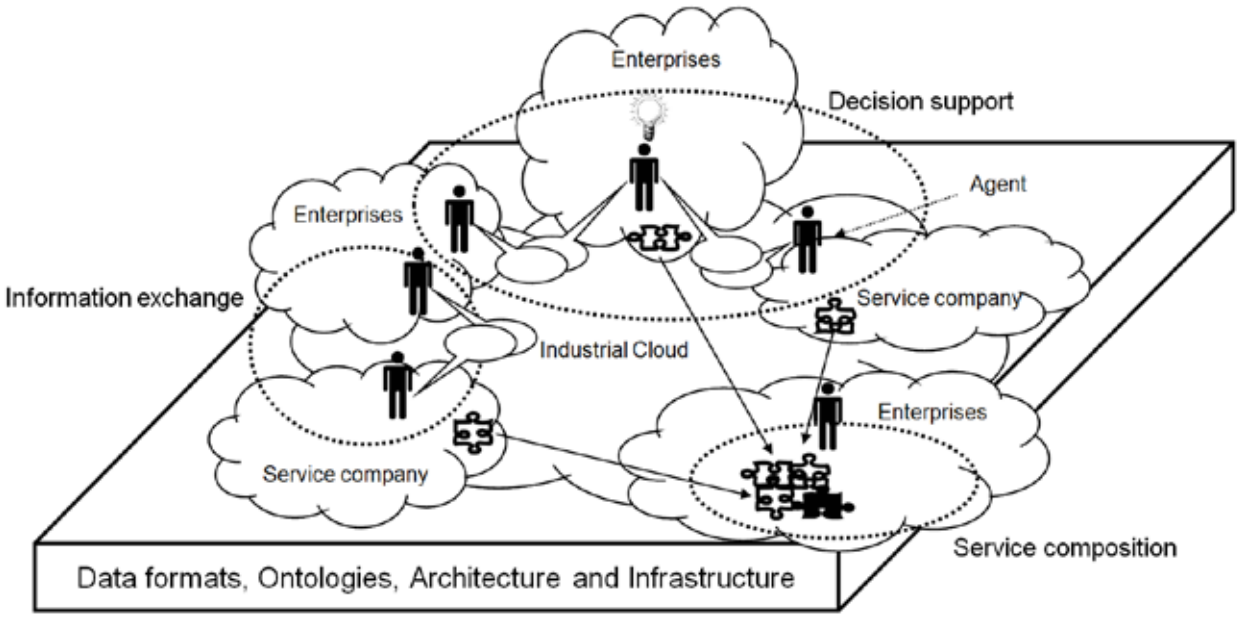

Figure 1: Integration, collaboration and composition in industrial cloud.

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When oil and water compete in porous rocks

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Oil and water do not mix. When they meet, there is surface tension along their boundary and any bending of this boundary creates forces that resist this. Attempting to shake oil and water together in a cocktail shaker for example will create a suspension of fluid bubbles. As soon as the shaking ends, the bubbles will start merging and after some time the two fluids have completely separated with the lighter fluid on the top. The reason for this is that the two fluids want as little interface between them as possible.

Rocks that are porous have a network of pores inside. The porosity, i.e. the fraction of the space the rock occupies that consists of pores, ranges from being close to zero to more than 0.99 – the latter case concerning aerogels, which are man-made materials. When the porosity is high enough, the pore network is connected throughout the rock and the transport of fluid is possible through the network. This fact makes the oil industry possible.

When there is oil and water in the porous (reservoir) rock, they will be competing for the same pore space. They will not mix, but set up interfaces between them. Since the two fluids are attracted differently to the pore walls – they have different wetting properties – the interfaces between the two fluids will end at the pore walls by coming in at a well-defined angle determined by the properties of the two fluids and the pore wall relative to each other. If the angle is zero, films of the fluid that wets the pore walls will form.

In a reservoir that has not been explored, oil and water will be well separated. They have different specific weights and over geological time gravity will have separated them just as oil and water shaken together separates in a glass when left alone.

If now the fluids in the reservoir start to move, e.g. due to exploration, the two fluids will start to compete. The interface between the fluids will typically be ustable and bubbles and clusters will form. These again will merge and then split up. At high enough flow rates a steady-state situation develops with a characteristic cluster size distribution.

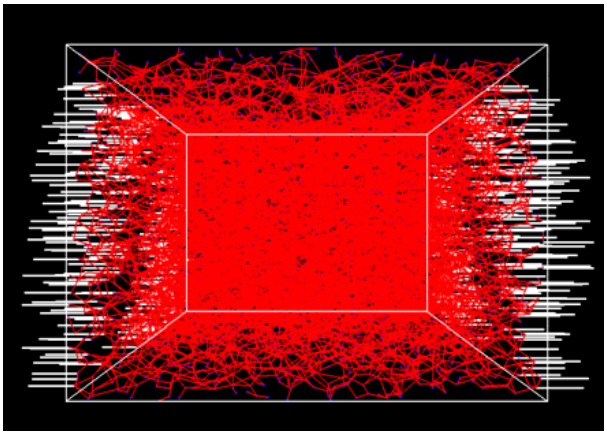

Figure 1: By slicing up a Berea sandstone its pore network has been identified and reconstructed.

It has been our goal in this project that started more than ten years ago, to construct a numerical model of immiscible two-fluid flow in porous rocks at the pore level. There are many fundamental questions that remain open in this field. We use our model as a numerical laboratory both to answer the open questions and to pose new questions. As an example of a lingering open question that we have answered is what happens when two immiscible fluids flow in parallel in a porous rock. It turns out that there is an instability producing a layer of bubbles of both types of fluids – a foam – at the interface. An example of a new question emerging from this work is why is the foam layer stable? It does not dissolve as commonsense would dictate. This is strange and we do not understand it.

Apart from the fundamental aspects of this project, there is also a practical side. The information that can be harvested from running our model on reconstructed reservoir rocks is exactly that which is needed as input for the reservoir simulators run by the oil industry. Today this information is obtained through routine but expensive core testing in the laboratory.

We have in the course of this work found strange relationships between fundamental variables occurring in the system. We believe that these relationships signal an alternative description and much deeper understanding of the physics of immiscible two-fluid flow in porous rocks. A practical consequence of this would be much more efficient computer codes. This is our goal for the future.

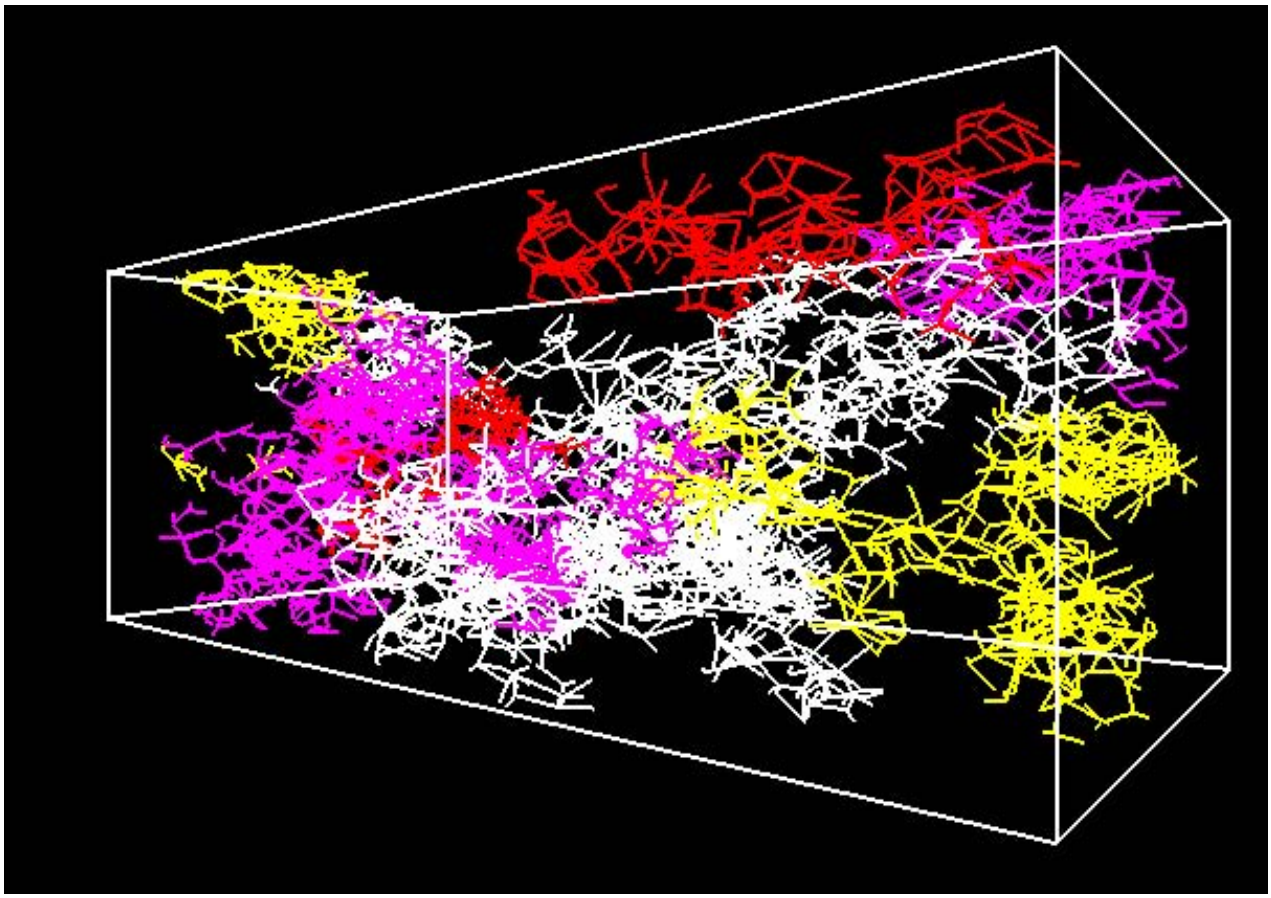

Figure 2: The reconstructed Berea sandstone pore network has initially been filled with two immiscible fluids which have been forced to move. The figure shows the largest clusters of non-wetting fluid after the systems reach steady state. The clusters are shown with different colours in order to distinguish them. The wetting fluid that surrounds the non-wetting fluid clusters is not shown.

Seismic imaging, modelling and inversion

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Reflection seismics is one of the most important methods for mapping the upper part of the crust of the earth. It is of great importance for the exploration of hydrocarbons and also for optimizing production from existing oil- and gas fields. New hydrocarbon reservoirs are increasingly harder to find and has forced exploration activities into ever more complex geological areas increasing the demand for new seismic imaging technology.

The raw material for creating seismic images of geological formations is reflected sound waves generated by an artificial source at the surface. The mechanical properties of the geological structures determine the strength and arrival times of the reflected seismic waves, implying that rock properties such as elastic moduli and density could in principle be obtained from seismic data. The elastic sound waves are described by elastodynamic differential equations, where the coefficients are the density and elastic moduli as functions of two horizontal coordinates and depth. In general there is a non-linear relationship between the coefficients and the measurements at the surface. To obtain estimates of the density and elastic moduli, a large, highly non-linear inverse problem must be solved. The full solution to this problem is not completely known and is the subject of research projects around the world. What is known is that even very approximate solutions requires large amounts of computing power, both in terms of storage capacity and CPU time.

SEISMIC IMAGING

Standard practice in the industry to solve the non-linear seismic inverse problem is to introduce gross simplifications and solve a set of simplified, approximate differential equations. In effect the problem is linearized around some initial estimate of the density and elastic moduli, and the output from these calculations is a correction of the initial estimate in the form of scattering or reflection coefficients. The approach is generally known as seismic migration or seismic imaging. A graphical display of the reflection coefficients gives an image which can be interpreted in terms of borders or interfaces between geological formations. An example of a seismic image is shown in Figure 1 (Arntsen et al. 2009), which was created from an input data file of approximately 100GB and required 21 days of computing on a cluster with 500 CPUs. Very often input datasets are much larger, in the order of tens of TB, requiring months of computing on large clusters.

Current research efforts have been concentrated on improving the accuracy of linearized solutions and recovering reliable quantitative information from the reflection coefficients, in addition to images of the subsurface.

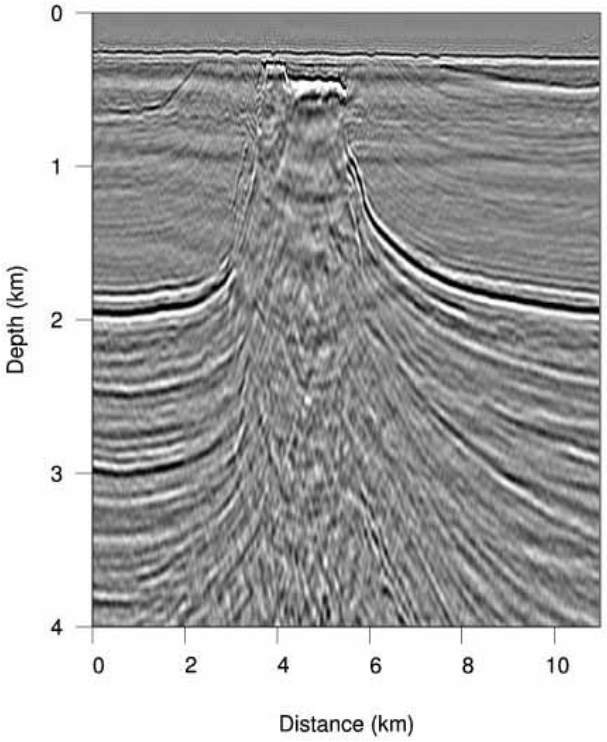

Figure 1: Image of the earth's upper crust, obtained from processing of seismic data

SEISMIC MODELLING

An important step towards the solution of the seismic non-linear inverse problem described above is the solution of the forward problem, i.e. solving the differential elastodynamic equations to obtain simulated measurements at the surface when the density and elastic moduli of the subsurface are known. This is a linear problem, and can be solved using standard numerical methods. An often used method is the finite-difference approach which involves discretization of the elastodynamic equations on a regular three-dimensional grid. Computationally there are two main challenges; the size of the grid and the number of simulations required to model a full seismic survey. The number of grid nodes is determined by the wavelengths of the waves and the size of the computational domain. For a realistic simulation this implies that the computational grids need between 1 and 100 GB of storage. Large simulations thus require either out-of-core solutions or the use of domain decomposition. With today's standard hardware a single simulation can be performed in a few hours on a single CPU. However, a realistic seismic survey may require several hundred thousand of simulations to be performed.

Each of these simulations are independent and are usually parallelized on a cluster with several thousand CPUs.

Apart from the solution of the inverse problem, the simulation of seismic surveys is extensively used for verifying and testing the layout of seismic sources and detectors before a real survey is performed. Figure 2 shows simulations of two surveys across the Heidrun

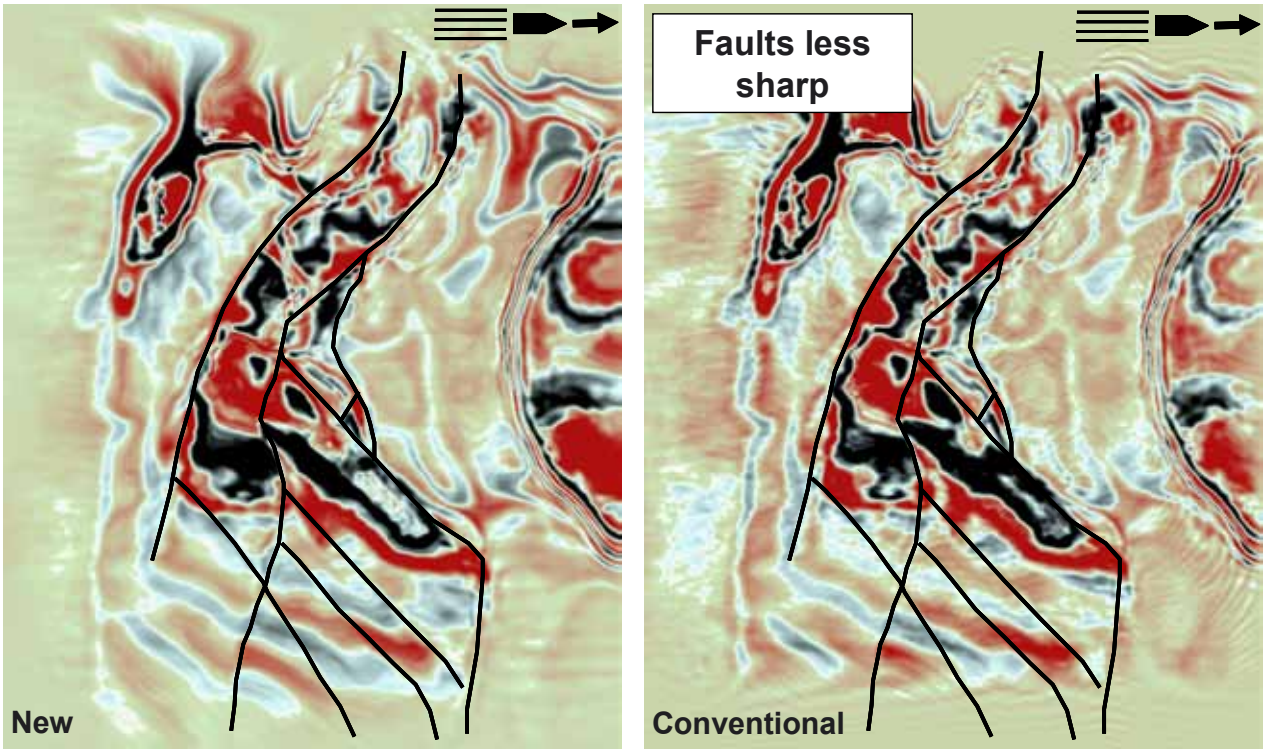

Figure 2: Seismic modeling of two different surveys on the Heidrun field showing the reflection strength on a horizontal slice of 20 x 20 km through the reservoir. The left-hand image shows simulated data using a new novel survey design, while the image on the right shows simulated data from a conventional survey design.

field in the North Sea (Houbiers et al. 2009). The computational time was approximately 12 days on a Linux cluster generating about 1.5 TB of output data for each of the surveys.

SEISMIC INVERSION

During the last twenty years, several attempts have been made to solve the full non-linear seismic inverse problem described above. The most successful attempts have used a least squares parameter estimation technique. The general idea is to compute simulated seismic data by solving the forward problem for some initial guess of the density and elastic parameters. The simulated measurements are then compared with real measurements and the difference is used to compute new estimates of the density and the elastic parameters. Usually several iterations, up to several hundred, are required before the solution converges. The computational effort is huge since a full seismic simulation is required for every iteration. Computing times of several months on large scale clusters with thousands of CPUs have been reported by research groups.

Seismic modelling, imaging and inversion are very important for the exploration and production of hydrocarbons. Current research indicates that a full solution of the seismic inverse problem is possible, but only through massive use of computing power. Typically clusters with fast storage systems of the order of hundreds of TB and computing power of tens of Tflops are necessary.

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High order methods for incompressible fluid flow: application to moving boundary problems

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Computational mechanics has seen unprecedented progress over the last few decades. This is partially due to the rapid progress in computational infrastructure, but equally important, progress in computational methods. Advances in mathematical modeling of such problems has also played an important role. Challenging new science and engineering projects are being planned, partially aided by the availability of more sophisticated simulation tools. For the Norwegian industry, we mention a few areas: marine technology, flow and energy transport, and materials processing.

Despite all this progress, there are still many important problems which cannot be solved sufficiently accurately (or not at all), either because of the enormous complexity of the mathematical model, or because of the large number of temporal and spatial scales to resolve. Some progress will "automatically" happen due to progress in computational infrastructure, however, it is utmost important to maintain a sustained research effort towards improving the computational methods. As larger and larger problems become amenable to simulation, it is important that the fundamental framework underpinning all the algorithms are properly understood, and it is important to never relent the search for doing things better, i.e., more accurately, more efficiently, more robustly, and more user-friendly.

We now discuss a couple of problems from computational mechanics (one of these perhaps with a Norwegian touch), and with the possibility of being amenable to different levels of mathematical and computational analysis. Both problems are very challenging.

First, we consider Benard-Marangoni convection where a thin fluid layer is heated from below. One of the intriguing features with this problem is the formation of hexagonal convection cells from random initial conditions; see Fig. 1 and Fig. 2. However, the free surface deformation associated with these cells has previously only been studied experimentally [1,2] or analyzed analytically using linear stability analysis [3]. It is known experimentally that the free surface

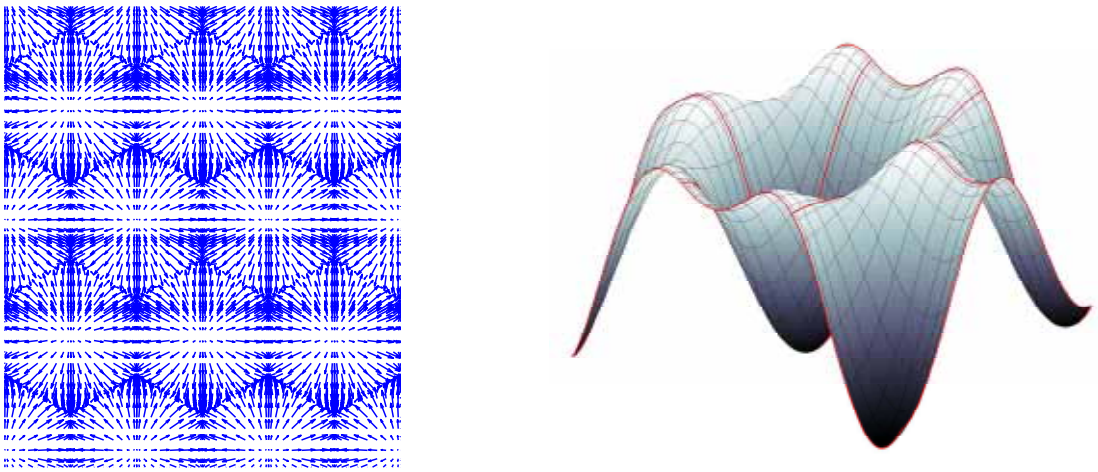

Figure 1: Three-dimensional simulation results for Marangoni number Ma=90, Rayleigh number Ra=0, and Prandtl number Pr=infinity. Periodic boundary conditions are imposed. The velocity field is shown to the left (top view), while the free surface deformation over a single (periodic) cell is shown on the right. The depressed free surface at the center of the cell is consistent with the fact that there are no buoyancy effects in this case, only surface-tension-gradient effects. To our knowledge, this type of surface deformation (although with a small amplitude) has never been computed before; only a fixed and flat "free surface" has been used in earlier work [8].

will either be depressed or elevated over each hexagonal cell, depending on whether surface-tension-gradient effects or buoyancy effects are dominating [2]. It should be remarked that Benard himself had an incorrect interpretation of which effect was dominating in his original experiments [1]; only several decades later were the experiments correctly interpreted through surface-tension-gradient effects [4,5].

Second, we consider a particular marine application. The development of high quality elastic fabric of low weight, high strength and relative low price has increased the use of fabric as construction material for marine applications. One example is a floating fabric container for transportation of fresh water [6]; see Fig. 3. Full-scale field tests have been done using this approach, with limited success.

The flexible fabric container gives rise to a hydroelastic problem, with major challenges in terms of predicting the shape of the membrane subject to external loads. The forces acting on the membrane can be modeled in a similar way as when modeling surface tension effects in fluids. In a hydrostatic analysis, the pressure jump across the fabric will depend on the local curvature. In order to predict the dynamic response, e.g., from waves or currents, the full three-dimensional Navier-Stokes equations will need to be solved in a time-dependent domain, and where the shape of the membrane needs to be determined as part of the solution. To simulate the dynamic response of a full-scale problem is completely out of reach with the current technology and will probably remain so for the foreseeable future. Nonetheless, this problem can still be used as a motivation and inspiration for research in computational methods for three-dimensional moving boundary problems, including accurate tracking of free surfaces, and accurate determination of the mean curvature for incorporation of surface tension effects.

From a computational point of view, a powerful framework for simulating moving boundary problems is provided by the Arbitrary Lagrangian Eulerian (ALE) formulation. Even though this framework is quite mature and is currently used in many commercial codes, it is still a subject of active research. Part of the current research in ALE methods is related to time integration [7]. One issue is the importance of satisfying the so-called geometric conservation laws. The conclusion is still not quite clear for general Navier-Stokes problems. A complicating factor in all this effort is the fact that it is not easy to measure and verify the overall temporal accuracy during a transient simulation. This is partially due to the lack of analytical solutions for moving boundary problems, in particular, for general free surface problems where both normal and tangen-

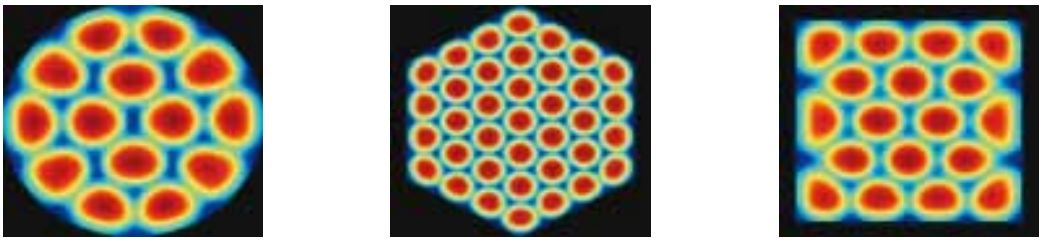

Figure 2: Temperature distribution along the top free surface due to the formation of hexagonal convection cells (Benard-Marangoni convection). The three-dimensional simulation results all correspond to Ma=105, Ra=48, Pr=890, but the computational domain is different (both in terms of the shape and the domain aspect ratio). A random initial temperature field is used together with a zero initial velocity field. At steady state (as above), hexagonal convection cells appear.

tial stress boundary conditions are imposed. This is an area where new mathematical contributions can help.

Special issues arise when trying to apply high order methods to free surface problems. Because the free surface is part of the overall time-dependent solution, it is, in general, nontrivial to update the domain boundary in such a way that the distribution of the surface points remains optimal from the initial time to the final time. This is due to the fact that the free surface displacement is fundamentally linked to the normal fluid velocity along the surface ("front-tracking"), while the tangential displacement of surface points is less well defined and open to different choices. Recently, new results related to geometry representation have been obtained, which opens up for more robust and more accurate ways to follow time-dependent interfaces.

ACKNOWLEDGMENT

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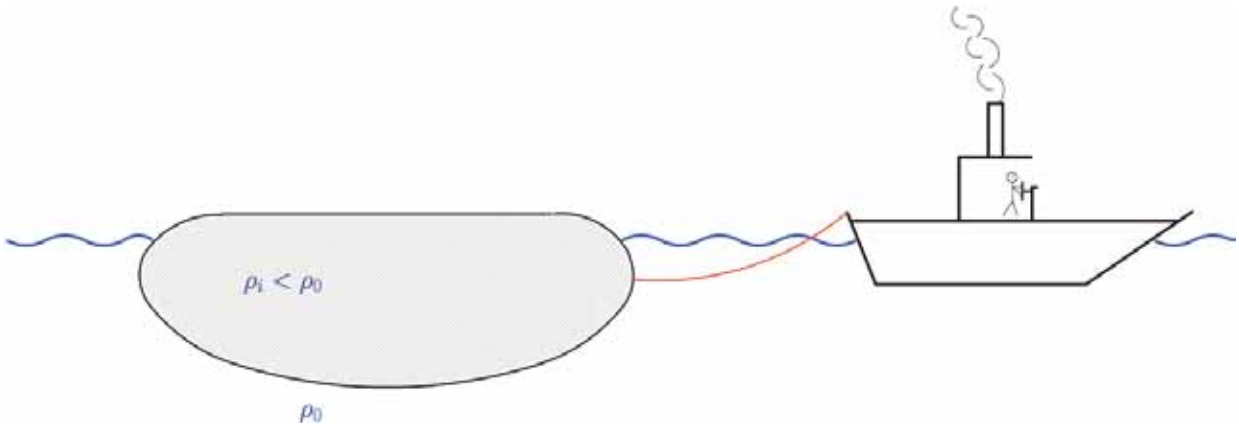

Figure 3: Transportation of fresh water using a flexible fabric container.

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Computational challenges in bioinformatics

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BIOINFORMATICS

Bioinformatics is a computer-based discipline where we use approaches from computer science to analyse complex data from molecular biology and medicine. There are many sources of complexity in bioinformatics, including exponentially growing data sets, incomplete data sets due to expensive or error prone experiments, time and size scales covering several orders of magnitude and communication barriers between different scientific disciplines. This makes bioinformatics both challenging and exciting as a research area. Bioinformatics is a prerequisite for modern molecular biology and an essential basis for complex challenges like Systems Biology. The research group on Bioinformatics and Gene Regulation is associated with Programme for Bioinformatics at NTNU and has worked on a range of bioinformatic challenges, some of which are briefly described below.

Large scale comparison of bacterial genomes

Bacterial genomes are dynamic during evolution, with frequent gene transfers and reorganizations of gene order. By comparing a large number of bacterial genomes we can identify functional constraints on this genomic plasticity; which genes are essential for survival, and how are these genes organized in the genome? This has been done by large scale sequence alignment of 113 bacterial genomes with dynamic programming, running Blast and OrthoMCL software on the NOTUR Stallo system. The analysis showed that essential genes are different with respect to the degree of co-regulation (operons), that these differences are caused by functional differences (pathways, interaction partners) and that this also affects the evolutionary rate of the relevant genes [1]. Figure 1 shows frequently occurring sets of co-regulated genes in bac-

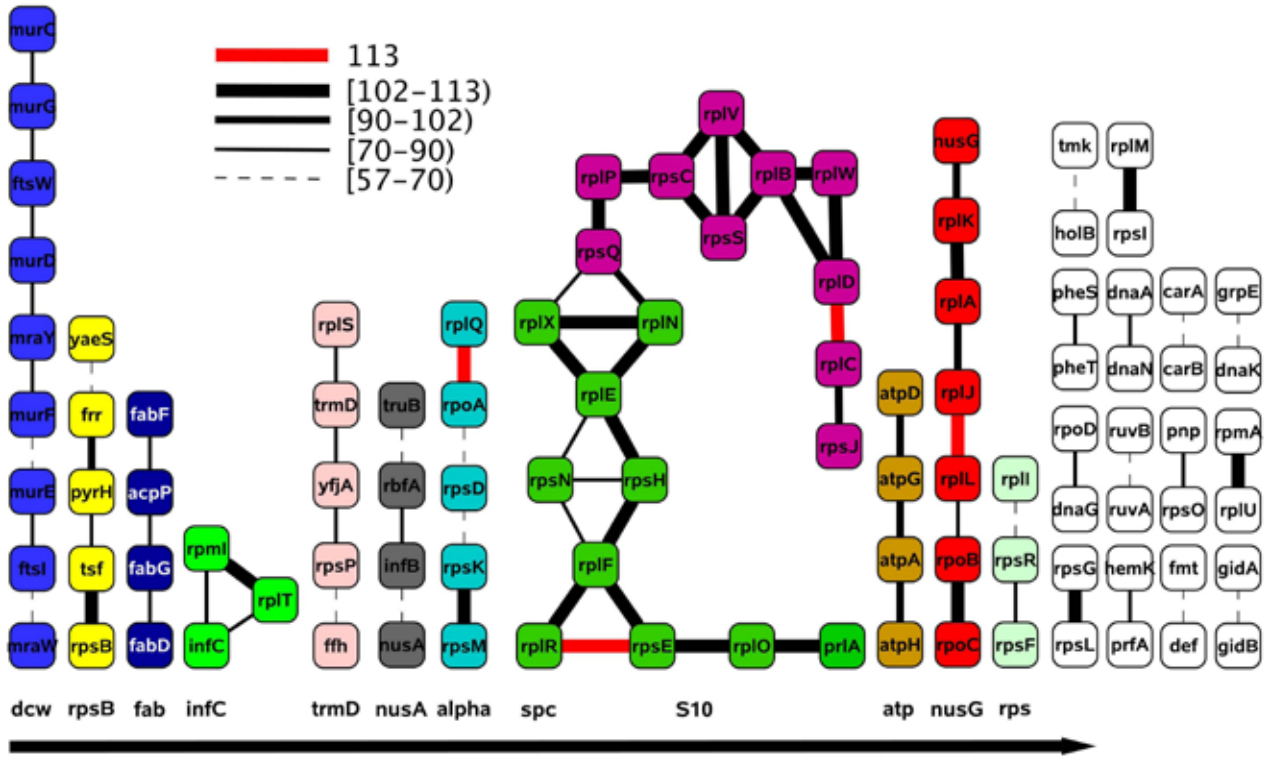

Figure 1: Conserved bacterial operons. Co-regulated gene sets (operons) that are conserved in most bacterial genomes have been identified by sequence similarity searching and clustering.

terial genomes. This information can help us to understand data from metagenomics, where large amounts of bacterial genomes from soil samples or oil wells, for example, are sequenced simultaneously.

Pattern discovery in genomic sequences

A genome sequence is basically a string of four basic building blocks, represented by the letters A, C, G and T. Specific proteins (e.g. transcription factors) or RNA molecules (e.g. microRNAs) are able to recognize short degenerate motifs within this sequence and affect gene regulation by binding to these motifs. We have developed motif discovery tools based on enumerative approaches [2], model based classification [3] and machine learning [4] for prediction of binding sites. The training process in machine learning may be computationally challenging, in particular if we want to run on genome-wide data. We have therefore used special purpose hardware (Interagon Pattern Matching Chip) and Field Programmable Gate Array (FPGA) technology to speed up applications [5], in addition to traditional multiprocessor technology. Other research groups have recently implemented GPU acceleration for similar tasks. Figure 2 shows genomic consensus

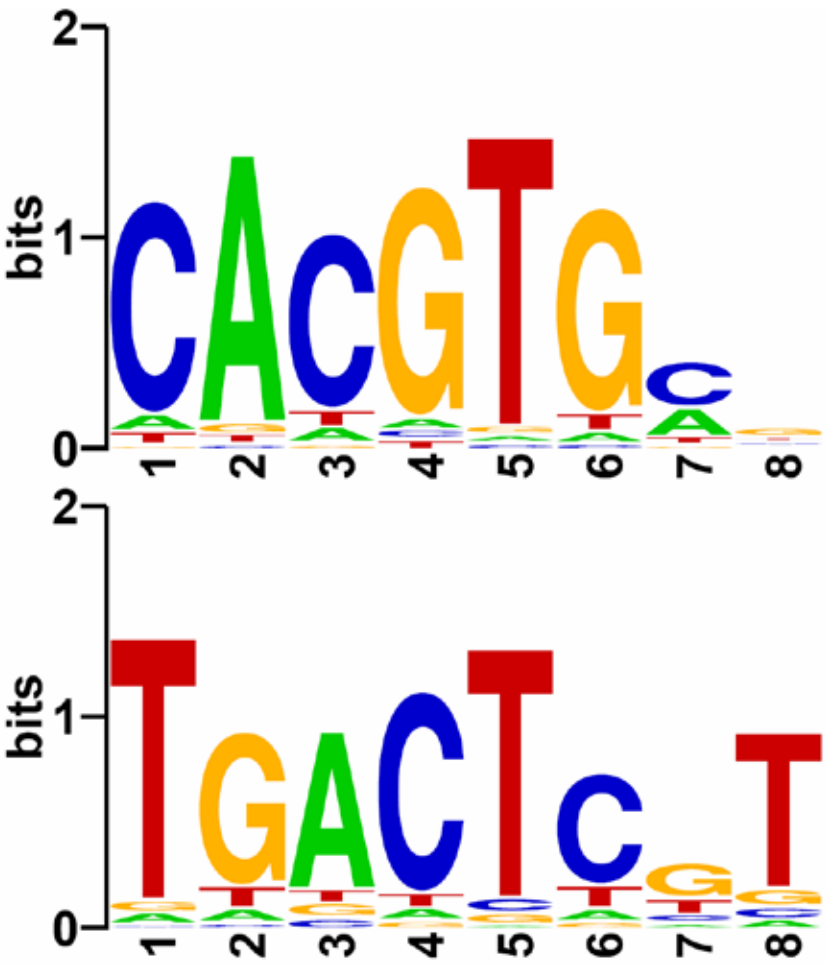

Figure 2: Gene regulatory motifs. Transcription factor binding site motifs have been identified for two transcription factors from yeast (Cbf1 and Bas1) using a novel two-step motif discovery process (TScan).

motifs for proteins involved in gene regulation (transcription factors), identified with a novel two-step motif discovery process [6]. This type of analysis is essential for understanding how genes are regulated, and potentially deregulated in cancer, for example.

Future challenges from ultra-throughput sequencing technologies

Sequencing is the process in going from a sample of genetic material to a symbolic representation of the genetic code (text string). This has been a time consuming and very expensive process; sequencing the human genome took more than 10 years at a total cost of at least USD 3 billion. However, over the last few years novel sequencing technologies have become available through companies like Roche (454), Illumina (Solexa) and Applied Biosciences (SOLiD). These technologies can do sequencing at much higher speed and lower cost; the 454 instrument sequenced a human genome in two months, and a bacterial genome can be sequenced in less than a day on a single machine. We are approaching a situation where the complete genetic profile of a person can be determined for less than USD 1000, enabling personalized medicine where treatment is adapted to the genetic profile of the patient. The increased sequencing capacity also enables new types of experiments. However, the high throughput is a challenge. A single machine can already produce 10-20 TB of data per year for bioinformatic analysis, and both the number of machines and the throughput of each machine are increasing rapidly. This represents very significant challenges with respect to bioinformatics competence and software for data analysis, but also regarding computer capacity for running the software, network capacity for data transfer and resources for data storage and archiving.

ACKNOWLEDGEMENTS

The Research Council of Norway is acknowledged for extensive support through the FUGE programme for technology platforms and computer time on the NOTUR resources. The work has also been supported through internal funding from NTNU and by the Svanhild and Arne Must Fund for Medical Research.

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Multiscale methods for subsurface flow

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Being able to understand and predict flow and transport processes in subsurface rocks is decisive for oil and gas recovery, carbon sequestration, and groundwater management. Porous rocks are typically highly heterogeneous and exhibit multiscale behaviour in the sense that small-scale flow paths dominate the overall displacement of fluids in a reservoir. Describing all pertinent flow processes with a single model is impossible and flow modelling is therefore divided into separate steps according to physical scales: from rock models on micro scale, via facies models and geological models, to simulation models on the macro scale, see Figure 1. Mathematical models must be calibrated against static and dynamic data of very different spatial (and temporal) resolution: thin sections, core samples, well logs, geological outcrops, seismic surveys, well tests, production data, etc.

Upscaling is inevitable to transfer parameters and effective properties up (and down) in the model hierarchy. Unfortunately, the turnaround time of upscaling workflows is relatively slow. Fundamental methodological development and automated approaches are therefore required.

This is particulary true for workflows like data integration, scenario modelling, risk/uncertainty asessment, and recovery optimization which typically require a large number of simulations of fluid flow. Ideally, each of these simulations should utilize all available data to improve modelling realism and run within minutes or seconds to enable exploration of the whole parameter space. Contemporary commercial simulators are far from delivering this computational capabilities and typically require the user to perform a time-consuming model reduction (upscaling) before simulation, thereby losing important features in the input data.

MULTISCALE METHODS

Multiscale methods [2] offer a systematic framework for model reduction and bridging scales. In these methods sub-scale information is incorporated into model equations on a coarser scale in a consistent way. In this paper, we discuss on upscaling from geological to simulation models and present a particular multiscale method [1] that provides mass-conservative flow fields on geocellular models at the cost of solving the flow equations on a much coarser simu-

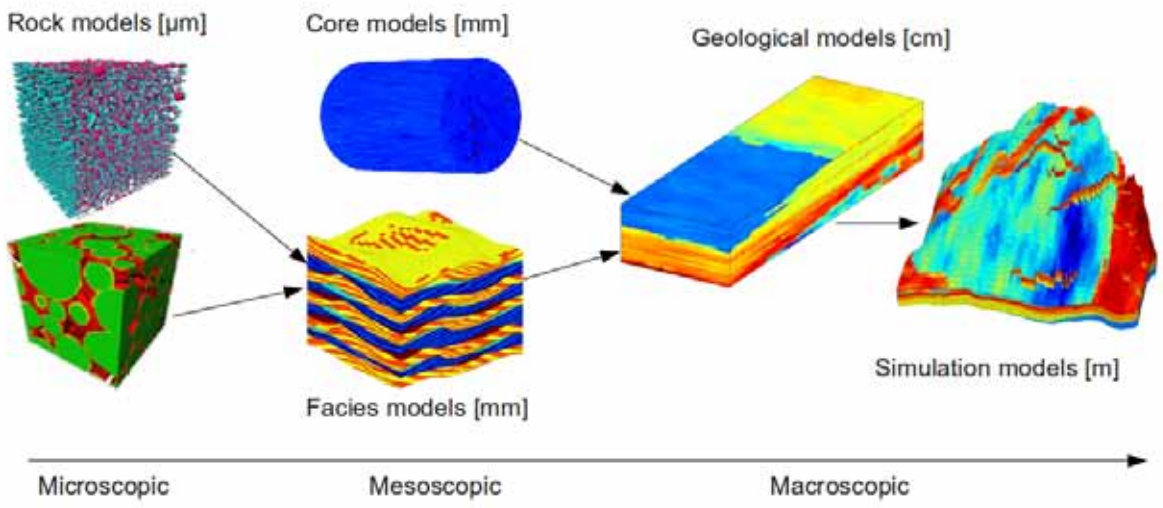


Figure 1: Illustration of four stages in subsurface modelling. The length scales are the vertical sizes of typical elements in the models.

lation grid. Key steps of the method are illustrated in Figure 2. In an upscaling method, one would make a coarse grid and solve local flow problems to compute effective properties associated with each coarse block. In a multiscale method, one retains the local solutions and uses them as building blocks (basis functions in FEM-terminology) to construct global solutions. This way, one is able to account for both effective coarse-scale properties and sub-scale variations and describe the flow on both the coarse computational scale and the underlying fine parameter scale.

The resulting method has appealing computational features. It is relatively insensitive to the coarsening factor, applicable to both structured and unstructured grids, and usually more accurate and robust than standard upscaling methods. The method is particularly efficient when the flow field must be updated repeatedly. Because temporal changes in the flow equations are moderate compared to the spatial variability, it is seldom necessary to recompute basis functions each time the flow field is recomputed. Instead, basis functions are computed initially as part of a preprocessing step and only updated if the

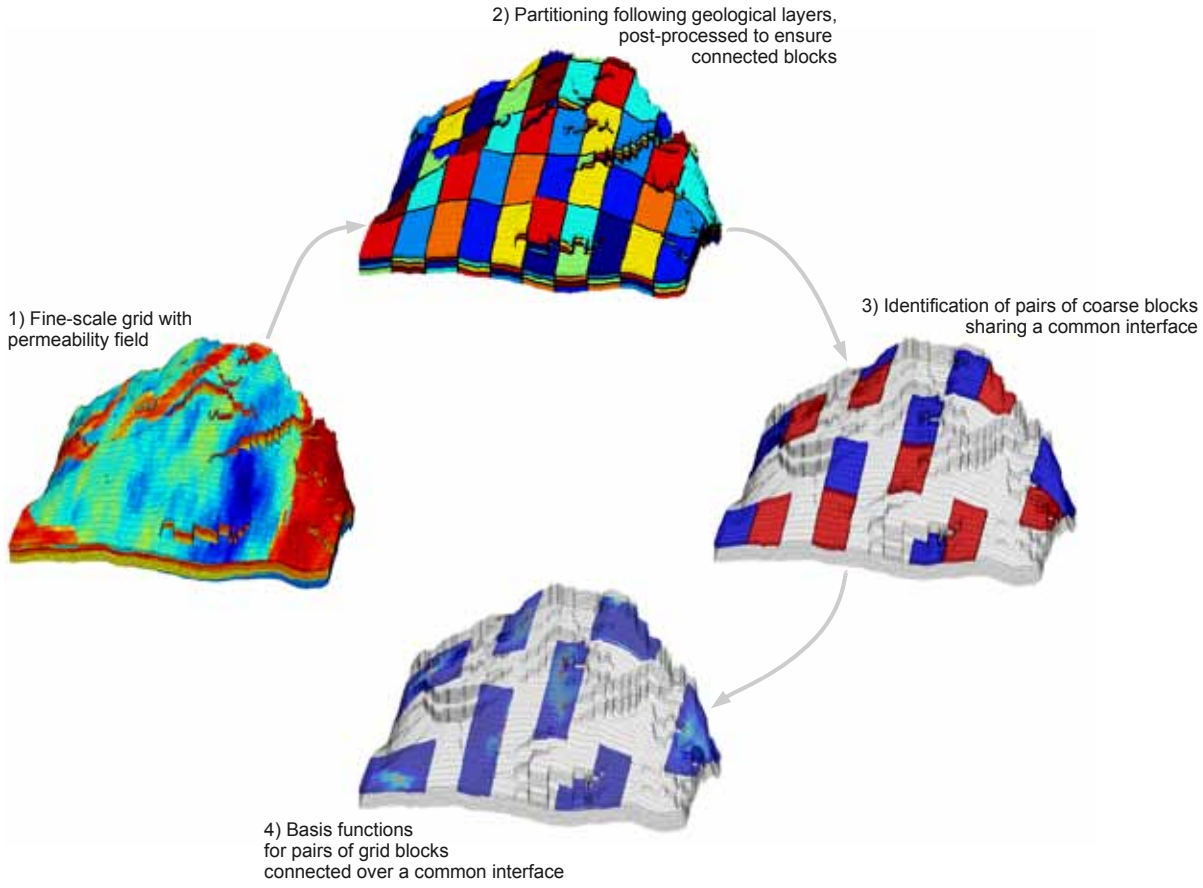


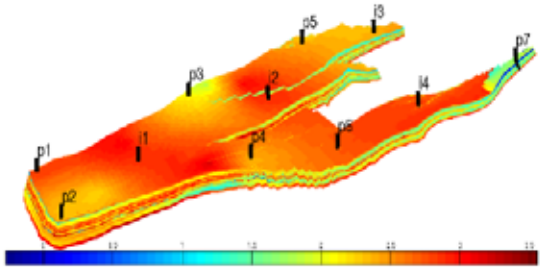
Figure 2: Illustration of key steps for the multiscale method. The model is courtesy of Arne Skorstad (NR) and the SAIGUP project.

coarse block is swept by a strong fluid front or if the global flow pattern changes significantly because of infill drilling, well conversion, or the like.

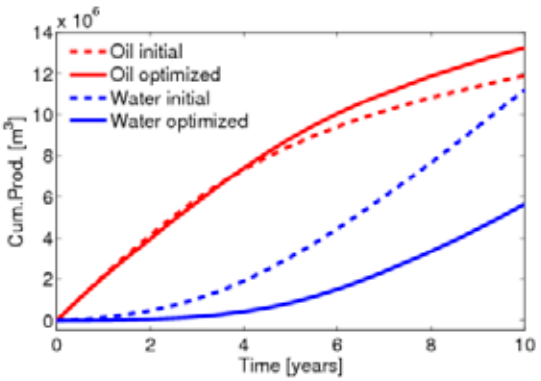
ACCELERATED SIMULATIONS

We will give three examples that illustrate the efficiency of our multiscale method:

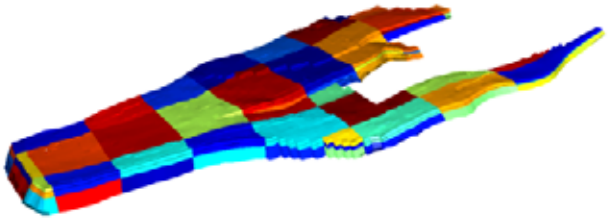
1. The 10th SPE benchmark study was designed to challenge contemporary upscaling techniques and has later become as an academic test bench for new computational methods. In 2004, our group could simulate the whole production history of the million-cell fine-grid model in less than 2.5 minutes on a standard workstation [5, paper III]. This was at least one order of magnitude faster than contemporary multigrid simulators.
2. By combining multiscale flow solvers with an efficient streamline-based inversion method, we were able to integrate seven years of water-cut data from 69 producers into a million-cell model in about seventeen minutes using a standard PC [4,5].
3. Figure 3 shows the use of multiscale simulation as a model reduction tool to accelerate the optimization of water flooding on a model from the Norwegian Sea. Sufficient accuracy in the forward simulations was obtained by using different coarse grids for flow and transport, and the net present value of the field was optimized within a few minutes in Matlab [3].



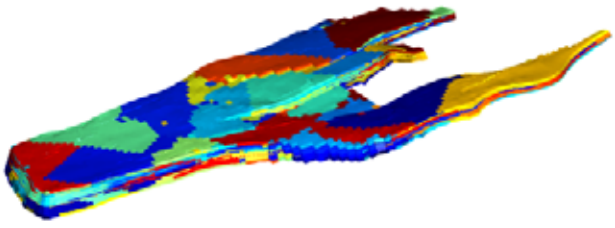
Permeability and well placement



Improvement in cumulative field production



Coarse grid for multiscale flow solver



Coarse grid for multiscale transport solver

Figure 3: Example of water-flood optimization on a model.

In neither of the examples above the underlying solvers exploited the natural parallelism of the multiscale method.

CONCLUDING REMARKS

Multiscale methods are generally very much in fashion. The most valuable conceptual feature of multiscale methods, and what distinguishes them from multigrid and domain-decomposition methods, is the focus on reuse of results from previous computations (as for reduced basis functions). By fiercely reusing computations and cleverly exploiting the inherent parallelism in multiscale methods, I believe that one can make a much needed step change in simulation capabilities. At the moment, the main challenge in my research group is how to most efficiently drive fine-scale residuals to zero and guarantee a prescribed pointwise accuracy. Our ultimate goal is to create a truly multiscale simulation tool that dynamically distributes computational power between upscaling and numerical solution of the multiphase flow equations to obtain the best possible representation of flow fields within a given computational limit. Meanwhile, the interested reader can test the multiscale method using our open-source Matlab Reservoir Simulation Toolbox (MRST) [6].

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Multicore challenges

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TECHNOLOGICAL TRENDS IN MULTICORE ARCHITECTURE AND PROGRAMMING

Multicore processors are now emerging in all markets from embedded systems, laptops and game consoles to servers and supercomputers. Intel predicts that in 2011 as much as 90% of all processors shipped in computers and servers will be multicores. This sudden change is a result of physical and engineering related problems in the processor industry: rapidly increasing power consumption, huge and growing processor-memory performance gap implying that processors have to wait for slow memory accesses, and limited instruction level parallelism (ILP) and clock frequency. These trends are often summarized as the power wall, the memory wall, and the ILP-wall — in total giving the brick wall. Remarkably, multicore designs reduce or circumvent all these problems. These technology changes have given "a new deal" with a rebirth of interest in parallel architecture research and a rapid propagation of parallel programming to other market segments in addition to the HPC community. A direct result is a rich diversity of multicore architectures: homogeneous multicores with different core-counts and different on-chip cache architectures, heterogeneous multicores such as the Cell processor and GPUs, and MPSoC systems typical within embedded systems. On the software side there is renewed interest in old parallel programming languages (e.g. Cilk) and new languages such as CUDA and OpenCL, and there are new techniques such as autotuning and OS-supported power management. We see new multicore programming products every week. In many ways, a programmer with a wish to be productive within CSE for the next 10-20 years will need a more architecture-oriented skill set than in previous years. In addition to parallelism and memory distribution, understanding of the consequences of multicore diversity and heterogeneity, cache and power awareness will be needed for efficient utilization of all future supercomputers and compute clusters.

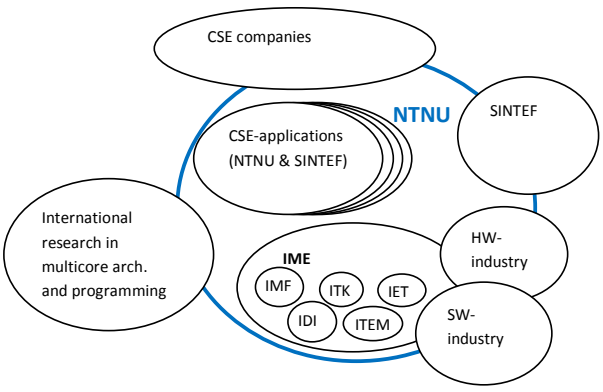

Figure 1: CSE in Trondheim: Contributors and consumers of multicore research in the Trondheim area.

TRONDHEIM — IN POLE POSITION TO BECOME A SIGNIFICANT CONTRIBUTOR TO MULTICORE RESEARCH

NTNU and SINTEF have a long tradition in teaching and research within a multitude of sub-disciplines central for multicore research and CSE. The situation is summarized in Figure 1. On the HW level, the Faculty of Information Technology, Mathematics and Electric Engineering (IME) has produced engineers and researchers at both MSc and PhD levels for the growing HW industry in Trondheim comprising companies such as ATMEL, Nordic Semiconductor and ARM. Three key departments in this area at IME are Electronics and Telecommunications, Engineering Cybernetics, and Computer and Information Science, which have been the main HW contributors. For the SW industry, with Microsoft and Yahoo! as examples, the departments of Engineering Cybernetics, and Computer and Information Science as well as the Department of Telematics have provided skilled personnel. Trondheim has also a significant mix of "CSE companies", many within the oil & gas industry but also within other sectors. There have been several startups and contributions from the Department of Computer and Information Science within both HW and SW for parallel databases. The Department of Mathematical Sciences has produced experts within numerical methods, mathematical modelling and scientific

computing. In this area, there has also been fruitful collaboration with SINTEF, including the Dept. of Applied Mathematics in Oslo. Both this group and the HPC lab at the Department of Computer and Information Science have currently much focus on heterogeneous multicores. At IME, two Special Interest Groups (SIGs) have recently been established to strengthen research within embedded systems (SIG Embedded) and multicore programming (SIG Multipro). Many of the challenges and techniques used in embedded systems are relevant for HPC, and vice versa. As an example, almost all new systems must balance energy consumption against performance. This challenge is an important part of "green computing"– at the heart of the collective endeavour named "Green IT".

"THE P6-MODEL" OF MULTICORE CHALLENGES AND OPPORTUNITIES

Parallel Processing is not a new concept. For more than 40 years the use of multiprocessors has been an alternative for achieving higher **performance**. For at least two decades researchers have seen the growing need and difficulties in combining high performance with **portability**. CSE application developers want to retain good performance when moving to a new supercomputer having a different architecture or software stack. With the overwhelming uptake of multicore processors – parallel programming is now a necessity for most programmers giving an increased focus on the productivity of programmers, i.e. how fast an application can be written. The term **programmability** is often used to denote the ease of developing parallel SW using a given language or tool. While a CSE/HPC project might be willing to sacrifice some programmability to achieve better performance, the recent increased popularity of heterogeneous computing might further reduce the programmer efficiency. Heterogeneous multicores (MPSoCs) have been used in more than 10 years within embedded systems, with better **power efficiency** as one motivational factor.

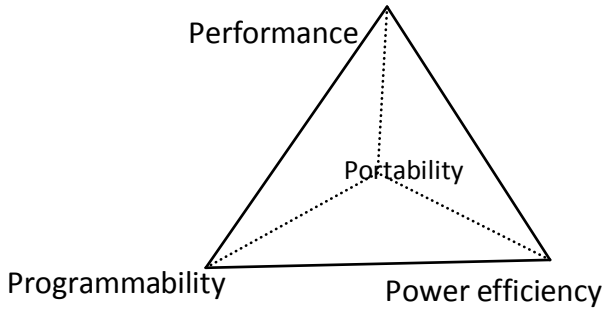

Figure 2: The P6-model: Parallel Processing challenges: Performance, Portability, Programmability and Power efficiency.

The rapidly changing technology continues to give new possibilities and constraints. It can be challenging enough to optimize for just one of the four directions given in Figure 2, and the various user groups have different needs. The real challenge, however, is how to combine the different optimization goals, since they very often are in conflict. The use of GPUs can potentially give very high performance, but programmability and portability might be reduced. Widespread high-level languages and libraries such as MPI and OpenMP will increase portability, but it is still an open question whether they will give optimal power efficiency or maximum performance on multicores. Optimizing for power efficiency means using slow and simple processor cores, and few levels of cache memory, and will give low performance. Optimizing for programmability means using high level abstractions, domain specific languages and powerful scripting languages such as MATLAB and python, but will not reach maximum performance. Tens or hundreds of thousands of researchers all around the world are doing research and development within this field of multicore challenges. This mainstream research is important both for society and industry. NTNU and SINTEF together with associated enterprises have a unique blend of competence to contribute to these opportunities. By joining forces and only focusing on a few areas – we can have a real impact. My proposal is that green computing becomes one of these.

Molecular dynamics simulations

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COMPUTATIONAL SIMULATION

Non-equilibrium *molecular dynamics simulation* (NEMD) was set up in our group in the early 1990 [1]. The idea was to simulate experiments on transport and assist in explaining the mechanisms behind observed trends. In the method, a box with thousands of particles is created (see Figure 1). Pairs or triplets of particles interact according to a prescribed potential, to be investigated, and their movements in a field are calculated using Newton's equations. By summing over particle properties, the macroscopic behaviour is determined.

With state-of-the-art techniques in 2009, not only trends can be understood. Realistic properties are being modelled, and computer simulations can in certain cases replace costly experiments, for instance in the modelling of phase diagrams or equilibrium structures. Modelling of molecular functions must still be done. Aside from these lines of research, molecular simulation plays an important role: It is indispensable in the development of new theory. The three examples below, report on recent activities to determine transport properties, to develop theory and to obtain insight where experiments are difficult, if not impossible.

THEORY VALIDATION IN COMPUTATIONAL SCIENCE

In the development of non-equilibrium thermodynamics theory, computational science is indispensable, because the system is under complete control. Validity of this theory rests on the assumption of local equilibrium. Thanks to NEMD simulations we have been able to define criteria for validity. The Onsager relations are also central in this theory. A first proof was given for these relations for nano-meter thick surfaces [2]. A snapshot of a surface studied in a temperature gradient for these purposes is generated between the liquid and gas in Figure 1.

COMPUTATIONAL SCIENCE GIVES MOLECULAR INSIGHTS IN TRANSPORT MECHANISMS

Flame modelling is a central topic in engineering, and the properties of reacting gases are integral to a hydrodynamic model. We have studied a simple chemical reaction in a large temperature gradient [3] and found that the chemical reaction changes the thermal conductivity and the diffusion. The interfaces of droplets are also special [4]. The interfacial thermal conductivity depends on the curvature when the droplet becomes small, cf. Figure 2, and at the interface, the temperature jumps.

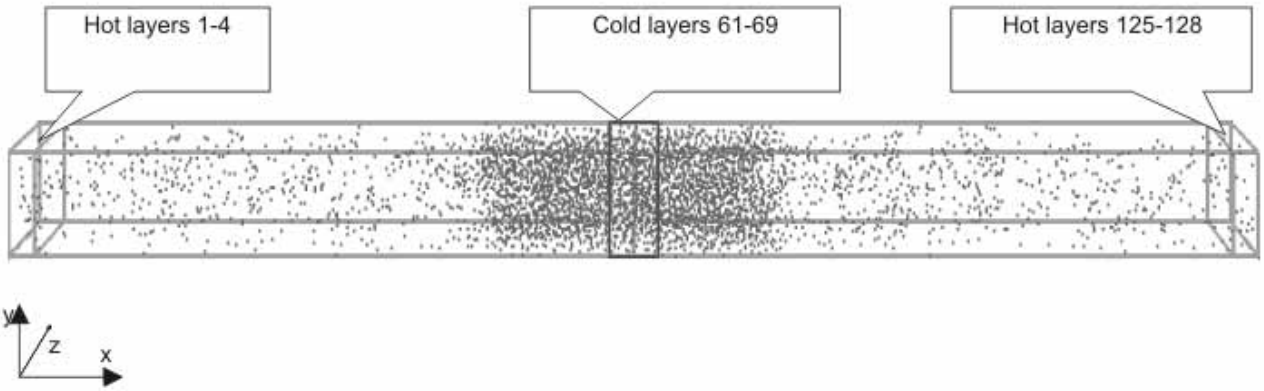

Figure 1: Snapshot of molecules in a box exposed to a temperature gradient. The box is symmetric and heat is taken out in the center and supplied at the ends. A vapor-liquid interface forms at the appropriate condition in each half-box.

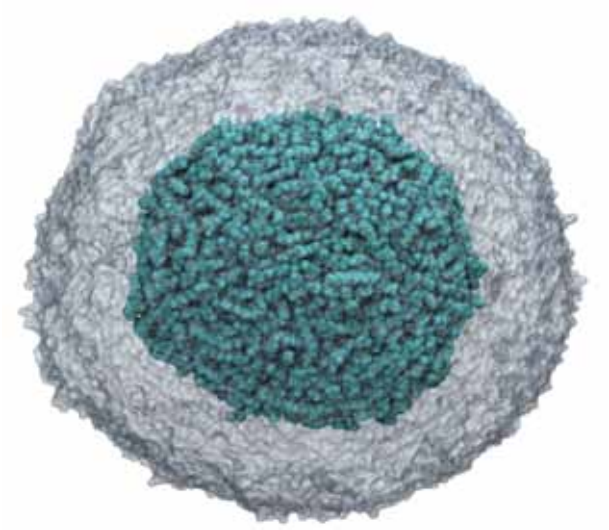

Figure 2: A decane drop surrounded by water has been used to study the heat transfer coefficient of curves interfaces.

COMPUTATIONAL SCIENCE – WHEN EXPERIMENTS ARE IMPOSSIBLE

Surfaces are technically very important; in catalysis, for adsorption, for heat transfer etc. The surface itself is often inaccessible for experimentation because of its molecular dimensions. However, the computer enables us to control the impurity levels, and interface layers can be created and studied separately from their adjacent homogeneous phases. The adsorption of butane into a zeolite catalyst was studied [5] (see Figure 3), revealing that the temperature gradient could be rate-limiting to the transport of chemicals to and from the catalyst surface. This may give new insights in catalysis.

OUTLOOK

Unlike the situation for equilibrium molecular dynamics simulations, where several commercial programs exist (i.e. GROMACS), computer programs for non-equilibrium studies are still being developed "in-house" by research groups. Structure-function relationships must be formulated by chemists' participation. Developments of new software will be greatly facilitated in an environment where interaction of experts can take place. The link between quantum mechanics and systems dynamics is yet to be made workable. This and other large multi-scale efforts, like enzyme behaviour, are waiting for us. A possibility to visualize results is sought. It will greatly enhance the understanding and help the generation of new ideas.

ACKNOWLEDGEMENT

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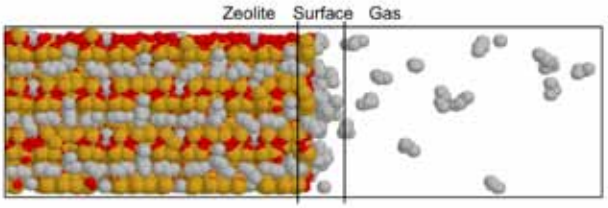

Figure 3: The zeolite gas interface. There is an adsorbed layer of butane molecules in the surface. Transport properties are obtained by exposing the system to fields.

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Computational science and engineering cybernetics

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Engineering cybernetics deals with real-time processing of data and information from process plants, machines and human operators for the purpose of automatic control and monitoring of their operation. The purpose is to secure quality, reliability, safety, efficiency and profitability of the operations.

Advanced solutions and products make use of sophisticated mathematical models, numerical simulation, numerical optimization, and statistical methods together with real-time data arriving at high data rates. Computational science is an enabling technology for the design, implementation and validation of these advanced information processing techniques. Even with the growing user-friendliness of software and the ever increasing capabilities of computer hardware, computational issues remain an important bottleneck and cost in the foreseeable future. As an example, availability of real-time computational power is a major obstacle to be able to handle model and data uncertainty in automated decision making and control, as well as in model-based decision support systems. As another example, numerical simulation and the associated development of mathematical models and software implementation are usually one of the main time-consuming activities in the development and validation of software-based control systems. Computational software with high flexibility, user-friendliness, efficiency and scalability is a key issue. This is further illustrated by the examples below.

OIL AND GAS PRODUCTION OPTIMIZATION

The diagram is a simplified illustration of the processing and control variables in an offshore production facility. In the optimization of production in order to maximize recovery of oil from the reservoir one must typically make decisions about valve settings of water and gas injection wells, the settings of gas lift and chokes for the production wells, various routing valve settings, and settings of valves in the separation and processing trains topside. This has to be based on massive amounts of real-time data from sensors and instruments regarding the state of the reservoir, wells and production equipment. This is a complicated task often conducted in an interdisciplinary team of reservoir and process plant expert operators and engineers. In order to take full advantage of the real-time data it is of great interest to extract key states, parameters and other useful information from the data in real time using mathematical models of the reservoir, well and equipment, together with estimation methods, numerical simulation and numerical optimization.

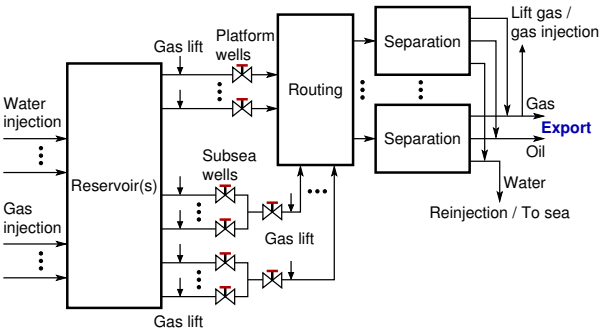

Figure 1: Main elements to be considered for production optimization of an offshore oil and gas production facility.

Figure 2: Topology of an integrated vessel control system.

This has been focused on in the following recent PhD theses [1,2].

There is considerable potential in combining such numerical methods with computation-based Monte Carlo type statistical estimation methods to be able to quantify and incorporate model and data uncertainty in a user-friendly and transparent manner into the automatic or manual decision process. In order to take full advantage of these methods and the available mathematical models, there is a call for advances in the application of computational methods.

SIMULATION-BASED DESIGN AND VERIFICATION OF VESSEL MANAGEMENT SYSTEMS AND DIESEL ELECTRIC MARINE POWER PLANT

Vessel Management Systems in diesel electric vessels used for offshore operations and maritime shipping applications are highly sophisticated integrated control systems which may have 10 000 or more measurement and data tags. The control system will take care of safety-critical functions such as steering, power, propulsion, positioning, ballast and cargo systems. Today, it is computationally and technically feasible to use numerical simulation in order to verify and validate the functionality and design of key modules such as a propulsion control system, a power management system, a power converter, a dynamic positioning system and similar using real-time hardware-in-the-loop simulations [3].

However, in order to achieve fully integrated design and validation of the power plant and control systems one needs to simultaneously simulate equipment such as electric drives with power converter electronics, circuit breakers, power generation equipment and diesel engines, thruster and other electric consumers, vessel motion subject to wind, wave and ocean current loads, etc. as an integrated system. Such integrated real-time simulations combining advanced hydrodynamics, power electronics, electric machines are highly interdisciplinary and extremely computationally demanding due to the dynamic range from microsecond dynamics of power converters to the second or minute range of the machines and vessel motion dynamics. Yet, as an example, this is required in order to be able to fully optimize the design with respect to power system harmonics, resonances, fuel consumption, as well as selectivity and breaker settings to verify power equipment failure scenarios.

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GENERAL OVERVIEW

The Department of Energy and Process Engineering at NTNU has a scientific staff of about 30 professors, 85 PhD students and postdocs, working in four groups; Thermal Energy, Industrial Process Technology, Energy and Indoor Environment, and Fluids Engineering. The department works with power production and energy conversion, transfer and distribution, as well as the end-use of energy, both offshore, sub sea and inland. This comprises from indoor environment and energy use in buildings to oil hydraulics, gas technology, aerodynamics, combustion, bio-energy, refrigeration, as well as the thermal processing of foodstuffs.

The department is involved in several large energy-related projects, both national and European projects. An example of this involvement is the participation of the department in five out of eight Centres for Environment-friendly Energy Research (FME), which were appointed by the government in 2009. At NTNU, the department ranks among the top three with respect to external project funding.

The research activities are combining comprehensive laboratory facilities (6000 m^2) with advanced computer simulation methodologies. For the latter, there is a comprehensive activity with fluid dynamics, combustion and dynamic process simulation.

The research activities in the department are balanced with 36 MSc-level courses and 34 PhD-level courses. Many of these courses, and in particular the PhD-level courses, are related to advanced computer simulation methodologies.

The department has extensive experience working with a number of other departments, both initiating new projects and running joint projects. Since 2003 the department has hosted the Gas Technology Centre NTNU-SINTEF and the Centre for Renewable Energy.

RESEARCH CHALLENGES

Computational fluid dynamics (CFD) is a major area of research within the Fluids Engineering Division and spans from development of improved computational techniques via mathematical modeling to computer-based experiments of complex flow phenomena. While CFD is a research field in itself, CFD is often a vital ingredient in energy and process engineering, notably computational combustion.

Computer-based experiments on turbulent flows are carried out in the 'numerical' wind tunnel', i.e. on high-performance computers (HPC) which are part of the national HPC infrastructure NOTUR. Although the mathematical model for single-phase flow is known, direct numerical simulations (DNS) of turbulence require all scales of the turbulence to be resolved on the discrete mesh. Such computer experiments are therefore feasible only if several million grid points are used. The demand for more efficient algorithms, more efficient supercomputers and advanced post-processing tools is therefore crucial. By means of such computer experiments, we want to reveal and understand complex flow phenomena which are beyond reach in a traditional laboratory.

CSE RELEVANT ACTIVITIES

Research and development

A major part of the research at the Department of Energy and Process Engineering is devoted to the use of computational tools to investigate and optimize fluid flow and heat transfer in energy and process engineering. Commercial software packages are heavily used.

Turbulence is an inevitable ingredient in most industrial flow problems. In practice, industrial CFD relies on phenomenological models since fully resolved simulations are out of reach. The number of unknowns is thus reduced to be compatible with standard computational resources. However, the shortcomings of the

approximate turbulence models have to be addressed. There are also considerable activities in the development of numerical methods and computer codes in particular for multiphase flow. Level set, phase field and volume of fluid methods have been developed for the incompressible Navier-Stokes equations. The lattice Boltzmann method has been devised as an alternative to simulate multiphase flow. Multiscale methods are under development to model the contact line dynamics, where molecular and macroscopic effects interact. Besides finite volume methods, spectral element methods and high order finite difference methods have been employed.

Teaching activities

The following master's courses are taught at the department: Computational Heat and Fluid Flow and System Simulation.

The following PhD courses are taught at the department: Dispersed Phase Modelling, Advanced Computational Fluid Dynamics, Modelling of Multiphase Flow, Turbulence, High Order Methods in Fluid Dynamics and Microfluidics.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The Department of Energy and Process Engineering can contribute broad experience and activity in CFD development, applications and teaching to a CSE centre. In research, our development of new methods for multiphase flow simulation will be of particular interest: modelling issues, sharp interface methods, multiscale methods, etc. We also have interesting activities on numerical methods for compressible flow involving high order methods and immersed boundary methods.

A field of great practical relevance is particle transport in turbulent flows. Tiny particles embedded in a fluid bring in yet another length scale. When the turbulent flow field stems from a DNS, the detailed particle dynamics can be explored. In particular, we can observe how and learn why certain particles tend towards a wall and why they accumulate in certain areas and leave from others.

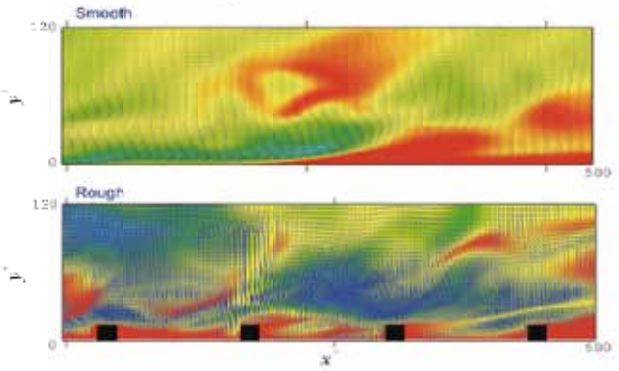


Figure 1: Turbulent flows in smooth and rough channels.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research themes

Direct and large eddy simulation of turbulence, multiphase flow methods, multiscale methods, high order methods.

Education

Master's and PhD courses on CFD, turbulence, etc.

Infrastructure

Experimental facilities for validation of numerical results.

We envisage that the future CSE centre will enhance our collaboration with other researchers at NTNU and SINTEF on multidisciplinary modeling related to energy and process engineering, the development of novel numerical methods for these multidisciplinary models, their efficient implementation on new computer architectures, and the development of corresponding post-processing tools.

GENERAL OVERVIEW

The department (IPM) has about 8 professors doing research with CSE relevant profiles. Of its students, about 5 Ph.D. and 40 M.Sc. candidates are working on computationally oriented projects.

RESEARCH ACTIVITIES

IPM has 4 main research areas:

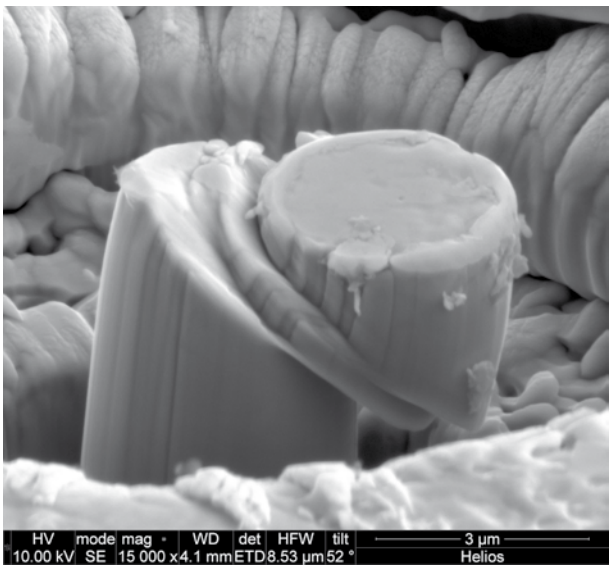
- Structural integrity
- Polymers and Composites
- Metal Forming
- Engineering Design

These areas entails research in tribology, surface technology, fatigue, fracture mechanics, metal forming, welding, long term properties, methodology for engineering design, finite elements and product simulation. IPM has been an active player in software development for more than 20 years, refer to the Fedem simulation code **www.fedem.com**, as well as contributions to more recent commercial efforts such as offshore wind turbine analysis by Virtual Prototyping AS; **www.virtualprototyping.com**.

The last few years atomistic and multiscale material modeling and testing has been introduced as a new activity at the department. A new course is in Atomistic Modeling of Materials Failure, with extensive use of the supercomputer, is now offered.

Teaching activities

About 10 of the courses taught from the department are computationally oriented. This include courses in the field of engineering design, Computer Aided Engineering (CAE), the Finite Element Method (FEM), dynamics, mechatronics, atomistic modeling of materials failure, tools for collaboration and tools for multidisciplinary simulation.



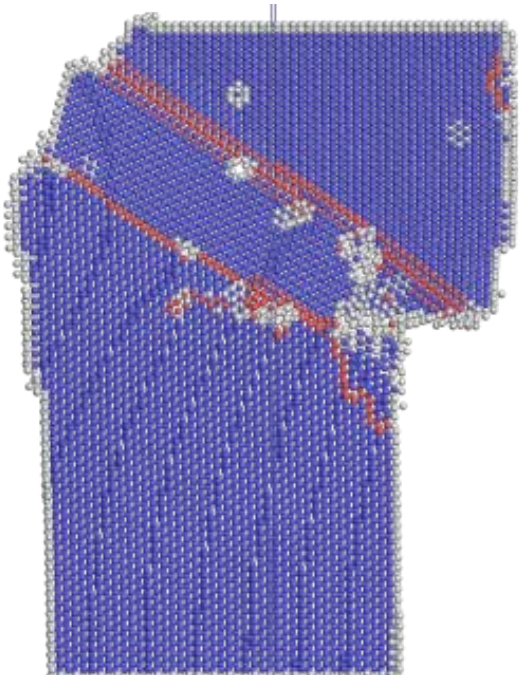


Figure 1: Testing and atomistic modeling of nanopillars made of steel. The pillars are machined with focused ion beam at NTNU NanoLab and compression tested with a nanoindenter. The atomistic modeling is performed with parallel processing at the NTNU supercomputer njord.hpc.ntnu.no. The deformation mechanics and generation of disclocations and twinning are examined.

RESEARCH CHALLENGES

Unsolved problems and bottlenecks

Predicting the behavior of advanced mechatronic systems such as radar tracking systems, active suspension systems for cars, have spurred the development of very advanced codes for nonlinear multidisciplinary analysis involving structural dynamics and controls. However, to further improve the design and optimization of such systems, one has seen the need for doing advanced frequency domain analysis for the coupled system at a given time and configuration. No tools today offer sufficient functionality in this field, and IPM has an ongoing research and development effort here. Screw extrusion is a novel production method for aluminum profiles with shredded or granular material as the starting point. Existing fluid codes are not able to handle the complex flow in the screw channel where the material goes from a granular compressible material to a incompressible fluid. This type of analysis, including the strong friction and lubrication (tribological) components are among the ongoing research efforts at the IPM.

The behaviour of materials under arctic conditions is a challenge for the oil and gas industry. Materials become brittle as the temperature is lowered, especially steel undergoes a dramatic shift from ductile to brittle behaviour as the temperature decreases. Understanding this transition is a major focus in ongoing research activities, including extensive use of FE and multiscale material modeling.

Long term properties of polymers are currently de-

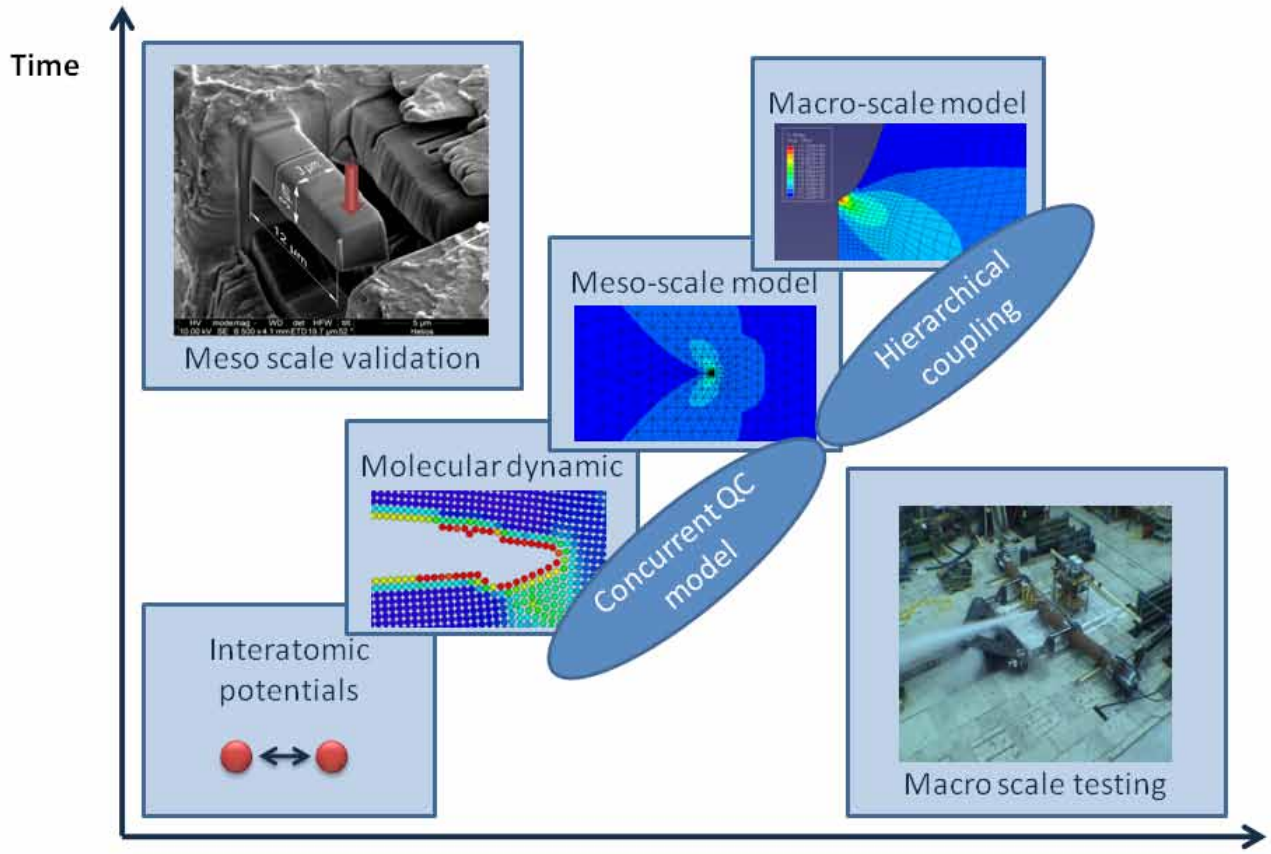


Figure 2: Multiscale material modeling and testing. We apply the Quasicontinuum model to transfer atomic calculations to macroscale behaviour.

scribed by macroscopic mostly empirical models. The degradation happens on an atomistic level where molecules interact. Establishing the link between atomostic interaction and global property change is a challenge that needs to be addressed. Two PhDs will work on this starting in fall 2010. The work is experimental, but extensive computational analysis will most likely be needed to understand the results.

Vision and ambitions

IPMs mission is to do research at an international level in all of its 4 research areas mentioned above. Through solid research activities, IPM seeks to form research partnerships outside the department, at NTNU, at SINTEF and internationally.

IPM has taken an initiative to develop simulation software that is "state of the art" simulation technology for its application.

IPM takes a key role in bridging the gap between engineering science and computer science using the study program *"Engineering science and ICT"* as a tool.

IPM is well equipped to head multidisciplinary simulation software development, and has over the last year strongly strengthened its ability to carry this out. IPM introduces nanotechnology for mechanical engineers. At this moment we are at the crossroads to a new era in engineering where humans, for the first time, start creating structures and technologies at the scale of single atoms and molecules, and with hierarchical features that enables a design from nano to macro. Such nanotechnology could revolutionize the way we live, learn and organize our lives in the decades to come. Computational modelling paired with advanced experimental techniques for validation, in particular atomistic and molecular simulation, is becoming increasingly important in the development of such new technologies. However, once the dimensions of materials reach the submicron length scale, the classical continuum description of materials is questionable and the full atomistic information about the material state is often necessary to study relevant materials phenomena. This presents an issue at the frontier of engineering science, and is particular important to describe phenomena such as deformation and failure of materials, or their behaviour under extreme conditions.

Need for computational methods

Commercial finite element codes are often difficult to use as research vehicles. Necessary "tweeks" are often impossible to do as the codes are seldom sufficiently open. In order to do in-depth research in areas such as screw-extrusion of aluminum, dynamic behavior of actively controlled structures, it is necessary to have sufficiently "open" numerical analysis tools available. Sufficiently open codes are usually either personally developed codes, or collaborative tools developed by centres such CSE.

The atomistic and multiscale modeling depends to a large degree on close cooperation with the development of novel software for parallel computation on supercomputers. IPM will take part in this development.

CSE RELEVANT ACTIVITIES

See previous sections.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Ongoing research and development

The ongoing research and development at IPM has large parts that have general uses for others, in addition to parts that are specialized for our purposes. IPM would very much see that such building blocks were improved through peer-review and use by others in the setting of a centre such as CSE.

IPM is an active participant in the Arctic Materials project, with SINTEF as project leader.

Fluid flow tools for analysis of matrix infusion for composite material structures such as wind turbine blades.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research themes

IPM looks forward to take part in development of the next generation of methods in computational mechanics. In particular, IPM envisions the need for collaboration with mathematicians and computer scientists to develop novel methods and computer software for handling multiscale phenomena.

Education

IPM envisions taking stronger part in providing courses in computational mechanics relevant for the "Engineering science and ICT" study program. A fruitful collaboration with researchers focusing on numerical methods and software development in a future CSE centre is considered beneficial for IPM to provide high quality courses for this study program.

Infrastructure and facilitation

Of great importance to IPMs vision of developing "state of the art" simulation tools are our physical testing laboratory facilities, considered essential to do validation of numerical methods. IPM will make the laboratories available to other partners in the CSE centre.

IPM has several computer laboratories dedicated to undergraduate and graduate students. However, IPM needs access to HPC infrastructure and user support, assuming this to be provided through a future CSE centre.

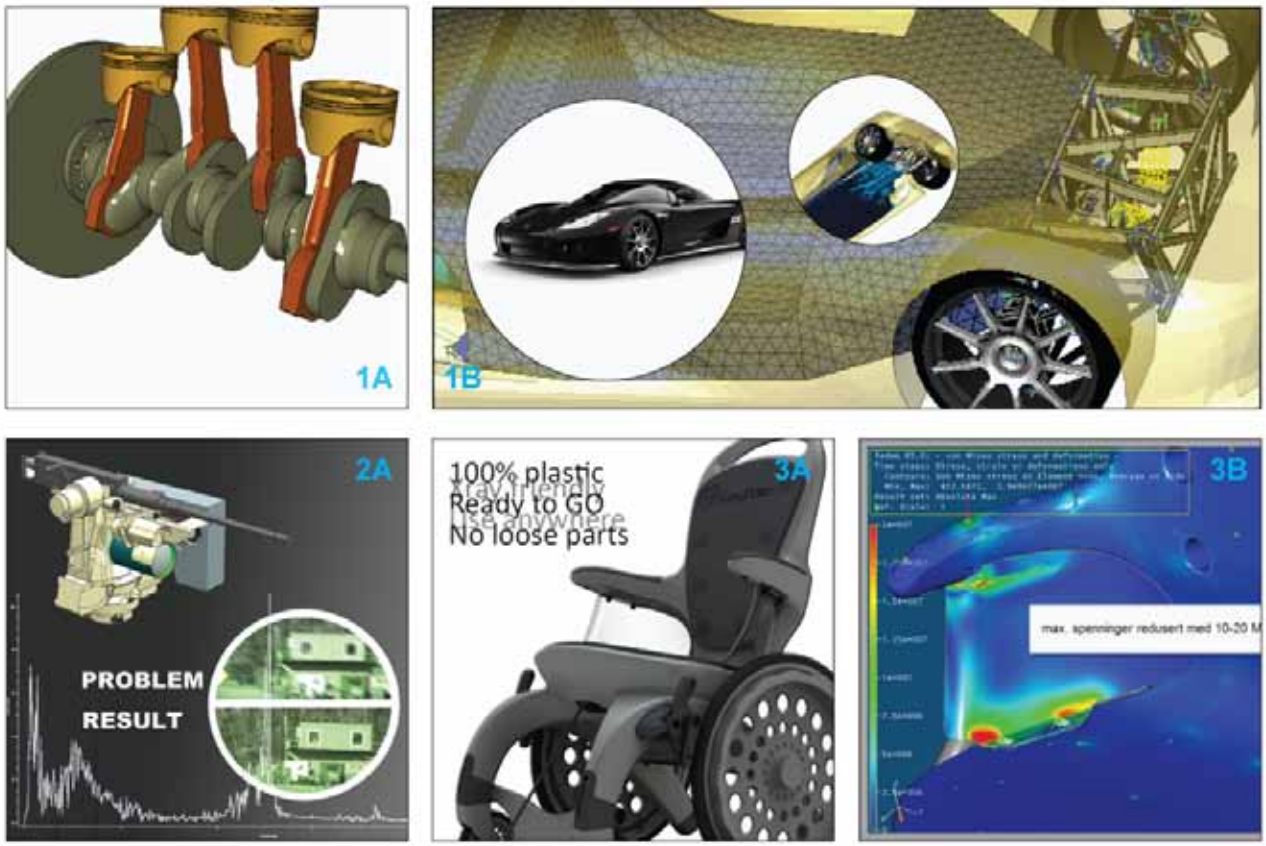


Figure 3: Example simulation applications: Engine (1A), Car suspension (1B), Remote weapon system (2A), Wheelchair (3A and 3B).

GENERAL OVERVIEW

Research activities

The research activities at the department are governed by the fact that the Norwegian marine industry operates in some of the harshest environment on the globe. A combination of strong winds, large waves, deep water, low temperatures and safety concerns requires unique technological solutions. The research activities are broad, spanning the disciplines of hydrodynamics, structural mechanics and cybernetics. The department is engaged in several strategic research programs

- Extreme wave load effects in sea structures
- Scenario-based risk assessment of ship collisions and groundings
- Marine computational fluid dynamics
- Material and structural integrity
- Performance in a seaway
- Energy from the north. Arctic technology
- Floating and fixed wind turbines at sea

Unique national laboratories are operated in cooperation with MARINTEK. These are: towing tank, ocean basin, marine cybernetic laboratory, wave tanks, cavitation tunnel, circulating water tunnel and marine structures laboratory.

These laboratories are becoming more and more important in their role as complementary tools to numerical simulations.

Teaching activities

Around 100 MSc students start their 5-years study every year and the department offers marine-related courses from the first year. In the last two years, all courses are given in English, coordinated with our International Master Program in Marine Technology. There are modeling, programming and simulation courses given from the third year.

RESEARCH CHALLENGES

The trend for marine structures is that they become more and more optimized and dynamically sensitive, where interaction effects between waves, wind, current, ice, soil and control system induced response increase. Laboratory testing can only be performed for parts of the total system. Hence, verification of new conceptual designs has to rely on virtual "testing", i.e. numerical testing to increasing extent. This requires thorough understanding and mathematical formulation of the governing physical processes. An example of this is installation of wind turbines offshore in relatively deep water where fully integrated analysis of the complete servo-areo-hydroelastic system is needed (Figure 1).

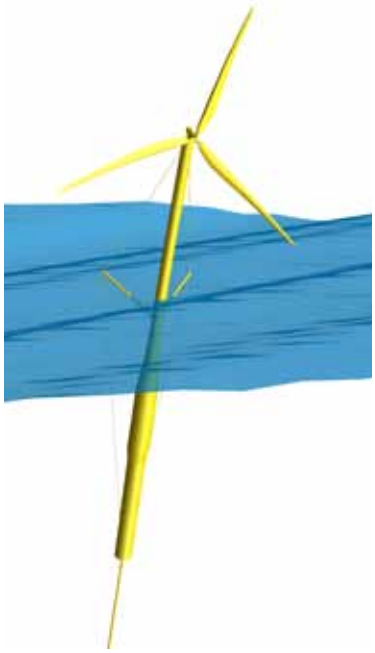


Figure 1: Floating wind turbine.

Another trend is exploration and production of oil and gas resources in deeper waters, often associated with high pressure and temperature wells. To minimize the costs and still ensuring structural integrity, more advanced models are needed to describe the structural behavior considering fluid-, soil-, and structural-interaction.

Deep water installation requires more accurate simulation of the physical process in order to meet the installation tolerances. This requires not only integrated analyses but also real time simulations with on-line monitoring of vessel motion, environmental loads etc. as illustrated in Figure 2.

Wind turbines and electrical power for more environmentally friendly oil and gas production both requires high voltage power cables for energy transmission. The lifetime reliability of these may both be governed by the local 3-dimensional stress state and electrical effects which require integrated electrical and structural models with a high degree of complexity.

The Norwegian marine industry have performed a huge amount of laboratory testing related to the above and have therefore ownership of a large amount of scientific data. Since these data can be used to calibrate computational models, the Norwegian research institutions are in an unique position to serve the worldwide industry with more advanced models. Extracting scientific knowledge from this data collection requires major research efforts.

Bottlenecks

The main bottlenecks are both related to computational and human resources. With the available computational resources, we are in the position of solving equations within the order of 5-10 million unknowns. However, in order to meet the future challenges this need to be scaled with a factor of more than 1000. This can most likely not be enabled by faster computers alone but requires increased focus on numerical code optimization. It is obvious that this requires a major effort both with respect to human and computational resources and also integration of the different disciplines involved. Effective data handling utilizing memory hierarchy, parallel processing and visualization and animation of results are examples.

CSE RELEVANT ACTIVITIES

Research and development

One group has participated over time in several CSE-focused user projects supported by NOTUR/NTNU IT. The use of Direct Numerical Simulation to simulate turbulent flow in CFD put a challenge on handling and

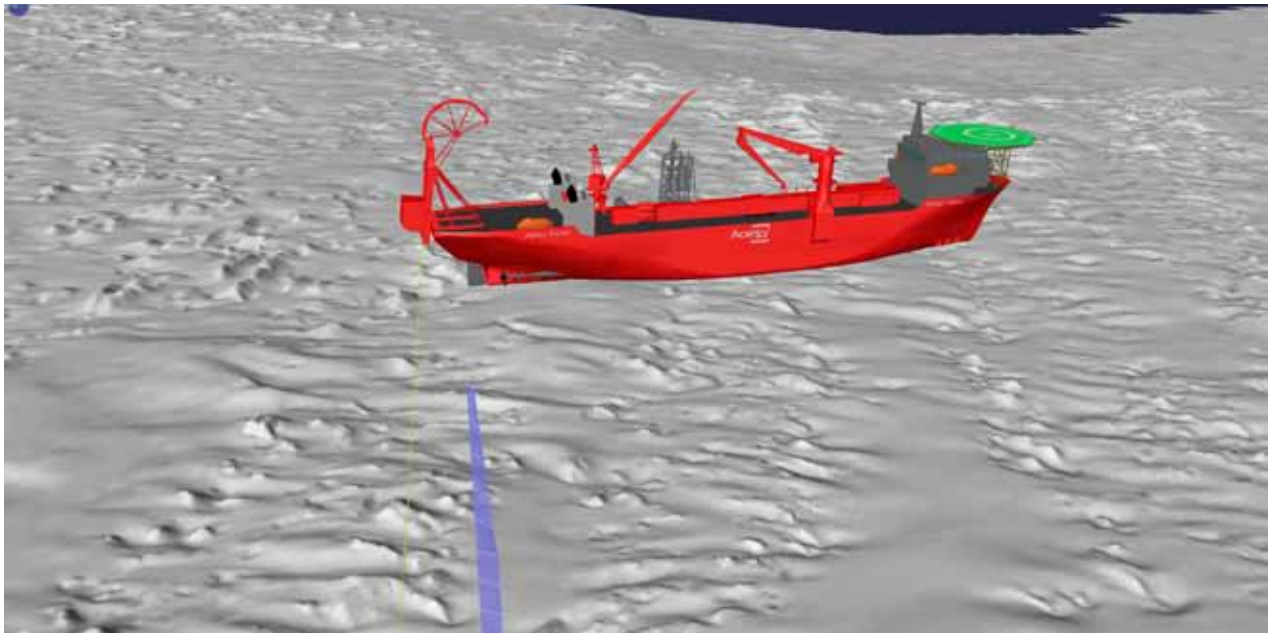


Figure 2: Simulation of installation process in deep water.

storing, on the fly, of large amount of data. Today we cannot use more than approximately 700 cores with our existing simulation code, but work is planned to break that limitation. This is necessary in order to expand the simulations to higher Reynolds numbers, and more practical flow situations.

Scenario based approach to risk analysis of ship collision and grounding: A major part of the activity is devoted to simulation of collision and grounding problems with the explicit solver (LS-DYNA). A particular challenge is related to high energy collisions between bergy-bit ice and ships. Severe damage to the outer shell is accepted for such accidental collisions, but the objective is to perform a fully integrated analysis where the mutual deformation of the bow and the ice is taken into account. The task involves considerable development of continuum mechanics modeling of ice.

The lifetime of subsea power cables is expected to be a critical factor with respect to large scale development of renewable offshore energy resources. Since the lifetime may be governed by the local 3-dimensional stress state, this requires a major development of methods that enable efficient solution problems including contact dynamics.

Teaching activities

In cooperation with DNV the department annually offers courses in the use of the DNV software suit SESAM in the MSc course Design of Offshore Strcutres (4th level). This also includes use of USFOS for analysis of the jacket response to extreme stochastic waves and simulation of offshore wind turbines subjected to transient -, fault- and emergency conditions. In their last year, MSc students are offered a course in CFD related to marine structures.

POSSIBLE CONTRIBUTION TO A CSE CENTRE

Ongoing research projects

Several of our 90 PhD-students are involved in simulation projects. They will represent a resource of knowledge, experience and competence. Since they are in different phases of their PhD-work, they may benefit from, and contribute to, the participation in a “pool” of collaborating students.

Planned

We will continue at this level for the next 5 years, with increasing focus on the integration of experiments and computational results with visualization and data mining tools.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research topics

Explore HPC problems and take responsibility for updated knowledge of marine CFD related applications in cooperation with SINTEF. Coordinate PhD students.

Education

We have teaching activities in modeling, programming and visualization. Several MSc-students are every year involved in detailed program development during their thesis and use of our visualization laboratory (Havrommet).

Infrastructure

We have at the moment no separate infrastructure (hardware) to offer our users, but we plan to install a dedicated cluster with discipline specific software, to be used for initial testing and upstart students. It will be highly integrated with the central HPC system at NTNU.

Of crucial importance is more advanced user support over time so we can concentrate on modelling and solving marine problems.

GENERAL OVERVIEW

Research activities at the department involve reservoir engineering, geophysics, rock physics/geomechanics, petroleum production, well drilling, CO2-storage and Integrated operations within petroleum industry.

The department gives approximately 40 MSc courses per year. 16 full time professors and 8 adjunct professors are responsible for teaching and supervision of the approximately 100 MSc students per year. About 40% of the MSc students are non-Norwegian. In addition approximately 60 PhD students are employed at the department, wherof more than 50% are non-Norwegian.

RESEARCH CHALLENGES

Development of geophysical methods for early detection of gas and CO2-leakage from subsurface layers. The main bottleneck for this research is the repeatability of time lapse measurements. Numerical inversion methods to correct data for acquisition footprints will demand development of computation methods.

Seismic imaging of complex structures such as below salt and basalt. The main bottleneck here will be to develop new algorithms for seismic velocity estimation and seismic wave propagation. There is also need for new acquisition methods for improved illumination. The computation methods needed are development of 3D wave propagation algorithms and full automatic velocity estimation.

Efficient use and integration of field data acquired at a producing oil field. A challenge here will be to develop a common platform for integration of diverse data. The computational methods will be semantic web and efficient data organization.

Drilling of long wells (up to 40 km). The main challenges here will be limited material strength of drilling equipment in addition to hydraulics systems and data transmission. The computation methods will simulation of material properties (development of new materials).

100 % recovery from hydrocarbon reservoirs. The main challenges here will be identification and mapping of the hydrocarbon reservoir. Also new recovery methods must be found. On the computational side a detailed fluid flow simulation from micro to macro scale will have to be developed.

Complete well downhole separation and injection. Bottlenecks here are availability for efficient maintainence and well interventions and reliability. Computer methods needs are data transmission and monitoring.

CSE RELEVANT ACTIVITIES

Seismic modeling: Development of finite difference (FD) modeling of three-dimensional anisotropic elastodynamic wave equation. This is strongly coupled to the mathematical inversion for the subsurface medium parameters. Realistic 3D FD models include 20000x20000x6000 grid cells, each containing up to nine medium parameters.

Reservoir simulation: FD modeling of 3 phase, 3-dimensional diffusion equation. History matching is a multidimensional inversion scheme enabling production forecasting. Realistic models include up to several million grid cells.

4D seismic: To identify undrained hydrocarbon pockets (100 % recovery) there is a strong need for efficient coupling of reservoir simulation and 4D (repeated) seismic. In addition, new methods for recovering trapped hydrocarbons within the pore system are needed. Simulation on micro-to-nano-pore scale (3 phase and 3D) is assumed to be an essential research topic.

Teaching activities at the department will use/benefit from CSE activities. Examples of this is 3D visualization for enhanced interpretation, model building and well planning. Here, a cooperation with the computer department at NTNU is vital to maintain the leading edge position of visualization. There is also need for improved systems for more realistic (3D) processing

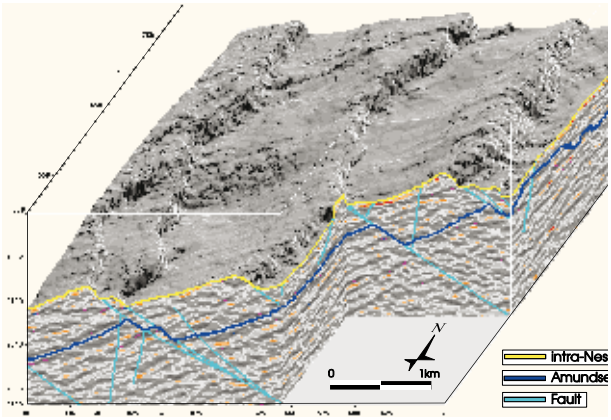


Figure 1: Reservoir model of the Gullfaks field, North Sea.

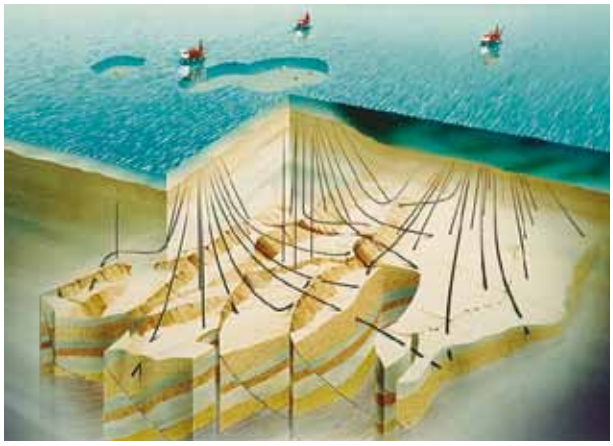


Figure 2: Seismic data from the Gullfaks field, North Sea.

of seismic data. Today, only 2D and simplified processing algorithms are used due to limited computer power and teaching personnel. Reservoir fluid flow simulations for education suffer from similar shortcomings. So far, at the department no teaching has been introduced for micro-to-nano pore scale simulations.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The following ongoing research projects at the department can be of benefit for a CSE centre:

- Strategic centre for research based innovation (CRI) within integrated operations within petroleum (IO-centre).
- Storage of CO2: This activity is a part of a centre for Environmental-friendly Energy Research.
- ROSE (Rock Seismic): Geophysical research for improved characterization of overburden and reservoir rocks.
- Unconventional hydrocarbon reservoirs.
- Test facility at the department for drilling, reservoir and geophysical studies (planned)
- New centre for improved oil recovery (planned)
- Continuation of the ROSE consortium including 20 industrial partners (planned)

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Development of numerical algorithms for new generation of 3D and 4D geophysical simulations. Todays computer facilities are not capable of solving such problems. Large international multi-computing cooperative initiatives are currently launched. However, even the Society of Exploration Geophysicists (SEG)-initiative involving a dozen of oil companies is in-sufficient. Therefore, there is a need for more efficient computer implementations.

Advanced simulation of fluid and pressure distributions both in reservoir and production systems. A typical fluid flow simulation within a petroleum recovery system requires several hours of CPU-time. Ideally, this should be done in seconds in order to achieve a more realistic scenario modeling, and improved updating of the reservoir model.

Education. The department has currently three experts in team villages: Gullfaks village, Norne village and the Virtual Reality village. All these villages will benefit from advanced CSE support. Students can cooperate with the CSE centre for dedicated computational problems.

Infrastructure. The department can provide three state of the art operation/visualization rooms to be used as an arena for scientific collaboration.

GENERAL OVERVIEW

The Department of Structural Engineering teaches the fundamental courses in solid state mechanics for all engineering programmes at NTNU. The department is particularly involved in the curriculum of the Master study programmes for Civil and Environmental Engineering and Engineering Science and ICT.

Research at the department is primarily concerned with experimental testing in well-equipped laboratories and numerical (program controlled) simulations. Our strength lies in the combination of these, while our theoretical foundation is mechanics. Research and development encompass the following disciplines and fields; (1) concrete structures and material technology, (2) biomechanics, (3) fracture mechanics and fatigue, (4) structural dynamics, (5) steel, light-weight material and timber structures, (6) nanomechanics, (7) numerical modeling and simulations, (8) software development, and (9) impact and energy absorption .

The department is heavily involved in two Centres for Research-based Innovation (SFI):

- SIMLab, the Structural Impact Laboratory, is hosted by the department.
- COIN, the Concrete Innovation Centre, is managed through SINTEF, but with the department as a research partner.

  The department participates in NTNUs Institutional Strategic Program (ISP) for Sustainable Infrastructure and the following large projects:
- ICADA – Integrated Computer Aided Design and Analysis
- Norlight – Crashworthiness of Light-Weight Automotive Structures
- RESIA – Residual Stress Simulation for Integrity Assessment

The Department of Structural Engineering has a total of 35 professors including associate, assistant and adjunct professors. In addition to the professors, more than 50 Ph.D. candidates, post docs and researchers are currently engaged in research activity at the department.

Our collaborative research partners include SINTEF, Statoil, Hydro, Det Norske Veritas and Simula Research Lab, in addition to companies in the building and construction industry, large and small.

RESEARCH CHALLENGES

One of the current activities in nanomechanics is the development of a multiscale modeling approach to engineer the microscale and nanoscale molecular characteristics in order to obtain designed mechanical and physical properties of the materials. The macro properties are determined by material microstructures which are further linked to their atomic/molecular structures. Therefore, multiscale modeling and simulation strategies to provide seamless coupling among various length and time scales are essential for nanomechanics. The current focus is the polymer particles and silicon materials. The research in nanomechanics and multiscale modeling is computation intensive and strongly depends on the super-computer infrastructure available in Norway.

The biomechanical activities was established about five years ago and have increased significantly over these years. Research has mainly been carried out along two axes: Computational cardio-vascular mechanics and computational bone mechanics. Two years ago the division joined the Simula Research Lab centre of excellence “Centre for biomedical computing” as a node. Our research input addresses patient specific models and computational methods for heart valves, blood flow and fluid-solid interaction in the heart and vessels. The other axis provides research input to ortopaedians. Here patient specific numerical analysis of hip prostheses and leg lengthening is addressed in order to give clinicians better tools for decision making.

Most of the biomechanics analyses must employ high performance computers in order to obtain results within reasonable time. We believe that improved numerical schemes coupled with parallelization on high

end computers are very important in order to provide original research results. So far we have addressed the modeling by means of the continuum mechanics approach. The current trend is to go down in scale (e.g. cells, microstructure). This trend requires multiscale methods and efficient algorithms, hence computer resources will be even more important.

The Department has long traditions in computational mechanics dating all the way back to the pioneering days of the computer based finite element methods in the 1960's. Since then the Department has been involved in a systematic development of the finite element method for use as a tool in engineering decision-making processes. Currently the Department participate in the KMB project ICADA where the objective is to integrate computer aided design and analysis based on a coherent representation for geometry and analysis. Although geometry is the foundation of analysis, modern methods of computational geometry have until recently had very little impact on computational mechanics. It now seem appropriate to look at more powerful descriptions of geometry to provide a new basis for computational mechanics. An important aspect of the ICADA project is to explore the new generation of computational mechanics procedures based on modern developments in computational geometry. In the ICADA project emphasis is on Isogeometric Analysis in which basis functions generated from NURBS (Non-Uniform Rational B-Splines) and T-Splines are employed to construct an exact geometric model.

While standard finite elements have a wide application spectrum, there are still limitations where they do not give acceptable results. One class of problems that finite elements are not able to capture sufficiently accurate are problems that involve strong and weak discontinuities, i.e. jump in the displacement and strain field, respectively:

- Fracture and computational failure mechanics that involves initiation and propagation of cracks (strong discontinuities)
- Coupled problems, that can be classified into solid-solid, solid-fluid and fluid-fluid interfaces (weak discontinuities)

In order to understand the variability of macroscopic properties of the various structural materials (e.g. concrete, wood, steel, aluminium, composites, etc.) and the underlying phenomena and to suitably describe them mathematically in a material model, the hierarchical microstructure of the material has to be considered. At sufficiently small length scales universal constituents common to the various structural materials as well as universal building principles may be identified. A mathematical formulation of the universal building principles results in a multiscale micromechanical model which links microstructural characteristics of the various material samples to macroscopic mechanical properties of these samples. First and second order homogenization techniques are employed for this purpose depending of the length scale of the heterogeneities.

In order to meet the future challenges and cope with the limitations of current analysis techniques the following research tasks are identified:

Figure 1: Translucent concrete bridge.

- Bridging the gap between design and analysis in industry through Isogeometric Analysis.
- Establish accurate and reliable solution techniques for solving problems that involve strong and weak discontinuities.
- Establish a multiscale design system for structural materials (e.g. wood and concrete) which integrates state-of-the-art multiscale analysis capabilities with material model calibration and validation. The theoretical framework is based on first and second order homogenization.

The following research areas connected to wood are currently paid special attention at the department; (1) material description and experimental parameter estimation based on experimental testing, (2) interaction phenomena between metallic fasteners and wooden material including fracture, (3) moisture, moisture gradient effects and moisture induced stresses, and (4) vibrations of wood based composite structures and sound insulation

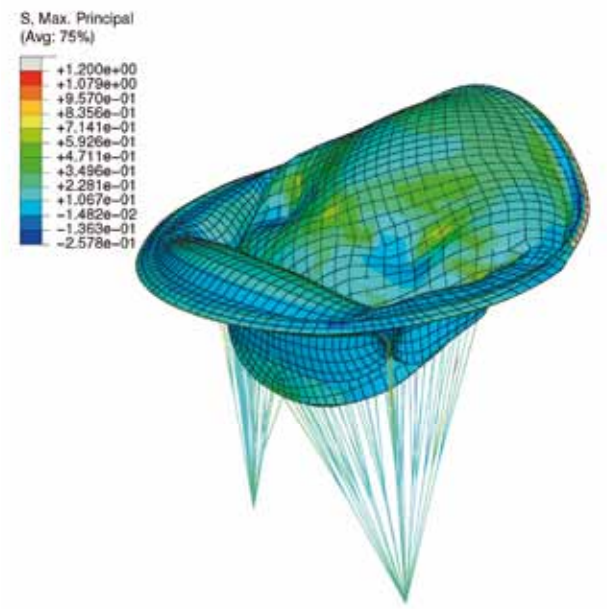


Figure 2: Principal stresses in the mitral valve at peak systole from finite element simulation.

There is a need for improved material models for wood based materials, but the development has to be performed in parallel and together with extensive laboratory testing in order to have confidence and valid parameters. It is well known that wooden material have considerable size effects and variability, and consequently statistical properties on several scales, including the structural scale used in most engineered structures, must be evaluated. The most critical issue related to the development of mathematical models for material description is the availability of and experimental facilities for exploring the physical behavior and parameter estimations.

The Department of Structural Engineering also has a long tradition in computational response calculations of stochastic load processes such as wind and earthquake induced loads. Future challenges will include high degree of non-linearity demanding the development of new and efficient real time computational methods. This includes better description of the in instantaneous stochastic wind field, the influence structures have on the wind field and the imposed loads by the wind field on structures.

Reliable response calculations for long spanning slender structures such as suspension bridges are already stretching present methods used in structural design. This will demands improved solution techniques for structural response from high wind speeds close to aerodynamic instabilities where material, geometrical as well as aerodynamic non-linearity's controls the response predictions.

Most calculations today are based on extensive wind tunnel tests which can be both time consuming and financial costly. A moderate use of wind tunnel test together with an increased use of CFD analyses can help to create new and improved load models for more efficient response solutions, making it possible to validate future groundbreaking bridge design.

Within the field of renewable energy production using

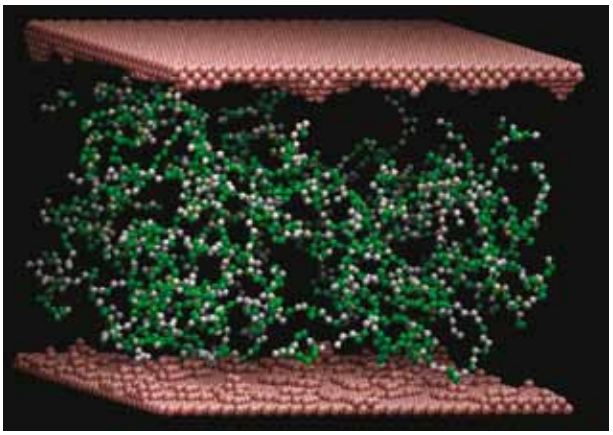


Figure 3: Nanomechanical properties of Polymer particles and polymer-metal interfaces – Metal-coated polymer interfaces.

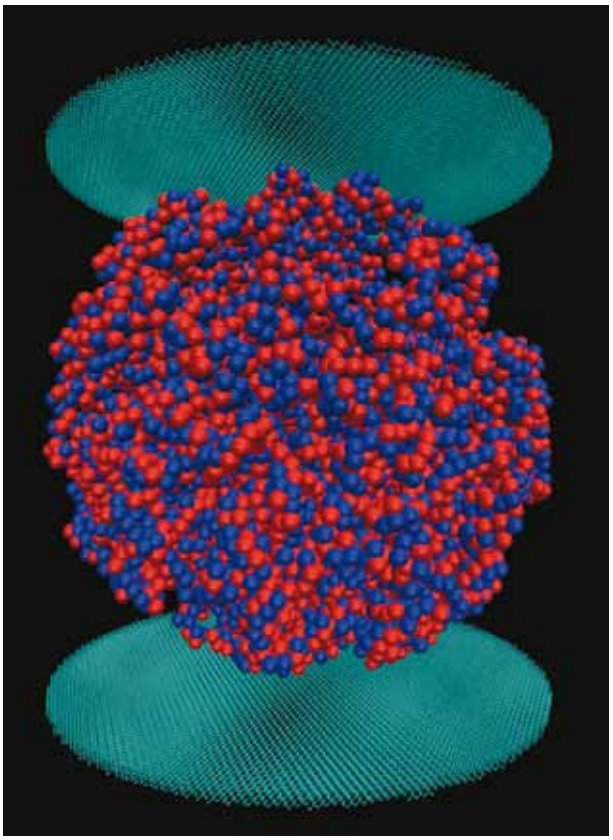


Figure 4: Nanomechanical properties of Polymer particles and polymer-metal interfaces – Metal-coated polymer particles.

off-shore windturbines are the demands for real time solutions of highly coupled problems of vital importance. It is necessary to use models which can predict the interaction between structural response, wind and wave loads, influence of the production unit to the wind field as well as control systems to create an efficient and economical viable power generation.

Real time calculations are of great interest for structural response where a high degree of structural load interaction controls the system. However, it is equally important to be able to predict the uncertainties of the processes. Better uncertainty predictions will require highly efficient methods to meet the increasing computational cost of solving large reliability problems. The effects of the inherent uncertainties in load models, the underlying statistical data as well as possible shortcomings in structural response calculations are areas of great interest.

Other activities that will demand computation solution under the influence of load structure interaction is the development of extremely long spanning submerged floating tunnels. These structures will demand new technological solutions to be able to span several kilometers to cross some of the largest fjords in Norway. Finally, another field of structural dynamics which can be of interest is wave propagation, particular regarding noise and vibration pollution of buildings. There is an ever continues increase of different sources such as technical installations in the modern society which must be combined with higher standards and increasing demands from the general public.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The research challenges addressed above are all CSE relevant activities that require efficient algorithms and dedicated software tailored to take advantage of the existing computer resources. Today both commercial software and software developed in-house are used for this purpose.

Ongoing research activities in for instance nanomechanics, biomechanics and multiscale modeling are relevant contributions to a CSE centre.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

In the context of structural engineering, it is important for our department to collaborate with a CSE Centre as this will enable us to improve and expand many of the research challenges addressed above.

The Department of Structural Engineering is in the process of establishing a virtual laboratory for design and testing of new engineering materials based on multiscale modeling and simulation. In this context a major challenge is to develop a multiscale design system that can take advantage of the practically unlimited design space at the fine scales. Many of the necessary experimental facilities to carry out extensive testing and validation are currently available at our department. However we need a better understanding of how to calibrate the design space at many different scales to the experimental data available. This effort would benefit from collaboration with a CSE Centre and hopefully vice versa.

GENERAL OVERVIEW

The research at the Department of Language and Communication Studies relate to CSE in two areas. One area combines natural language processing and formal linguistics, namely *e-linguistics* and *grammar engineering*. The other area is that of technological applications within the area of *Norwegian as a Foreign Language*.

E-linguistics is an emerging term for a family of methodologies that uses computational tools to combine linguistic analysis with the advantages of modern database technology and the possibilities offered by the World Wide Web (the Cloud). A rising need for sharing data resources is one of the driving forces of this research; a growing insight into the potential offered by modern communication technology for the advancement of research itself and the publication of its results is the other force behind this development. New standards emerge in the for generating reusable resources, and to create the linguistic tools that allow computational handling of language data without demanding special computational skills or background of the user.

Grammar engineering is the building of computational parsers and generators reflecting the rules of linguistic grammars, with the possibility of representing the semantic content of parsed sentences in ways such as to interlink the sentences with knowledge bases, automatic translators, artificial agents, and more.

The main current projects in these areas are, respectively, *TypeCraft* (http://www.typecraft.org), an annotation editor combined with a database and a wiki (see figure 1), and *NorSource* (http://www.typecraft.org/tc2wiki/Norwegian_HPSG_grammar_NorSource), a computational parser for Norwegian.

Both developments have a certain commercial potential; also, both applications represent a considerable intellectual value. It therefore is of importance that the intellectual rights connected to these applications are assessed. To deal with this issue has so far been beyond the scope of what can be done within the ISK.

The sustainability of tools developed within research projects and the question of intellectual property

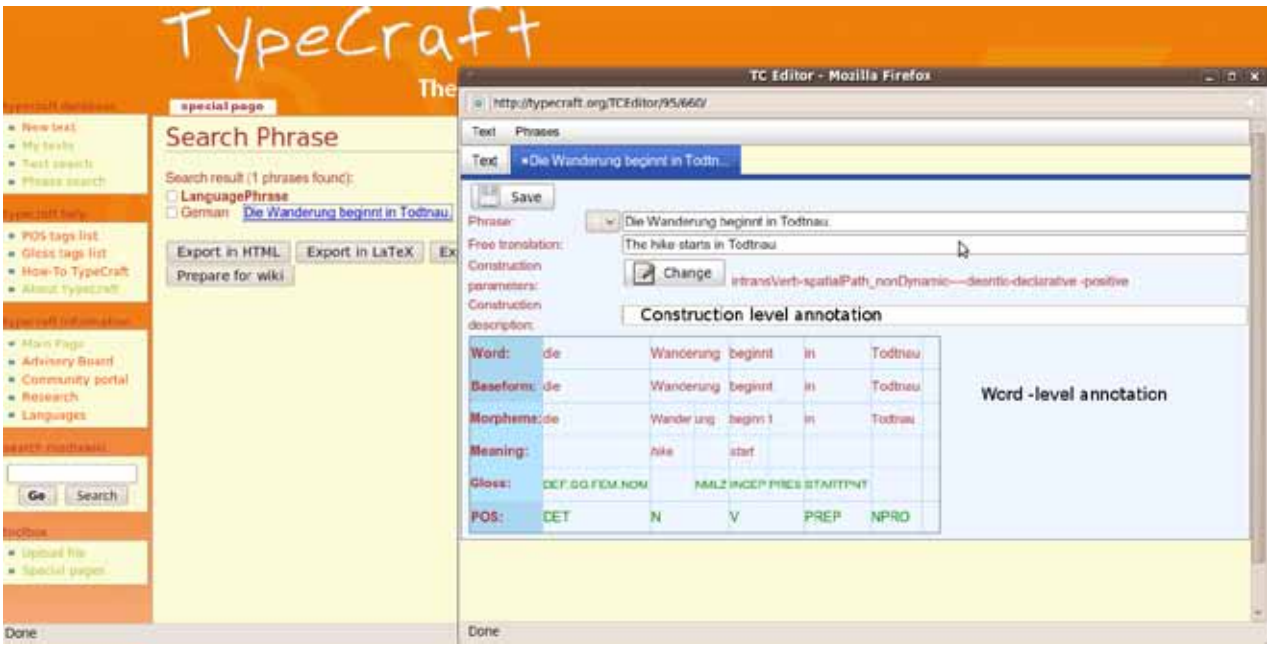


Figure 1: The online annotation and database interface of TypeCraft.

rights are also relevant in other projects in ISK. In the area of *Norwegian as a Foreign Language*, two projects started on August 1, 2009. Both projects integrate research directly into the teaching practice for foreign students and employees at NTNU.

The first project, WIN, aims to develop an internally funded computer-assisted language learning (CALL) course, and will offer web-based Norwegian courses for beginners. One of its goals is the development of interaction platforms in which L2 (second language) learners can communicate with each other and with their Norwegian teachers through a web interface. Both the WIN learning environment and that of CALST (see below) have the potential of extension of its use to very large groups of L2 learners, and its platforms should be sustained long past the projects' lifetime.

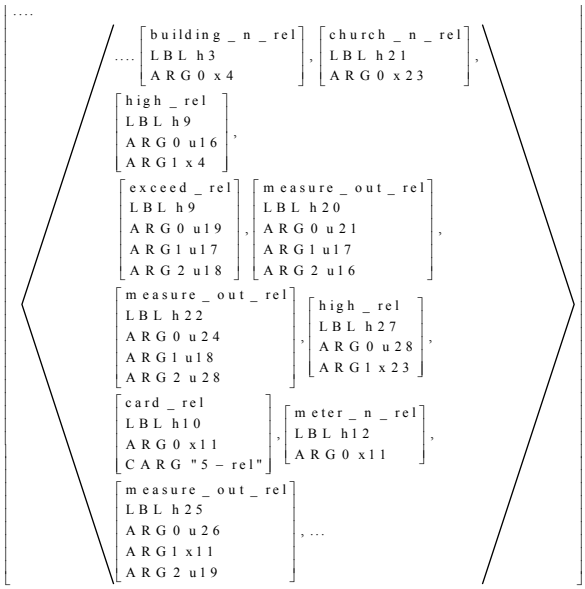


Figure 2: Knowledge-explicit representation for the sentence "This building is 5 meters higher than the church", as produced by a parser like NorSource and amendable to input in further processors (d1 = u17, d2 = u18, d3 = u19).

The second project, CALST (Computer-Assisted Listening and Speaking Tutor), is funded by the Faculty of Arts together with Norgesuniversitetet. This project focuses on pronunciation and will develop a web-based service based on the VILLE system for CAPT (Computer-Assisted Pronunciation Teaching, http://www.speech.kth.se/ville) developed by KTH in Stockholm, who are also one of the partners in the project. This project must not only enable simultaneous use of the system through the internet by a large number of users (like WIN), but also record users' learning progress in the form of test results and speech recordings. Together with personal information about the students, this data shall be collected over many years and thus form a rich basis for the phonetic analysis of L2 learning behaviour. It is expected that the use of web-based interfaces and the collection of databases over the web fit well within the scope of CSE.

RESEARCH CHALLENGES

In the areas of the above projects, challenging areas include:

– solving the *bottleneck problem of Artificial Intelligence,* namely an adequate and computable representation of natural language, texts as well as speech. To serve as inputs to expert systems, advanced machine translation, robot control, and more, such representations should be 'calculation-sharp'; for example, when it comes to expressions of measurement, the representations delivered should provide a breakdown of exactly what is being measured and which values are being assigned. For instance, for *This building is 5 meters higher than the church*, a calculation-sharp analysis should provide a representation corresponding to the quasi-paraphrase (see figure 2):

> "For a degree *d1* and a degree *d2* such that *d1* is the height of the building and *d2* is the height of the church, *d1* exceeds *d2* to an extent *d3*, and *5 meter*s measures out *d3*."

– *rapid language resource building,* by computational methods for extracting from text and speech corpora grammars and dictionaries for poorly documented languages. With the current rate of language endangerment and death, this is one of the main challenges for Linguistics research groups across the world, with a need to develop tools which are both easy to handle, provide safe storage of data, and allow for maximal sharing of data through online 'shared methodologies'.

– *user-assisting integrated language tools,* in settings like tourism, introducing visitors and new citizens into a new society, which includes guiding language learners into salient aspects of a community (like educational institutions, legal help, health services, etc.).

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Cooperation with a future CSE centre will involve

- Opportunities for interdisciplinary training and education, including training of assistants, cooperation in "Experts in Teamwork".
- Support in resource development, software licenses, software security, software storage.
- Support in intellectual rights questions.

The areas mentioned above are computation intensive, both in calculation of massive data (for fullfledged text and speech processing) and in model design and interconnecting technologies. For instance, the development of technological approaches to pronounciation training uses special processing approaches to extract relevant signal properties for the evaluation and training of foreigners' pronounciation. The processing of grammatical, semantic and pragmatic information jointly in unification-based technologies raise significant challenges with regard to sequencing and interaction of processes. While the modeling of speech signal processes may bear some relation to computer simulation, one of th etarget areas of CSE, the modeling of SEMANTIC space and its connection to linguistic dynamics lies in very different area of complexity. Our hope will be that CSE can with time broaden its scope to take on even challenges of such an area.

GENERAL OVERVIEW

The department is part of the Faculty of Information Technology, Mathematics and Electrical Engineering (IME) at the Norwegian University of Science and Technology (NTNU) in Trondheim, Norway.

Research activities

The department research activity overview is limited to areas of assumed interest to computational science and engineering (CSE), including high performance computing, computer architecture and design, database systems, software engineering, self-organizing systems, knowledge-based systems and algorithm development. Within those areas, the main topics of research are

- supercomputing, cluster and grid computing, parallel algorithms for accelerators (notably GPU's), performance analysis and benchmarking of HPC platforms, auto-tunable algorithms, computational steering and software environments for testing, developing parallel scientific codes (high performance computing)

Figure 1: A detailed polygon model of the West Front of the Nidaros Cathedral. The model is based on laser scans using the Riegl LMS-Z420i scanner. The scan accuracy is approximately 10mm. A major challenge is reduction of the vast amount of data generated by the scanner.

- evolvable hardware, and parallel computer architectures, improved understanding of the interplay between application, algorithm and architecture in parallel computers, processor-memory performance gap, performance evaluation, green computing, graphics, visualisation and virtual reality, 3D rendering, tracking and animation (computer architecture and design)
- distributed and heterogeneous data, parallel and object oriented data bases, high capacity transaction oriented databases, large data volumes, parallel technology and methods in database systems, performance engineering (database systems)
- software quality, software process improvement, component-based development, cooperation technology, ubiqutous computing (software engineering)
- computational neuroethology (self-organizing systems)
- data mining (knowledge-based systems)
- genetic algorithms, similarity search, metric indexing (algorithms)

Teaching activities

The department provides 74 courses in computer and information science, with a mixture of basic information technology, courses at bachelor level and master courses in artificial intelligence, software engineering, software architecture, software quality, programming languages, advanced database management systems, distributed systems, parallel computing, compiler technology, performance evaluation, computer architecture, hardware design, bioinformatics, management of very large data volumes and additional special courses at the Ph.D. level.

RESEARCH CHALLENGES

Computer Science is a necessary ingredient in every grand challenge problem, in terms of the inevitable multidisciplinary cooperation needed to address such problems.

High performance application software development

Figure 2: Real-time modeling of over 2 million particles harnessing the computational powers of modern graphics cards. The snow simulator incorporating a fluid model for the wind, shown here by PhD student Rune E. Jensen and advisor Anne C. Elster, is developed over several years by students in her research group. (T. Vik et al., ParCo 2003; I. Saltvik et al. PARA 2006; A. Gjermundsen, A.C. Elster PARA 2010).
Photo: Kai T. Dragland (NTNU)

is a research challenge in itself. Processor and related accelerator technologies are evolving at a rapid pace, still approximating Moore's law. Software complexity keeps on evolving, adapting to accelerator technologies, multi-scale problems and spatially non-uniform domains of computation. Currently, increases in hardware performance are realised primarily by increasing chip core counts and by including several levels of caches and large memories on-chip to address the memory gap.

High performance file systems are needed to address the ever increasing amounts of simulation data from increased computational capabilities. High performance disk I/O is realised by very large numbers of RAID'ed disks operating in parallel, with a high aggregate bandwidth. High bandwidth often comes at the expense of larger transfer sizes and more expensive metadata retrieval. Utilising this technology to access larger data volumes requires a different programming approach, exploiting the memory subsystem and interconnection hardware of the system.

Software development tools, programming languages and compilers are not able to take advantage of recent developments in hardware technology, posing large research challenges in these areas. Challenges also include developing adaptive algorithms and integrating visualisation techniques with software development tools.

CSE RELEVANT ACTIVITIES

Research and development

Current research of multicore and accelerator technologies (mainly GPU technology), including multicore cache hierarchy technologies, are core constituents. However, research in software engineering, programming languages, management of large data volumes and performance evaluation should be considered important ingredients in addressing the software side of Computational Science and Engineering. The software gap is not necessarily closed by solely adding more software engineering capability to the development teams; advances in computer science is also considered a key ingredient.

Teaching activities

CSE Centre-related courses currently offered include parallel computing, performance evaluation, grid technology and heterogeneous computing, distributed systems, computer architecture, compiler technology, visualisation and image techniques, computer vision, algorithms and data structures, data modeling and databases and management of very large data volumes.

Figure 3: Real-time Ray-tracing Using NVIDIA OptiX (H. Ludvigsen, A.C. Elster EuroGraphics 2010).

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Ongoing research projects

Research on multicore and GPU computing. The HPC-lab is currently collaborating with several departments associated with the CSE centre, including Chemistry, Cybernetics, Mathematical Sciences, Medical Technology and Petroleum Engineering on projects to take advantage of GPU computing. These collaborations would be strengthened with a CSE centre in place. A special interest group (SIG) on multicore computing is recently established at the faculty level to foster inter-departmental research, publication and development om multicore computing (http://www.ime.ntnu.no/multipro). Visualisations and image processing projects will also be of relevance to the CSE Centre.

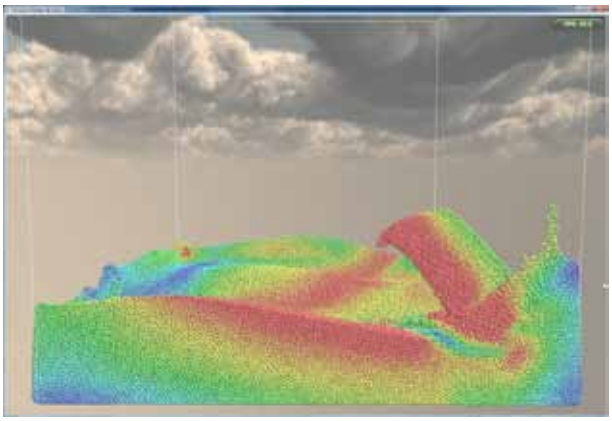


Figure 4: Real-time fluid simulations using SPH smoothed particle hydrodynamics (Ø. Krog, A.C. Elster, PARA 2010).

Planned

In addition to the above activities, we expect a CSE centre can strengthen joint proposals and serve as an internationally visible umbrella for such projects.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research themes

Multicore computing and visualisation of large and complex data seta are becoming increasingly important in major national focus areas such as medicine, bioinformatics, oil and gas, marine technology and meteorology. In order to take advantage if the computational power of current and future multicore architectures, including graphics processors (GPUs) and multicore processors, countless challenges within computer science and engineering remain.

Current relevant computer science research themes include advances in key areas as parallel programming models, abstractions, languages and algorithms, software development, compilation debugging and visualisation tools, platforms for parallel architectures and scientific computing, frameworks for automatic parallelisation, optimised code generation and dynamic run-time execution, scalable mechanisms for concurrency control and synchronization in heterogeneous environments, virtualisation for optimized performance, and power-aware scheduling algorithms and load balancing schemes.

Education

The Department has several courses and seminars that would be of interest to the CSE centre. It would also strengthen both if researchers from other departments could teach as adjuncts in our department and vice versa, including applying for joint Post Docs.

Infrastructure and facilitation

A future CSE centre should add value not only to the application areas at NTNU, but also be of added value to the Computer Science department. Human capital is a key resource in this context. Several research groups within the Department already are close to sub-critical in terms of manpower. Establishing a CSE centre at NTNU/SINTEF must not drain human resources at the Department to provide software support type of services. It needs to strengthen our grand challenge capabilities and provide added value to both computer science and its collaborative partners.

GENERAL OVERVIEW

The Department of Engineering Cybernetics is involved in a wide variety of research activities. This ranges from research on general purpose methods for control, estimation, embedded systems and information processing, to interdisciplinary research in application areas such as maritime, offshore, robotics, new energy, oil and gas, aquaculture and fisheries, medicine, automotive, process industries, and others. The department is heavily involved in the following ongoing research activities, in addition to several other projects:

- Center for Integrated Operations in the Petroleum Industry (IO-Center)
- Center for Gas Technology
- Center for Ships and Ocean Structures (CeSOS)
- CREATE – Center for research-based innovation in aquaculture technology
- Strategic University Program on Computational Methods in Nonlinear Motion Control (NFR)
- Strategic University Program on Control, Information and Communication Systems for Environmental and Safety Critical Systems (NFR)
- NTNU/SINTEF Gemini centre on Advanced Robotics

Two of the three research groups were given the evaluation "Excellent" by the national evaluation conducted by NFR in 2002. The department had in 2008 the highest score on "publications per professor" among the technology departments at NTNU. The department has 14 full time professors, and 6-7 PhDs graduate in a typical year. The Master-program on Engineering Cybernetics admits about 100 students every year, and the department provides courses at all levels in topics such as control theory and engineering, embedded and real-time computer systems, dynamic modeling, simulation and optimization.

RESEARCH CHALLENGES

The field of control engineering has matured considerably over the last 50 years. Still, several problems remain unsolved, and new challenges emerge driven by the development of new applications and technologies. The key challenges include systematic methods for handling of nonlinear phenomena, scalability and efficiency of methods to deal with large scale problems, accommodating more advanced control functionality with higher level of coordination among multiple systems, and achieving high reliability and safety of the implementation in industrial computer and communication systems. Computational methods are vital in all the above mentioned challenges, and it is clear that computational methods will be at hearth in the vision of a single general purpose control method or algorithm. The closest thing we have to fulfill this vision today is nonlinear model predictive control, which is currently limited by scalability, numerical issues, computational complexity, and similar issues.
The Department of Engineering Cybernetics is a leading international player in the area of control engineering. It is an ambition to be at the leading edge of developing, demonstrating and introducing new and advanced methods in challenging applications. Much of the research involves new theoretical developments in combination with experimental validation at our laboratories or in collaboration with industrial partners or other universities. Focus is given on areas of vital importance for the Norwegian industry and society, such as the maritime, oil and gas, new energy, fisheries and aquaculture, medicine and automation industries.

CSE RELEVANT ACTIVITIES

Mathematical models and computational methods are at the hearth of control engineering and cybernetics

- Numerical simulation is the key tool for validation and verification of control system design and implementation. This may involve mathematical models of different complexities for early concept and design studies (from ODE to PDE), algorithm development, verification and validation using real-time hardware-in-the-loop simulation, pre-tuning and operational simulations. Conventional modeling

Figure 1: Large scale industrial process monitoring and control require numerical computations for dynamic estimation, simulation and optimization. Plants may have 1000's of decision variables and measurements, sometimes leading to numerical problems with 100.000 or more variables to be solved in real time with guarantees on accuracy and reliability.

and simulation are concerned with the conservation of mass, energy and momentum. In cybernetics and control engineering one adds the key concept of information and takes advantage of information processing techniques to shape the characteristics, extract information, and add functionality to the systems. Information processing needs to account for cause, effect and timing, which adds to the requirements to simulation systems beyond the laws of nature.

- Numerical optimization is widely applied for control and management of complex industrial processes. With industrial plants having 1000's of sensors to process and decide in real time, optimization is today the main practical tool for such plant-wide control in the context of model predictive control. With hard real time computational constraints, the computational efficiency and reliability of linear, nonlinear and mixed-integer numerical solvers is a key issue.

- Cybernetics applications are characterized by real-time processing of data in order to extract relevant information, often in terms of parameter or state estimation. This includes statistical model based methods such as the Kalman filter and computational methods such as Monte Carlo simulation.

It is common for industrial projects related to cybernetics and control that more than 50% of resources are spent using computational methods on mathematical modeling, simulation, and data processing. The use of numerical methods is essential in research and courses at all levels. In the MSc program there are two dedicated courses, Modelling and Simulation and Optimization and Control, in addition to other courses where numerical methods are also important but not the main topic.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

There are several ongoing activities that are highly related to a CSE centre, including the Center for Integrated Operations (in offshore oil and gas production), Center for Ships and Ocean Structures (CeSOS), the Strategic University Program on Computational Methods in Nonlinear Motion Control, the Gemini Center on Advanced Robotics, and the Special Interest Group on Multi-core programming at NTNU. There are sev-

eral emerging activities that will be highly relevant contributions to a CSE centre.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research themes: Interdisciplinary modeling, numerical optimization, integrated simulation systems, real-time simulation, estimation and data processing, data assimilation in distributed parameter systems, advanced robotics, numerical methods for optimal control, exploiting multi-core computer architectures, control of fluid flow, embedded optimization algorithms and unmanned vehicles. Joint research projects involving two or more groups associated with the CSE centre, facilitated by the infrastructure of the centre.

Education: Enhanced opportunities for interdisciplinary training for our MSc students, through joint projects, MSc theses, Experts in Teamwork (EiT), etc. where they can work with state of the art software tools in groups involving students of different background.

Infrastructure: Seminar series, software licenses and support for numerical simulation and optimization, resource network.

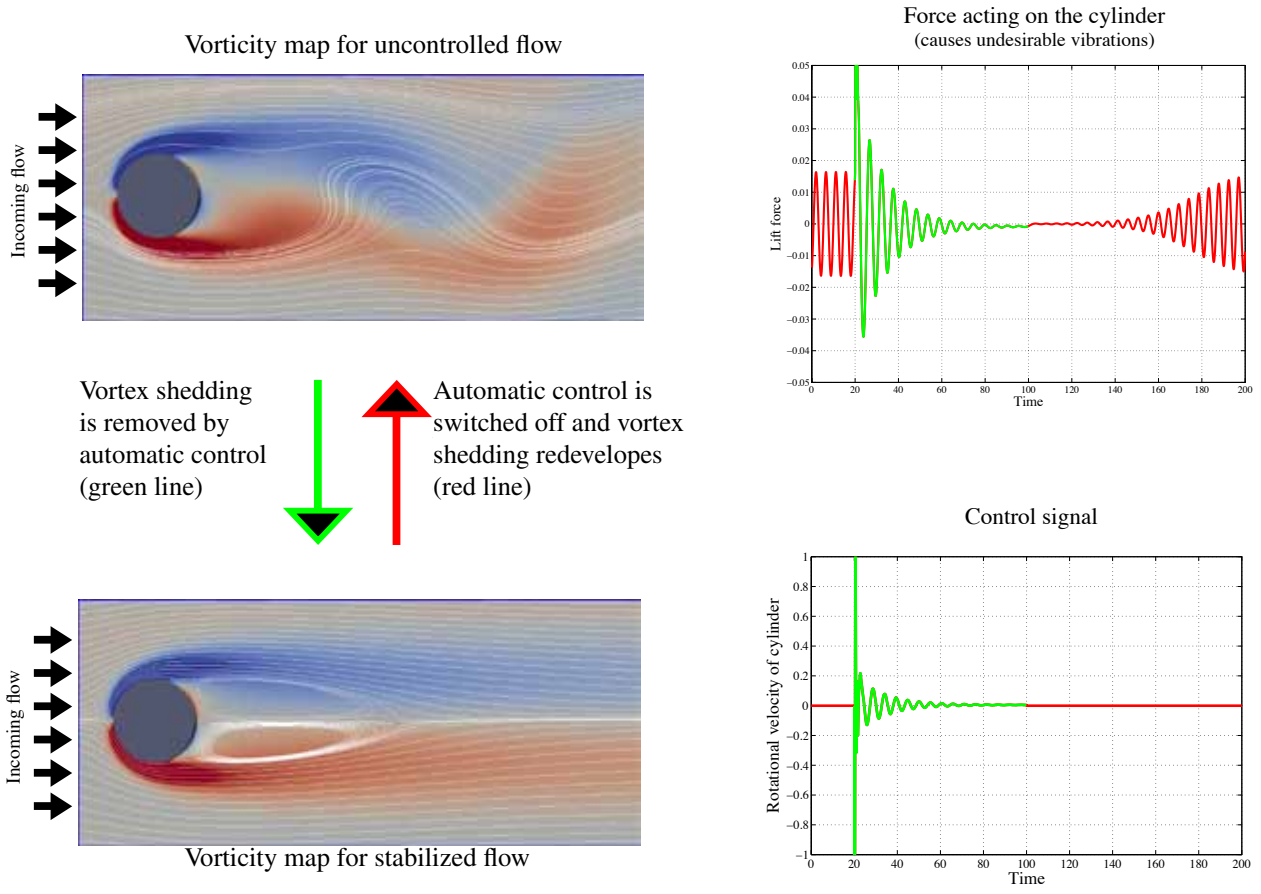


Figure 2: Computationally intensive automatic control alters the behavior of viscid fluid flows.

GENERAL OVERVIEW

Mathematics is the language of science and technology and an essential part of our cultural heritage. Vibrant research activity both in pure and applied mathematics brings constant advance in the subject and influences progress in other branches of science.

The research activity of the department is organized as nine research groups: Algebra, Differential equations, Functional analysis, Complex and harmonic analysis, Geometry/Topology, Numerical analysis, and Statistics.

By teaching the basic courses in mathematics and statistics, the department shoulders substantial responsibility for the quality of education for all engineering students at NTNU. The MSc programme Applied Physics and Mathematics is unique in Norway as it is the only programme in physics and mathematics with an emphasis on technology. The programme consists of two common years of basic training in mathematics and physics as well as some chemistry, mechanics and computer science. There are three majors to choose from in the last three years, one of which is *Industrial Mathematics*. Typically 30-50 students graduate with this major every year. Students easily find jobs in business, industry, and the R&D and governmental sector. The education in Industrial Mathematics provides an excellent preparation for PhD studies in the physical and mathematical sciences, as well as other branches of technology.

RESEARCH CHALLENGES

New computational resources coupled with advances in mathematical theories have moved the frontier of what can be achieved by computer simulations. Norwegian industry has much to gain from this progress, both in terms of international competitiveness in the race for limited resources and in increased production at home.

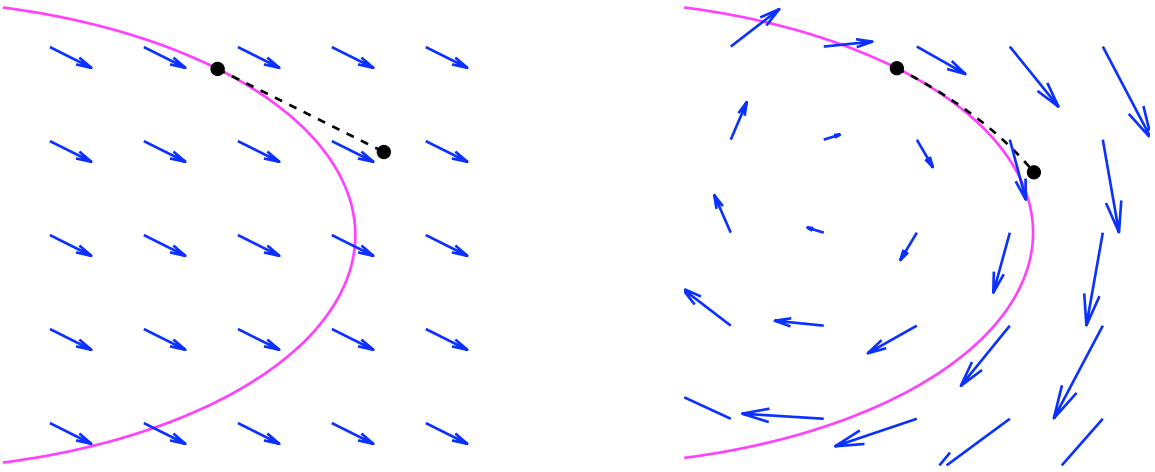


Figure 1: Standard numerical integrators use translations along straight line segments as building blocks, whereas geometric Lie group integrators allow for movements along curves in order to adapt the numerical solution to the dynamics intrinsic to the problem at hand. This is illustrated here by the explicit Euler method applied to the Dung oscillator, in the standard version the increment is a straight line, whereas to the right the translation has been replaced by a nontrivial Lie group action.

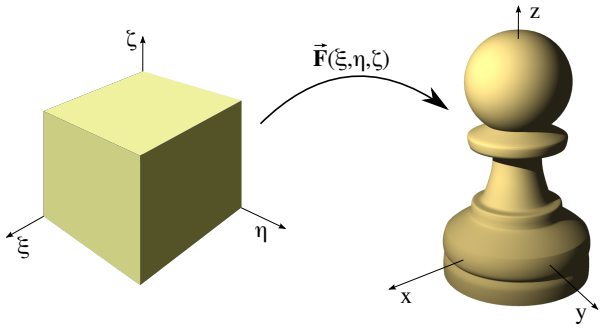


Figure 2: Isogeometric analysis is using the power of the NURBS technology, perfected by the CAD community for decades, to allow for extremely efficient parameterisation. Even seemingly complex models like this chess pawn piece can be created using only 681 degrees of freedom and can be constructed by an inexperienced user.

Overall vision/goal:

Developing and using mathematics to model and simulate scientific and engineering systems accurately and fast.

Challenges to achieve this:

- better fundamental understanding of numerical approximations of continuous systems
- modelling and simulation of complex systems (multiscale and multiphysics)
- lower the computational complexity to solve a given problem to a prescribed accuracy
- accurate long term prediction of dynamical systems and preservation of invariants
- exploit underlying geometric structure for improved simulation methods
- develop methods suitable to exploit new computational infrastructure
- simulation of models including statistical effects

Some relevant examples of mathematical methods: Multiscale modelling, compatible methods, reduced order models, geometric numerical integration, methods for highly oscillatory problems, integrators for differential-algebraic problems adaptive methods with error control. Whereas topics as hardware adapted numerics and development of numerical software are linked to computer science.

CSE RELEVANT ACTIVITIES

Differential equations arise in many areas of science and technology. Unfortunately, only a very limited subset of the differential equations allow for solutions in closed form by analytical methods. The bulk part of them can not be solved exactly, but their solutions can in most cases be well approximated by means of computer simulations. The way these simulations are realized, the mathematics involved in the method construction, as well as the derivation of reliable error estimation for the approximating formulas, are crucial aspects in all applied sciences. Not only is it of importance to quantify the error in a simulation, it is also necessary in practical simulations to be able to efficiently control the error by deriving appropriate control devices on the discretisation parameters, like mesh sizes, approximation order etc.

The expertise of the Numerical Analysis group at the Department of Mathematical Sciences lies within these areas. One may divide the collective expertise of the group into two categories: The development and analysis of numerical methods for differential equations and optimization, and the application of such methods to particular differential equations or mathematical models for certain applications. The group has worked on methods relevant to solving problems in solid and fluid mechanics, problems of interaction of fluid and structures, flow around marine structures, control of marine offshore structures, perceptual completion models, chemical engineering models, circuit simulation, electrochemical models for the human heart, seismic source modelling, aluminium extrusion models, nonlinear wave problems, neural learning models.

The expertise of the Statistics group is within statistical modelling and uncertainty quantification in reservoir evaluation, spatial statistics and Bayesian com-

puting. The main focus in these areas is to identify, develop and evaluate mathematically and physically based models for assessment of uncertainties in reservoir evaluation, construct computational efficient models for spatial statistics and to construct efficient methods for Bayesian inference. Efficient spatial models is important for analysing space-time environmental data like temperature and pressure measured regularly in time at various stations around the world, and the methods for Bayesian inference is required to analyse these models.

As examples on CSE-relevant projects we here briefly mention the URE and ICADA project:

The Uncertainty in Reservoir Evaluation (URE) project which is a collaboration between Department of Mathematical Sciences and Department of Petroleum Engineering and Applied Geophysics has as the objective: Identify, develop and evaluate mathematically and physically based models for assessment of uncertainties in reservoir evaluation, and distribute information and provide training about these models through education, publishing and seminars.

The Integrated Computer Aided Design and Analysis (ICADA) project which is collaboration between Department of Applied Mathematics at SINTEF ICT, and the Department of Mathematical Sciences and the Department of Structural Engineering at NTNU has as the objective: Build competence in Norway for taking advantage of Integrated Computer Aided Design and Analysis based on a coherent representation for geometry and analysis.

POSSIBLE CONTRIBUTION TO A CSE CENTRE

Ongoing activities

The Department of Mathematical Sciences may con-

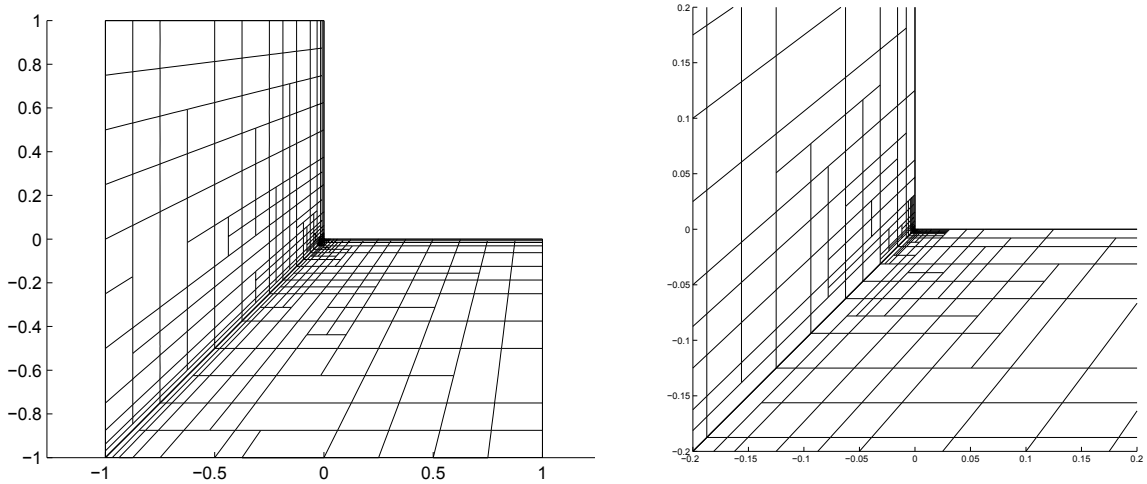


Figure 3: For problems with singularities at the boundary e.g. at certain points there is a need for local refinement in order to avoid "pollution" i.e. reduced order of convergence when using regular refinement. Isogeometric analysis based on B-spline or NURBS are structured grids, but may be enhanced by means of "T-splines" to achieve local refinements. In the figure above we show adaptively refined T-spline grids for a L-shape domain with a point singularity. To the left we see the whole domain, whereas to the right we see a zoomed in version nearby the singularity.

tribute to a CSE centre by means of educating candidates with a strong competence in Industrial Mathematics (both MSc and PhD) as well as provide relevant education in computational mathematics of students in other areas of science and technology. Furthermore, it may be a driving force behind initiatives similar to "ICT and Mathematics" that was a collaboration between the Department of Mathematical Sciences and the ICT departments at the Faculty of computer science, mathematics and electronics (IME). The main objective was to strengthen and promote theoretical research in ICT at the IME faculty by increasing the scientific collaboration with the Department of Mathematical Sciences.

The Department of Mathematical Sciences may contribute to a CSE centre by means of being partners in multidisciplinary research projects like e.g. URE and ICADA, as well as doing more generic development of methodology and research software, i.e. "numerical infrastructure" that together with computer infrastructure are important as enabling technology for a CSE centre.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

The Department of Mathematical Sciences aims to be the driving force to move the frontiers in Computational Science and Engineering (CSE), and be a focal point at NTNU for technology transfer of advances in mathematics to other areas in science and technology. To this end, we envision a truly multidisciplinary collaboration in which application specialists collaborate closely with mathematicians and computer scientists to take advantage of recent advances in mathematics and develop methods to resolve challenging problems in science and engineering. In particular, we consider multiscale and multiphysics problems (that may involve many scientific sub-disciplines) as classes of problems that are highly relevant for such collaborations.

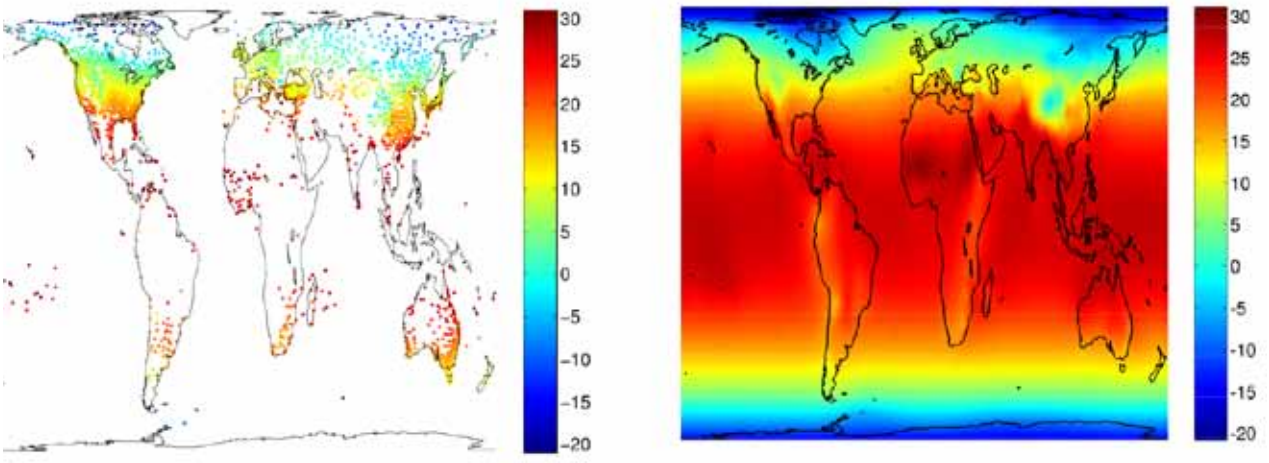


Figure 4: The left figure displays the mean temperature for 1980 for about 2500 different measuring stations around the world. The right figure shows the estimated mean temperature for 1980, extracted from a spatio-temporal model which incorporate both "climate" and "weather". Both the modeling and inference is made possible using state-of-the-art methodology involving stochastic partial differential equations, non-stationary Gaussian fields, numerical linear algebra for sparse matrices and approximate Bayesian inference.

GENERAL OVERVIEW

The department is responsible for teaching and research in fundamental chemistry. The department provides a large portion of the teaching of basic courses in chemistry to the study program in Industrial chemistry and biotechnology as well as the bachelor and master programs in chemistry, and contributes to other study programs at the faculty as nanotechnology, biotechnology, and biology.

The activities in theory and modelling are located in the physical chemistry group, with around five faculty members in modelling. The research in theoretical/computational chemistry includes most aspects of molecular modelling as quantum chemistry, molecular mechanics, molecular dynamics and statistical thermodynamics, irreversible thermodynamics and chemoinformatics/chemometrics. The research has a focus on method development combined with applications often in collaboration with experimental groups. Correspondingly, around five advanced courses are given on the master and ph.d. levels on these subjects.

RESEARCH CHALLENGES

One basic philosophy is to design molecules and materials with novel properties, another is to aid in the development of new theories. Chemical modifications by exchanging functional groups, chemical doping or isotope substitution result in different properties at the nano and macroscopic scales. Modelling and computations give a detailed understanding of the basic mechanisms and provide results with comparable accuracy as experiments. Assumptions made in theories can be tested. Molecular modelling has in general a prominent role not only in chemistry, but also in materials science, nanotechnology, chemical engineering, chemical physics, and molecular medicine. Ap-

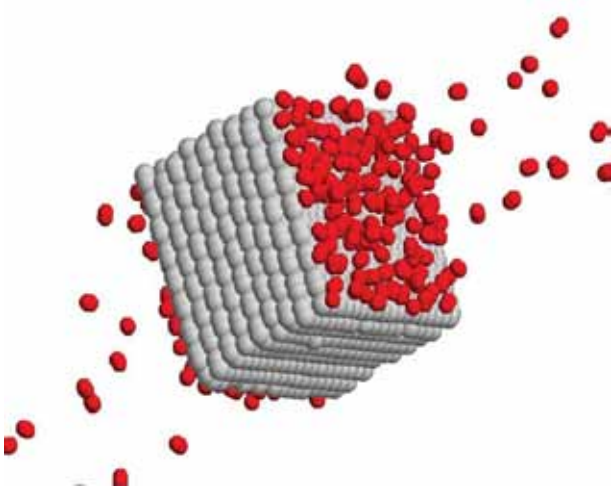


Figure 1: Molecular dynamics simulation of hydrogen on graphite. Snaphot showing the equilibrium between hydrogen (red) and graphite (grey) at 90 K. The model uses an atomic description of graphite and hydrogen. Reference: O.E. Haas, J.M. Simon and S. Kjelstrup, Surface self diffusion and mean displacement of hydrogen on graphite and a PEM fuel cell catalyst support, J. Phys. Chem. B, 113 20281-20289 (2009).

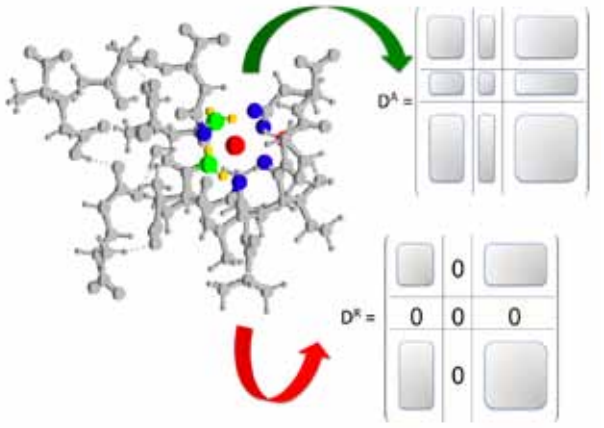


Figure 2: Development of new computational techniques in quantum chemistry for large molecular systems. The active part (A) of the molecule has been selected as the colored atoms and the gray colored atoms are the remainder (R). Computational reductions are obtained using method specific Cholesky decomposition. Reference: L. Boman, H. Koch and A. Sanchez de Meras, Method specific Cholesky decomposition: Coulomb and exchange energies, J. Chem. Phys. 129, 134107 (2008).

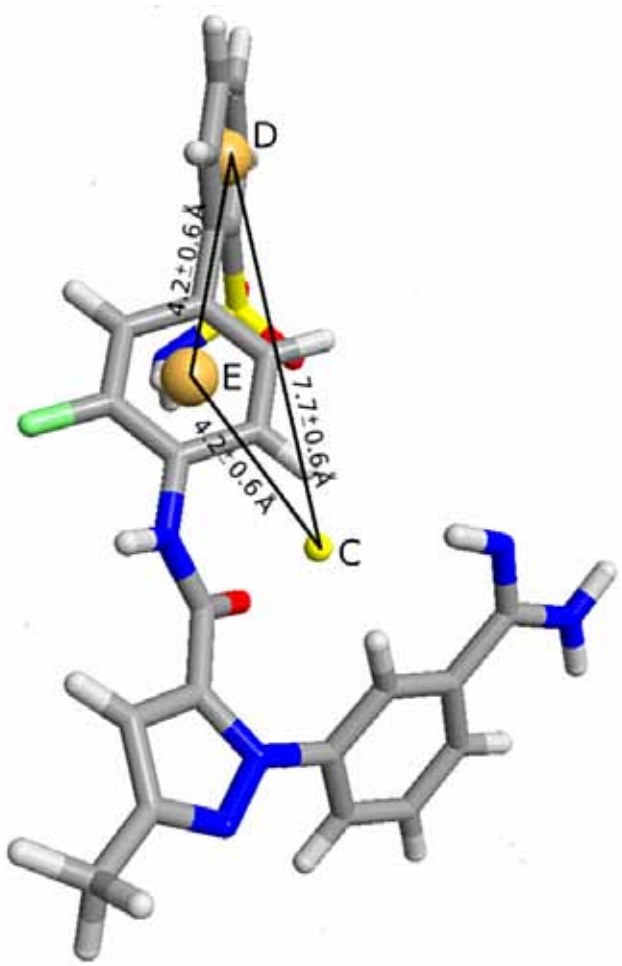


Figure 3: How can the 3D structure of molecules best be represented in a computer? One approach to generate pharmacophore rules about activity is to use a set of molecular interaction fields (MIFs) in combination with data compression and the non-attribute based machine learning method Inductive Logic Programming (ILP). The figure shows an example molecule together with three MIF minima points (two golden and one yellow) representing one of the predictive rules generated by ILP. Reference: B. Buttingsrud, R. D. King, B. K. Alsberg, An alignment-free methodology for modelling field-based 3D-structure activity relationships using inductive logic programming, J. Chemometrics 21,509-519 (2007).

plications in our group include, but are not restricted to, design of new catalysts, development of fuel cells, drug design, and the development of biofuels.

During the last two decades, the focus in theoretical and computational chemistry has shifted from method development to applications. Many methods are included in standard programs used by non-experts and computational chemistry has in many ways become a standard tool in chemistry. Still a major portion of our research activities are devoted to model development and many methodological problems remain unsolved. Certain areas of study, like surfaces, can only be studied in a well defined manner by computer modeling. In some cases a rethinking of the basic physics of the problem is prompted by simulation results, in some cases entirely new algorithms are necessary, and in some cases optimization and parallellization of existing models would improve the performance and extend the application area considerably. Some more fundamental grand challenges include:

- The scaling of methods with an atomistic resolution with the size of the system. Often only a very small portion of the system is actually included in the study, and in some cases the surroundings are described with less sophisicated models than the core of the system.
- The different time scales relevant for chemical events. Chemical reactions occur on the femtosecond-scale, whereas proteins fold in times often longer than one microsecond.
- We work on the boarderline between classical and quantum mechanics. For example, classical molecular dynamics is used to simulate liquids whereas vibrational motion in for example hydrogen bonds in liquid water can be measured in infrared spectroscopy indicating a quantum mechanical behaviour.
- The multiple minimum problem. Clusters, proteins, etc. exhibit a huge number of local minima of around equal importance often separated by relatively large energy barriers.

- The number of possible combinations of molecular fragments, functional groups, etc., leads to a huge combinatorial problem in the design of novel molecules and materials. For example in drug design, libraries of millions of ligands exist for e.g. inhibition of an enzyme, which requires efficient and accurate prescreening procedures.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The department can primarily contribute with expertise and experience in methodology development within most aspects of molecular modelling, including quantum chemistry, molecular mechanics, statistical mechanics, thermodynamics and chemometrics.

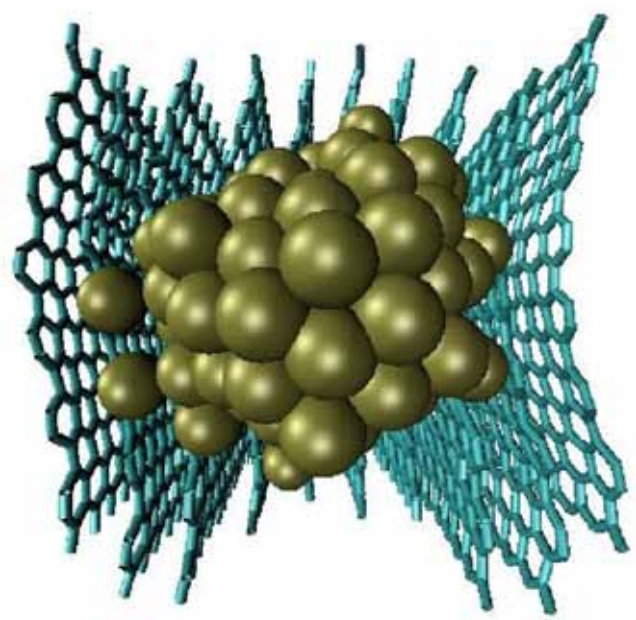


Figure 4: Molecular dynamics simulation of a platinum cluster interacting with carbon platelets with the purpose to improve the catalytic activity of platinum in for example hydrogen production. Reference: C.F. Sanz-Navarro, P.-O. Åstrand, D. Chen, M. Rønning, A. C. T. van Duin, T. Jacob, W. A. Goddard III, Molecular dynamics simulations of the interactions between platinum clusters and carbon platelets, J. Phys. Chem. A 112, 1392-1402, (2008).

We anticipate that atomistic particle models to a larger extent will be coupled to mesoscopic particle models as well as finite-element methods. In this respect, both novel algorithms and new software need to be developed. In general, we would like to contribute to the development of multiscale and multiphysics approaches in materials and biological sciences.

In addition, a graduate school in computational science and engineering would provide better suited students and researchers to address the present challenges in molecular modelling.

Computational chemistry is traditionally one of the largest users of high-performance computing resources, and a top-level computational facility is required.

An infrastructure for software development should be provided. The cost for developing and maintaining software is today higher than for the actual computations.

The number of possible collaborative projects and application areas in molecular modelling is end-less with numerous unsolved problems in for example the development of fuel cells, catalysts, processes for CO_2 storage, biofuels, drug design, novel molecular materials for nonlinear optics and solar cells, etc. To quote the famous statement by Richard Feynman from 1959: *There's Plenty of Room at the Bottom.*

GENERAL OVERVIEW

Research Activities

The department research activities are mainly related to NTNU strategic areas

Energy & Petroleum - Resources & Environment: 3rd generation solar cell, Climate processes in the atmosphere and space technology, Oil and gas reservoir studies, Catalysis, Materials and processes for improved environment.

Information and communication technology: Quantum communication, Laser physics, Spintronics, Traffic flow.

Materials: Functional materials, Materials for energy technology, Charge and spin transport, Soft materials and biomaterials, Optical and laser materials, Surfaces and interfaces, Nanostructured materials, aluminium.

Medical technology: Biomaterials, Bionanotechnology, Medical physics (x-ray, CT, PET, imaging), Spectroscopic imaging techniques, Radiobiophysics, Drug delivery. In addition there are department prioritized areas as astro- and particle physics and science education.

Main laboratory facilities: Spectorscopy laboratories in optics, laser physics and biophysics, Molecular imaging laboratory (FUGE) and cell culture lab, Photoemission-, Transmission electron microscopy-, Scanning tunnelig microscopy- and X-ray-laboratories, thin film laboratory and solar radiation observatory.

Teaching activities

The department provides 55 differenct courses in physics with a mixture of basic physics courses at bachelor level and master courses in astroparticle physics, biophysics and medical technology, condensed matter physics theory and experiment, en-

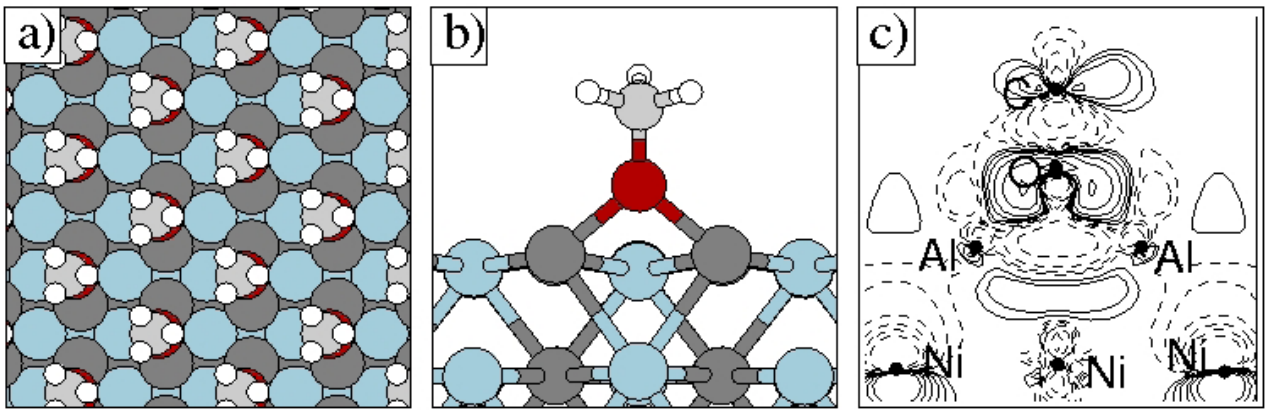


Figure 1: The optimum adsorption geometry of methoxy (CH3O) adsorbed on NiAl(110) as predicted by density functional theory calculations shown in (a) top view and (b) side view. Al atoms are represented by grey circles and Ni atoms as light blue cirles. (c) Contour plot of the the calculated electron density difference for methoxy on NiAl(110) in a plane through the C and O atom centres of methoxy and the bonding Al atoms. Solid (dashed) lines indicate gain (loss) of electron density as compared to the gas phase methoxy and the clean surface. This plot can be used to gain insight into the bonding mechanism of methoxy on NiAl(110).

vironmental physics, instrumentation, optics, science education in addition to special courses at ph.d. level.

RESEARCH CHALLENGES

Contemporary challenges in physics entail to an increasing degree complex problems where a close collaboration between experimental, theoretical and computational methods needs to be used. Computational physics is an essential ingredient in such collaborations, and it cannot be over-emphasised how important this is to the physics research activity at NTNU.

The main areas where there is a need for computational science is hard and soft condensed matter physics and complex systems. Examples of unsolved problems (bottlenecks) in condensed matter physics is the critical slowing down of systems close to second order phase transitions. Here, there is an essential need for the development of efficient new algorithms involving cluster algorithms for circumventing this serious problem. In particular, in many-particle systems with long-range interactions of various degrees of freedom both in space and time, there is an urgent need for new such alorithms in order to make real progress, in addition to an increase in computing power. Using computers with an operation speed of 100-1000 TFLOPS, in combination with new designs for algorithms imply that problems that have hitherto been impossible to attack in any real sense, will be within reach. Examples of such unsolved and central problems are spin systems with disorder, low-dimensional interacting fermion systems, multi-component interacting bose systems with and without disorder, just to mention a few examples. It is the vision of the department of physics to contribute in a real sense to development of new and effiicient algorithms as well as applications of these to solve real problems such as those mentioned above, in a future CSE. There is no doubt that physicists ought to play an essential role in such an environment.

CSE RELEVANT ACTIVITIES

Research and development

Superfluids, superconductors, and quantum antiferromagnets. There is an extensive activity within the department on large-scale Monte Carlo simulations of Ginzburg-Landau type of models for multi-component superfluids, superconductors, and gauge-teories of quantum antiferromagnets. These are massively parallell computations. The research group carrying out these simulations are among the largest users of the national high-performance computing facilities. The overarching theme which ties these three research topics together is the issue of mutual influence on critical phenomena of several simultaneously and spontaneously broken synmetries. The individual sectors of these theories may be characterised by symmetries whose restoration is facilitated by the proliferation of topological defects. On the other hand, with several such symmetries being broken, the issue arises what the character of the possibly composite topological objects are. This question is of fundamental importance. The use of large-scale computational facilities is one of the most useful tools to attack these difficult and important problems. In addition, the same research group has recently initiated a long-term research program on large-scale Monte Carlo simulations of extended dissipative field theories. Very little work has ever been done on such systems. The models are motivated by the physics of high-temperature superconducting copper oxides, and are believed to be at the heart of the problem of describing putative quantum critical points that have the potential for explaining the enigmatic anomalous tnormal state transport properties of these systems.

Department of Physics has also for many years had an activity within density functional theory calculations closely connected to advanced characterization techniques in condensed matters physics. Examples are electronic structure studies with electron spectroscopy; surface structures and catalytic properties and high resolution transmission electron microscopy;

atomic structure of early precipitation of metastable hardening phases in Al alloys. These first principles calculations here give valuable input related to the geometric and electronic structure on the atomistic level, complementing experimental results and predicting properties of hypothetical materials. Figure 1 shows an example of this type of work on surfaces relevant to catalysts.

There is also, within the department, and extensive numerical effort on simulating two-phase flows.

Teaching activities

There is one specific physics course related to CSE, TFY4235 Computational physics, where the goal of the course is to equip the students with a tool box of numerical methods in use in computational physics.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Ongoing research project within

1. Large-scale Monte Carlo simulations of multi-component superfluids and Bose-Einstein condensates and extended dissipative quantum field theories.
2. Large-scale numerical investigations of two-phase flow.
3. Density functional theory calculations in condenced matters physics.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

The department of physics has faculty members with broad experience in research on themes that are in common and complimentary to several research topics that one could envisage would form a part of the CSE, and correspondingly in teaching. The department sees it as vitally important that research collaboration between faculty members of the department and other elements of the CSE is initiated in a vigorous fashion whenever this is possible. It is difficult to be more specific at this stage, before one has more precise information about the constitution of the CSE.

GENERAL OVERVIEW

Research activities and organization

SINTEF Building and Infrastructure is a leading international research institute solving challenges linked to the entire construction process. The institute offers specialist expertise in technical fields ranging from architecture, construction physics and material science to the management, operation and the maintenance of all kinds of buildings and infrastructure. We focus on most of the built environment from details in private houses to large scale infrastructure like roads, bridges and tunnels, coast and harbour facilities, mines and underground hydro power plants, oil and gas caverns etc. An important aim for us is to contribute to sustainable development and knowledge dissemination in the building and construction sector. By means of our knowledge systems, publishing house and the SINTEF Certification system, we have established a unique knowledge dissemination platform which serves the greater part of the construction sector.

Together with NTNU we run comprehensive and well-equipped, large scale laboratories within our field of activities. These cover the laboratories for Construction Materials, Acoustics, Heating and Ventilation, Sanitation, Water Chemistry, Concrete and natural stone, Rock Mechanics, Geotechnology, Engineering Geology, Highway Technology and the Coast and Harbour Laboratory. Laboratory testing and field investigation has been and is becoming increasingly important in their role as the provider of the input data to numerical simulations. Advanced numerical analyses have shown their ability as a tool to interpret and understand phenomena observed in the laboratory.

SINTEF Building and Infrastructure comprises 4 departments; Materials and structures, Buildings, Infrastructure and Knowledge systems and certification. The subsidiary company SINTEF NBL is a part of our research division.

Teaching activities

Our laboratories play a central role in the NTNU's teaching and research activities. Our personell serves as co-supervisors to many MSc and PhD students at NTNU, Faculty of Engineering Science and Technology and Faculty of Architecture and Fine Art. Several of our senior/chief scientists are adjunct professors at NTNU and thus greatly involved in teaching activities at NTNU. Our chief scientist/adjunct professor Ming Lu , lectures e.g. for the course 'Numerical analysis for rock engineering' for both undergraduate and Ph.D students.

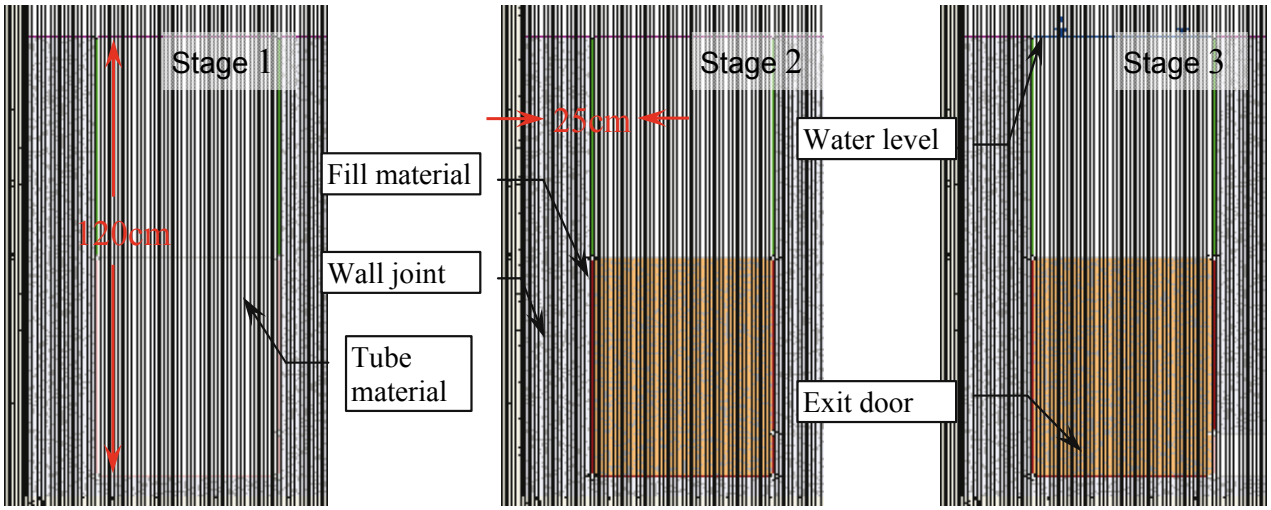


Figure 1: Example of a model for tunnel cave-in test.

Figure 2: Example of a small natural stone pavement for a road and the damage.

Through our research projects in general, and the Research Centre on Zero Emission Buildings (ZEB) and our centre for research-based innovation, Concrete Innovation Centre (COIN) in particular (see below), NTNU and SINTEF are able to announce and realize more than 20 PhD- and Post.doc-positions within the next 4-8 years. These and other projects/research programmes have also made a large number of MRC-studies possible.

RESEARCH CHALLENGES

Vision and ambitions

SINTEF Building and Infrastructure wish to establish a cutting edge international arena for research-based innovation and research training in order to develop knowledge and solutions promoting innovative buildings and infrastructure that support sustainable development.

Unsolved problems and bottlenecks

Both at global and national level, the society is faced with two big challenges where SINTEF Building and Infrastructure will and can contribute through further research and development; within energy shortage and consequences of climate changes. Based on our mulitidisiplinary fields of activities, some main challenges and research needs may be highlighted in this respect:

High-performance, climate adapted, energy- and cost-efficient buildings: Through the Research Centre on Zero Emission Buildings (ZEB), we are developing new solutions for the built environment of the future. By means of a broad spectrum of other projects, we have developed methods and technical solutions for

energy efficient buildings, as well as buildings and infrastructure which are adapted to the challenges presented by future climate change. In collaboration with Enova and Norwegian industry, we have completed a number of demonstration projects aimed at achieving our goal of energy-efficient and environmentally-friendly buildings.

Sustainable solutions for the cement and concrete industry: Through the SFI Centre COIN - Concrete Innovation, research is focused on enhancing the capability of the business sector to innovate by focusing on long-term research based on close alliances between research-intensive enterprises and prominent research groups. COIN works to create more attractive concrete buildings and constructions. Attractiveness implies aesthetics, functionality, sustainability, energy efficiency, indoor climate, industrialised construction, improved work environment, and cost efficiency during the whole service life.

Sustainable solutions connected to e.g. Geohazards, water supply, arctic climate etc.: SINTEF Building and Infrastructure are involved in several projects within these fields. Further research effort is essential to meet a broad set of challanges in coming years.

Need for computional methods

Towards the above mentioned main challenges and research items, numerical analyses will play an integrated part. Numerical analysis has become the major modelling tool on both material and structural levels. It is now widely used in analyzing the structure safety, reinforcement and optimization of design. However, the demanding on more accurate and reliable numerical tools has ever been increasing.

As a whole, SINTEF Building and infrastructure will continue to use and further develop computional methods and the interrelationship between laboratory testing and numerical simulations in our research activities. We see that such research activities will become increasingly important input to many of the challenges that the industry and the whole society are facing today and in the future.

CSE RELEVANT ACTIVITIES

The Finite Element Method (FEM) is the best developed versatile tool that has been used for structural analysis for several decades and within several fields at SINTEF. SINTEF Building and Infrastructure have done research on advanced material modelling and developed several new models for use with FEM. Research has also performed with the newly developed numerical methods such as Discontinuous Deformation analysis (DDA) and Numerical Manifold Method (NMM) for simulating the most sophisticated behaviour of rock joints. Personell within the institute has developed several computer programs in various fields and use a number of programs such as ABAQUS, PLAXIS, UDEC, FLAC, DYNA, DIANA and PHASE for a wide variety of projects especially within Rock and Soil Engineering. Ming Lu, our specialist in this field, was one of the initiators and key researchers of a five-year research program "Computational Mechanics in Civil Engineering" (CMC), which was the largest research project in this field ever financed by the Research Council of Norway. Through CMC, SINTEF Building and Infrastructure has built top competence in integrated, numerical analyses together with NTNU and other institutes at SINTEF. SINTEF Rock and Soil Mechanics organized the 6th International Conference on Analysis of Discontinuous Deformation in Trondheim in 2003 and together with NTNU hosted an ISRM sponsored international symposium on in-situ rock stress at the university campus in 2006, where numerical analysis within this field was highly focused.

In recent years SINTEF Building and Infrastructure have been involved in several projects utilizing several advanced models (2D and 3D) in areas including e.g.:

- Location, design and stability of new and existing underground facilities, like mines, hydropower plants and oil and gas storage caverns
- Capacity for anchors for oil drilling platforms, bore-

hole stability and sand-production for petroleum engineering
- Stability of weak zones and modelling and evaluation of geohazards
- Performance prediction of roads and analyses of reinforcement in soil and roads
- Analyses of concrete floors and natural stone pavements with concentrated loads
- Cyclic behaviour and energy absorption of reinforced concrete slabs
- Concept evaluation of pipes and tanks for ultra deep water purposes
- Rehabilitation of water and wastewater networks
- Optimisation of water distribution systems
- Distribution of pollution in the water system Modelling and analyses of coast and harbour structures
- Energy related questions in buildings and in particular analyses of heat and moisture transfer using commercial programmes like THERM and WUFI.

As an important example, SINTEF and NTNU has for more than 40 years performed rock stress analyses and numerical modelling in order to assist in dimensioning and stability evaluations of mines and other underground structures at home and abroad. Increasing the extraction rate in underground mines is of high economic importance. Rock stress measurements have revealed a relatively high horizontally rock stress regime at many locations in Norway. These stresses have considerably changed the mine design in many mines (wider span), with increasing economy as a result. 2 or 3 dimensional numerical modelling has been and still are a very useful tool to determine a stable mine geometry when rock stress measurement results are available.

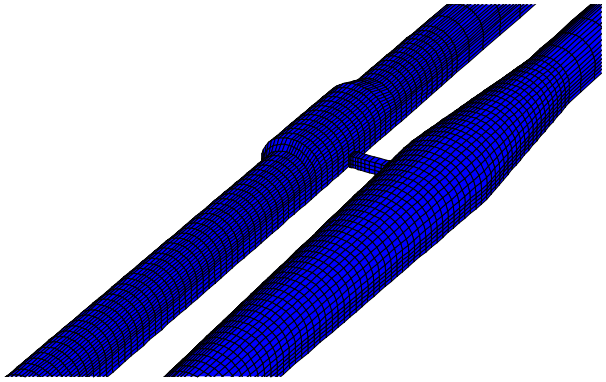


Figure 3: 3-D modelling of world's longest twin-tube road tunnel in China

POSSIBLE CONTRIBUTION TO A CSE CENTRE

With reference to chapter 3, SINTEF Building and infrastructure may bring in competent skills and personell in this field into a joint CSE- centre and of value for the work of the centre also research topics of vital importance for further sustainable development of industry and society.

In addition to commissioned research, SINTEF Building and Infrastructure has recently also put own effort and money internally through the SEP project FELABI (Finite Element Analysis of Buildings and Infrastructure) aiming at creating a platform or a forum to encourage numerical model users to communicate and exchange their experience. By gathering the people in SINTEF and NTNU with experience in this field the expertise could be better utilised and the volume of projects could be increased. We hope to work further along this line and the ideas and plans for a broader CSE centre at SINTEF and NTNU is in good agreement with what SINTEF Building and Infrastructure also search for.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

SINTEF Building and Infrastructure has research personell with broad and comprehensive experience, knowledge and understanding in numerical simulation-based research and at a multi-disiplinary level that should form a good contribution to and could be an important part of a joint CSE, both with respect to research themes and education. Work already performed in developing and improving numerical analyses and programmes is also envisioned to form the basis for further collaboration with a future CSE centre.

GENERAL OVERVIEW

Research activities

The core of the scientific field of cybernetics is **on-line control of dynamic systems**. The system's behaviour is observed through measurements and sensing, desired control inputs are calculated and applied to the system to adjust it to reach a desired behaviour. The goal is to obtain a desired behaviour of a physical system, or bring the system to a desired state and keep it there despite the influence of other, uncontrolled influences to the system.

The dynamic system may be mechanical, such as a robot, a ship, a missile or a prosthesis, a biological system, a process plant or any other dynamic system.

Figure 1: Anna Konda – the world's biggest and strongest snake robot. Multi-joint robots offer great traversability, but also numerous challenges in modeling, design and control due to a large number of interconnected links and complex dynamics.

Our main fields of expertise are dynamic modelling and data analysis, motion control, process control, real time control systems, safety critical real time systems.

Cybernetic research can be applied to very different types of dynamic systems, and the applications addressed in our department have varied over time. The **main applications** addressed are currently natural gas processes, distillation, petroleum processes, robotics, development of ship control systems, off-shore automatic shutdown and safety systems.

SINTEF ICT Applied Cybernetics is also chair of the Gemini Centre for Advanced Robotics.

Teaching activities / Curriculum

Our personell serves as co-advisors to many masters and PhD students at NTNU Engineering Cybernetics and Chemical Engineering, and one of our senior scientists is also an associate professor at NTNU.

RESEARCH CHALLENGES

Unsolved problems and bottlenecks

Dynamic models play an essential role both for off-line analysis of processes and systems behaviour and control system design, but even more so in an on-line real time setting. On-line use of a model is typically for estimation of unmeasured variables, for real-time optimization control.

As control involves using measurements (outputs) from the process/system in order to calculate necessary manipulations (inputs) to the system, the focus within cybernetics is on the input output behaviour of the process. This is also reflected in how the models are constructed and state space representation is a preferred form.

The focus on input to output behaviour also guides which level of accuracy is targeted in the modelling effort. The focus is on representation on phenomena

and behaviour which is actually observed through the measurements. If the model is to be run on-line, the real-time performance aspects are vital and governed by the sampling rates of the process which typically lies in the range of seconds or less.

Key challenge is within modelling and simulation within control is

- Obtaining a model which represents dynamic input-output behaviour with a sufficient degree of accuracy yet meeting real-time requirements and with a reasonable modelling effort.

Often, the development of a model is only one step on the way in the development of a control algorithm, an optimizer or an estimation solution. The modelling effort is therefore another important aspect. At the same time, the complexity of the systems to be modelled increases due to e.g. energy integration and recycling in process plants, or the sheer size of problems to be analysed. On the other hand, for many process plants there exist other models, such as design models. There is a potential for better utilization of such models in order to obtain control relevant models with less modelling effort. Accessibility of a model across different computer platforms, different data formats and protocols, and different software applications are also very important topics to address.

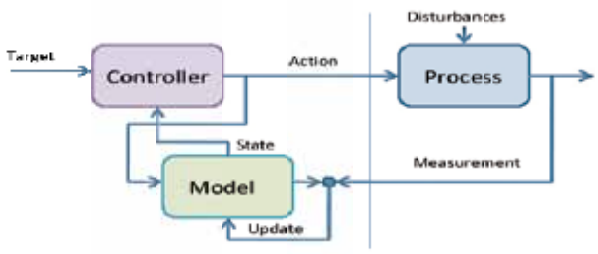


Figure 2: A model based control block diagram. The Controller calculates optimal actions to be implemented on the real process based on a real-time updated model and the desired process behavior.

Vision and ambitions

In regards to our modelling activities:

- To develop new methods and a toolbox for efficient development of control relevant models from rigorous simulation models, and to reach an international level within this area
- To further develop methodological basis for on-line updating of large simulation model
- To be able to analyse closed loop behaviour of complex systems and how the behaviour depends on control and feedback strategies and interactions with the system environment

Need for computational methods

Handling of larger and more complex models in a more efficient manner will be the tool to develop better and more accurate methods for control and optimization. This is related to much more than increasing the CPU-speed. Model formulation, utilization of possibilities for parallelization, numerical solution methods, model access and computational server access protocols, handling of large problems and also large amounts of data are just some of the key issues.

CSE RELEVANT ACTIVITIES

Research and development

In a CSE context, our vision is to focus on methodology for development and use of models for a variety of calculations for control relevant purposes. There are several challenges in efficient model development, model representation, software implementation, system modularity and hardware allocation. In dynamic simulation, dynamic models are used to compute time behaviour of a system. Such models can also be integrated into model based controllers and in state and parameter estimators. The real-time requirement in such applications demands high attention on effective computation and suitable complexity, both on the model part and on the cybernetic algorithms. Other applications may require other types of model calculations, like calculation of derivatives and sensitivities.

This is needed both for detailed controllability analysis and for different types of optimization tasks like real-time optimisation or in optimal control structure design. Safety system analysis, condition monitoring and fault detection are also important issues.

A vision is to be able to extract the required information for any kind of wanted model information or model computation. Such a mega-model that could serve all kind of purposes is probably utopian. However, issues like model extraction and model reduction are always important in view of handling more and more advanced models within real-time constraints with more and more advanced control algorithms.

The development of computer power through the last decades has made it possible to implement complex control algorithms that were simply impossible to realize just a few years ago. Thus, the research into how more advanced cybernetic algorithms actually can be realised with the upcoming computer power is a very important area.

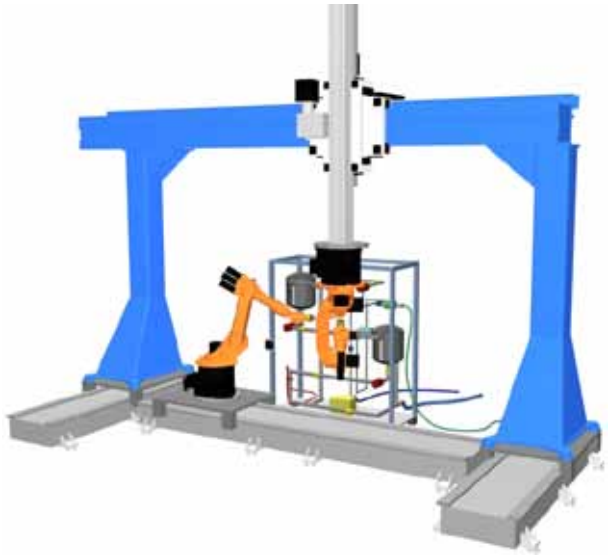


Figure 3: Two robots cooperate on an offshore inspection and maintenance operation. Real-time model-based collision avoidance control systems and multi-sensor fusion algorithms are required in order to ensure safe and robust remote operations.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Model development and efficient implementation for a suitable accurate and fast enough computation is normally part of any activity at Applied Cybernetics. Handling of closed loop feedback systems and the real-time requirements that arise for all control and monitoring applications are very central subjects.

In the area of advanced robotics there are several tasks that are computationally challenging. One example is motion planning and control that ensures collision avoidance. Vision and other high data rate sensor systems require efficient processing and handling. These tasks normally require cross-discipline collaboration.

In the process control direction, model based control optimizing control e.g. energy-optimal operation, and new methodology within control structure design are areas that set new requirements both to algorithm development and to fit for purpose model development.

ENVISIONED COLLABORATION WITH A FUTURE CSECENTRE

- Model reduction techniques. Extracting lean, dynamic models for on-line use from rigorous models.
- Further development of methods for on-line updating of (rigorous) simulation models in collaboration with “model owners” in CSE.
- On-line scalability of models used for orientation in non-structured environments.
- Interface and functional specifications for specific application types

Infrastructure (including facilitation)

Standard PCs with scientific software, with Matlab as the general tool. Embedded software development. General software development. Dynamic simulator development.

SINTEF Information and Communication Technology

Department of Applied Mathematics

GENERAL OVERVIEW

The department focuses on robust and efficient computational methods and software. Areas of expertise include computational geometry, discrete optimization, heterogeneous computing, numerical solution of partial differential equations, visualization, and software development. Scientific activity at the department comes in the form of research contracts with industry, the public sector, the European Union, and the Research Council of Norway.

The permanent staff consists of about 35 researchers and programmers. In addition, we have 6-10 associated PhD and postdoctoral students.

Research activities

- Robust and efficient numerical methods for computational mechanics and geophysical flows, including adaptive FEM and isogeometric analysis.
- Computational methods for subsurface flow, with particular emphasis on multiscale methods, fast transport solvers, and open-access software.
- Heterogeneous computing on multicore and data-stream processors.
- Computational geometry, visualization, and 3D technology for the IT industry.
- Discrete (including mixed continuous/discrete) optimization with applications within transportation, (maritime) logistics, health-care planning, finance, and sports.

The department is an active partner in three centres:

- *Centre of Mathematics for Applications*, a national centre-of-excellence at the University of Oslo
- *Centre for Integrated Operations in the Petroleum Industry*, a national centre for research-based innovation at NTNU
- *Norwegian Research Centre for Offshore Wind Technology (Nowitech)*, a national centre for environment-friendly energy research

Teaching activities

Several of the senior staff at the Department hold part-time positions at universities and university colleges (NTNU, UiO, UiB, HiN, and Jyväskylä). Each year we supervise 10-20 master, PhD, and postdoctoral students.

Figure 1: Simulation of sloshing using smoothed particle hydrodynamics implemented on GPUs.

RESEARCH CHALLENGES

Unsolved problems and bottlenecks

Physical and man-made systems can be described at many levels, from quantum mechanics and molecular dynamics, via the mesoscale or nano-level, to continuum and system-level descriptions. In a multiscale problem, the macroscopic behaviour is strongly affected by processes and properties from micro- and mesoscales. Solving the 'whole' problem at once is seldom possible, even on today's largest supercomputers, as it would involve too many variables to be tractable. Examples on application areas the department aims to address:

- *Subsurface flow* is a truly multiscale phenomenon and upscaling techniques are inevitable to transfer effects and parameters between models on different physical scales. Upscaling methods are both inaccurate and costly in terms of man-hours. Multscale methods form a promising alternative, but have not yet been applied to study systems of industry-standard complexity.
- *Materials failure* is described today mostly by macroscopic models using continuum mechanics. This approach has worked fairly well for traditional engineering materials. However, inhomogeneous materials with an internal structure at the molecular/nano level cannot be properly described by the classical methods. Such materials would be human tissue, most biological materials, membranes, nano-composites and nano-modified polymers used as liners or coatings.
- *Terrain induced turbulence* at airports or wake vortexes induced by airplane or wind turbines are multiscale problems that are among the most challenging problems within computational mechanics of great importance for the society at large. New mathematical and numerical models are needed as well as proper validation facilities.

Optimization problems arise very often in engineering and it is often challenging to develop robust and efficient methods for industrial cases. Here we mention

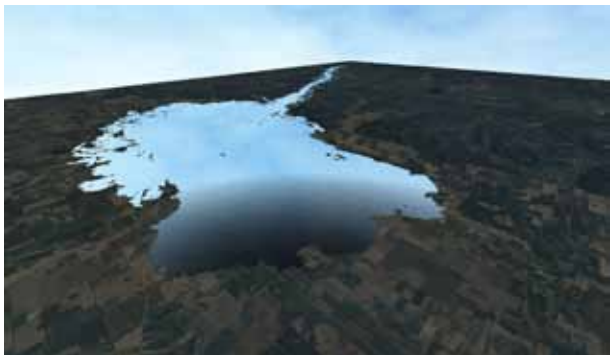


Figure 2: The sudden and unexpected collapse of the Malpasset Dam in France led to considerable loss of life. The figure shows the result of a many-core simulation of the incidence on a graphics card. For this type of simulations graphics cards can potentially replace huge computational clusters and enable the use of interactive simulations in flood prevention.

some challenges that the department aims to address:

- Computational methodologies for data integration, optimization, and risk assessment of petroleum production and subsurface carbon sequestration require reliable simulation responses within minutes or seconds. Current simulators spend hours on forward simulations.
- A serious challenge in real-life discrete optimization problems is quality vs. response time performance of optimization algorithms. Heuristic algorithms for discrete optimization need a time-consuming tuning of parameters. There is a strong need for self-adaptive methods that alleviate this problem. Exact methods and approximation algorithms based on heuristics have complementary strengths and weaknesses. How to combine these types of methods is a challenge. The novel parallel architectures offer special opportunities and challenges.

Future increases in computing capacities will come from parallel processing. Still, the majority of simulation and optimization software are based on serial algorithms for single-core CPUs. Similarly, unprecedented computational performance is gained by introducing specialized processors, making current computing

systems heterogeneous. Traditional computational methods do not map to new heterogeneous processor architectures. Hence, one needs to develop *hardware-adapted numerical methods*, i.e., numerical methods that map well to the new emerging hardware.

Computer Aided Design (CAD) and Finite Element Analysis (FEA) are essential technologies in modern product development. However, the interoperability of these technologies is severely disturbed by inconsistencies in the mathematical approaches used. The current lack of efficient interoperability of CAD and FEA makes refinement and adaptation of the analysis model cumbersome, slow, and expensive. The new paradigm of *isogeometric analysis*, which was introduced by Professor Thomas J. R. Hughes and coworkers in 2005, demonstrates that much is to be gained with respect to efficiency, quality and accuracy in analysis by replacing traditional Finite Elements by volumetric higher-order Non-Uniform Rational B-Splines (NURBS) elements. However, open problems like user-friendly making of isogeometric consistent CAD-models and efficient and reliable local refinement techniques remain to be addressed.

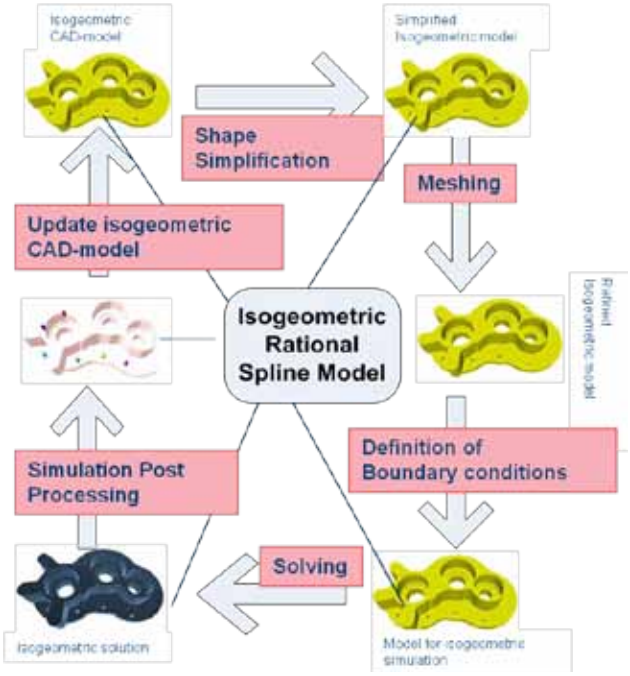


Figure 3: Figure depicts the envisioned interoperability of CAD and analysis offered by isogeometric analysis augmented with adaptive isogeometric methods. From the CAD model, where objects are represented as a patchwork of surfaces representing the outer and inner hulls, an isogeometric spline model is made representing the model as tri-parametric rational spline volumes. This allows the results of the analysis to update the isogeometric CAD-model, and directly refine this when the analysis needs more degrees of freedom.

Visions

Design once, use everywhere: complete descriptions of realities and their behavior through one coherent representation for simulation, modeling and visualization:

- Full integration of CAD and finite element analysis by introducing common basis representation (isogeometric analysis).
- Direct simulation of geological models using multiscale methods.
- Multiscale simulation of local wind fields around airports and wind power parks
- High performance, self-adaptable, parallel, hybrid methods in discrete optimization
- Interactive simulation and visualization in the cloud.

Open-source software modules relevant for:

- Subsurface flow (petroleum, CO_2-storage, etc).
- Continuum mechanics (both structural, solid and fluid)
- Multiscale modeling from atomistic to continuum mechanics

All application areas studied at the department require new computational methods to enable new value creation. Developing such methods is the core content of our research.

CSE RELEVANT ACTIVITIES

Research and development

Key strategic research areas include multiscale simulation, isogeometric analysis, heterogeneous computing, discrete optimization and visualization.

Examples on ongoing projects within multiscale simulations are *GeoScale – reservoir simulation on a geological scale*, where we have set an ambitious goal aiming to develop capabilities for multiscale, multi-fidelity simulation of flow and transport in porous media for applications in petroleum production and CO2 storage. This is done through GeoScale, a portfolio of strategic research projects funded by the Research Council of Norway and various industry partners. Another multiscale project is Local wind prediction around airports which is funded by AVINOR. The main aim of this project is to predict terrain-induced turbulence at various airports in Norway. The microscale code called SIMRA, developed by SINTEF, makes use of meteorological data from the Norwegian Meteorological Institute and produces more detailed wind prediction around a number of Norwegian airports. It has been approved by the Norwegian Civil Aviation Authority (NCCA) and has been fully operative since 1st of July 2009.

Within the area *Isogeometric analysis*, the department has initiated two major projects denoted Isogeometry and ICADA that are both co-funded by the Research Council of Norway and Norwegian industry. Furthermore, the department is a central partner in the EU-funded project *EXCITING*. Through these projects, we will for the first time make spline-based finite elements available for integrated design and analysis of industrial relevant problems in civil, mechanical and naval engineering. In particular, we will

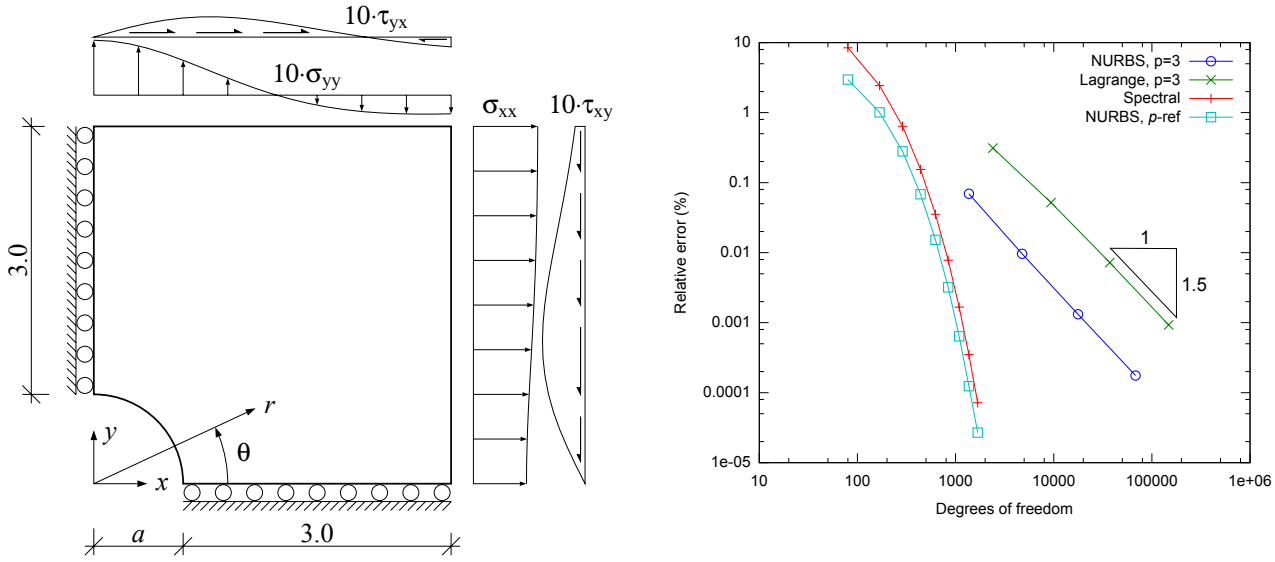


Figure 4: Comparison of the accuracy of different finite element shape functions and refinement schemes. The figure to the left displays the problem definition for the smooth problem denoted Hole. To the right we compare h-refinement using classical Lagrangian shape functions with NURBs, and we see that the convergence rate is the same but that the error is a factor 10 lower for the NURBs.Next we compare p-refinement using Spectral elements with NURBs, and again the NURBs gives less error for similar number of degrees of freedom. Notice the exponential convergence rate obtained using p-refinement! For smooth problems or properly refined non-smooth problems high order NURBs may increase the computational efficiency significantly.

address topics such as modelling of isogeometric-consistent CAD-models and goal-oriented adaptive mesh refinement using locally-refined splines.

The future is parallel and the department is involved in a number of projects where utilisation of emerging parallel computer hardware is the key point. We focus on *heterogeneous computing,* which aims to combine the parallelism of traditional multi-core CPUs and accelerator cores to deliver unprecedented levels of performance for simulation and visualization. The project *Interactive simulation and visualisation* in the cloud has as objective to develop methods for high-quality interactive simulation and visualization of large-scale coherent models on workstations and web-based clients. Novel methods will be developed for simulation and visualization of exact and compactly stored higher-order models. The use of heterogeneous computers will be central for both interactive simulation and visualization. The department's track record of research within heterogeneous computing is substantial, and has reached such a level of recognition by peers, that NVIDIA has selected the department as one of the inaugural CUDA Research Centers.

The department has a long tradition in doing discrete optimization and has many projects within this area of applied mathematics. During the past few years we have worked on complex projects in the following application within transportation, health care, finance, and sports.

Teaching activities

The department has organised the annual Geilo winter school in computational mathematics/eScience the last ten years and will continue to do so the next five years.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Department of Applied Mathematics aims to be the driving force to move frontiers in CSE, and be a focal point at SINTEF for technology transfer of advanced simulation technologies to the involved application areas. To this end, we envision a truly multidisciplinary environment in which application specialists collaborate closely with our mathematicians and computer scientists to take advantages of recent advances in computational methods and hardware to solve challenging problems in materials science, geoscience,

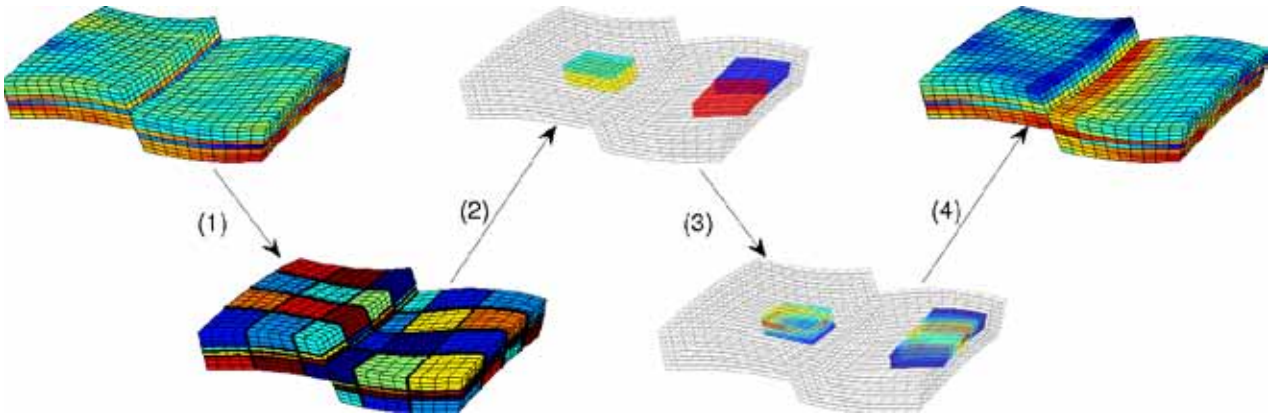


Figure 5: Key steps of the multiscale method: (1) blocks in the coarse grid are defined as connected collections of cells from the fine grid; (2) a local flow problem is defined for all pairs of blocks sharing a common face; (3) the local flow problems are solved and the solutions are collected as basis functions (reconstruction operators); and (4) the global coarse-system (8) is assembled and solved, then a fine-scale solution can be reconstructed.

process technology, etc. In particular, we will contribute with expertise on multiscale methods, isogeometric analysis adaptivity, error estimation, parallelisation, visualization, and heterogeneous computing.

Our researchers have long experience and traditions for developing highly efficient and maintainable computational software using principles of modern software development (object orientation, generic programming, testing, verification, etc). In recent years, we have gained a lot of experience in developing libraries under open-source software licenses, which will be the main model in the centre for licensing, protection of IP rights, and establishment and preservation of an efficient and well-maintained software infrastructure.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research themes

A CSE centre at NTNU and SINTEF is envisioned as a true collaboration between NTNU and SINTEF to achieve synergy between the two institutions complementary advantages: NTNU educating qualified personnel and SINTEF enabling continuity in building numerical infrastructure such that NTNU and SINTEF in a combine effort may do both high quality long term basis research as well as industrial relevant applied research.

The department will be a driving force in developing a sustainable numerical infrastructure, i.e., software for numerical simulation of challenging problems in science and engineering. In particular we may contribute to develop software that takes fully advantage of emerging computer hardware.

On the other hand, we anticipate a fruitful collaboration with application scientists focusing on theoretical modelling for development of novel mathematical and numerical models within targeted areas within science and technology. Furthermore, we look forward to collaborate with application scientist in charge of

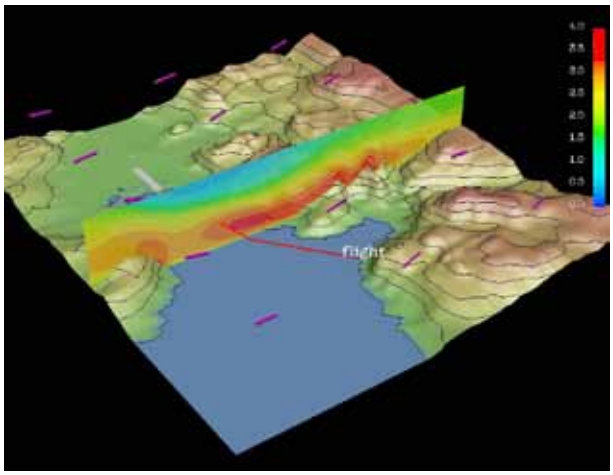


Figure 6: Estimation of turbulence intensity in the vicinity of Værnes airport using Computational Fluid Dynamics code SIMRA for 23rd Feb 2007 with real meteorological conditions. Flight operations were interrupted on the particular day due to intense turbulent conditions. The simulation confirmed the prevalence of dangerous flight conditions (Turbuelnce intensity above 3.5m/s is considered dangerous) as shown in the figure.

experimental facilities that may be used for validation of mathematical and numerical simulation tools developed in the centre.

Education

Senior scientists at our department will co-supervise master and doctoral students, and may be giving short courses on advanced computing methods and modern methods for software development.

Infrastructure

The department envisions the needs for establishing larger computing laboratories based on multicore and heterogeneous architectures, and are ready to take part in sharing cost facilities.

We also anticipate that support and development of basic numerical infrastructure may be a topic for a future CSE centre, and we are ready to be a driving force for such activities.

GENERAL OVERVIEW

The Department for Cooperative and Trusted Systems (CTS) provides research-based expertise in model-driven software engineering and service oriented systems, quality and security technology, and human-computer interaction. Through this expertise we provide advanced methods, techniques and tooling for constructing, executing and evolving complex software systems. Currently our research is focusing in the fields of Future Internet, such as *Internet of Services, Internet of Things,* and Internet of Content, where we have special emphasis on Ubiquitous Computing, and Dynamic Service Systems.

The research is applied in a diverse set of application areas, such as Intelligent Transport Systems, Scientific Software (see below), Enterprise Systems, Advanced Industrial Real-TimeEmbedded Systems, and Command, Control, Communication, Computer, and Intelligence Systems (C4I), such as Emergency / Crisis Management Systems.

At the University of Oslo the department holds several courses related to the research activities performed, in particular Model Based System Development, and Unassailable IT-systems.

RESEARCH CHALLENGES

The software engineering discipline has been challenged with continuous increase in the complexity of the software systems to develop. The history of software engineering shows that it has been exploring technologies applicable to a wider range and usable in the more general context. The first computer systems were running on one machine and typically computed relatively dedicated and simple but time consuming problems. Today computer systems are networked, ubiquitous and perform distributed computing in dynamic and heterogeneous execution environments. They compute advanced and generic problems in almost all thinkable contexts ranging from control of nuclear installations and space ships to information management, electronic commerce, short and long distance communication, entertainment, environmental model simulations, and intelligent homes. Thus, managing complexity is still something computer scientists, engineers, and programmers have to fight.

In our research the ambition is to tackle the complexity of software engineering in general and in particular to provide methods and technologies for constructing and executing high quality cooperative and trusted systems that can interoperate and adapt to various application domain and system contexts. We believe that better abstractions and advanced separation of concern supported with sophisticated tools are key elements in order to cope with the complexity.

CSE RELEVANT ACTIVITIES

IEEE computer had a special issue on Developing Scientific Software [Software, IEEE Volume 25, Issue 4, Date: July-Aug. 2008], where particular challenges of developing scientific software is enlightened. One particularity that is reported is that the domain expert very often is also the software and system expert. This is the case since a problem domain can be so complex that it is only the domain expert that really understands the problem, the requirements and the solution. Thus, the consequence is that domain experts also have a major role in designing and implementing the computer based solution (see the citation box to the right). Furthermore, the current state-of-the-practise in developing scientific software is also due the fact that it is organized as a highly explorative process. That is, most of the requirements of the specific domain regarding computational means, such as models and algorithms, are identified in parallel and often interleaved with the actual construction of the software solution itself. This is very different to the state-of-the art within Software Engineering, where the artefacts (e.g., models and algorithms) describing the problem domain and the corresponding software solution are not interleaved neither as abstract artefacts nor at the process level.

Therefore, our department currently do research to understand better the particularities of developing scientific software aiming to deliver methods, techniques and tooling that are well suited for such development. In particular we want to provide a tool supported methodology as an integrated development environment for developing scientific software. We follow a model driven approach where we will support both modelling of the software system applying MDE technologies such as UML and SysML and also modelling of the computational domain using appropriate computation modelling technologies and tools such as Mathlab/Simulink and Modelica.

As part of the integrated development environment we provide tutorials and lectures/courses, which also will be part of our University courses and for other dedicated lectures. In addition we will have both Master and PhD students address relevant aspects of scientific software development for their respective thesis projects.

POSSIBLE CONTRIBUTION TO A CSE CENTRE

In our research projects, which mostly are of generic nature, there are several topics that should be of interest to stakeholders in the field of Computational and Scientific Engineering, such as

- methods and tools for developing sustainable software which can be maintained and changed easily over time,
- ensuring quality and confidence by rigorous verification of the relation between the abstract computational models and algorithmic structures defined and the actual software executing the programs for these models and structures, and

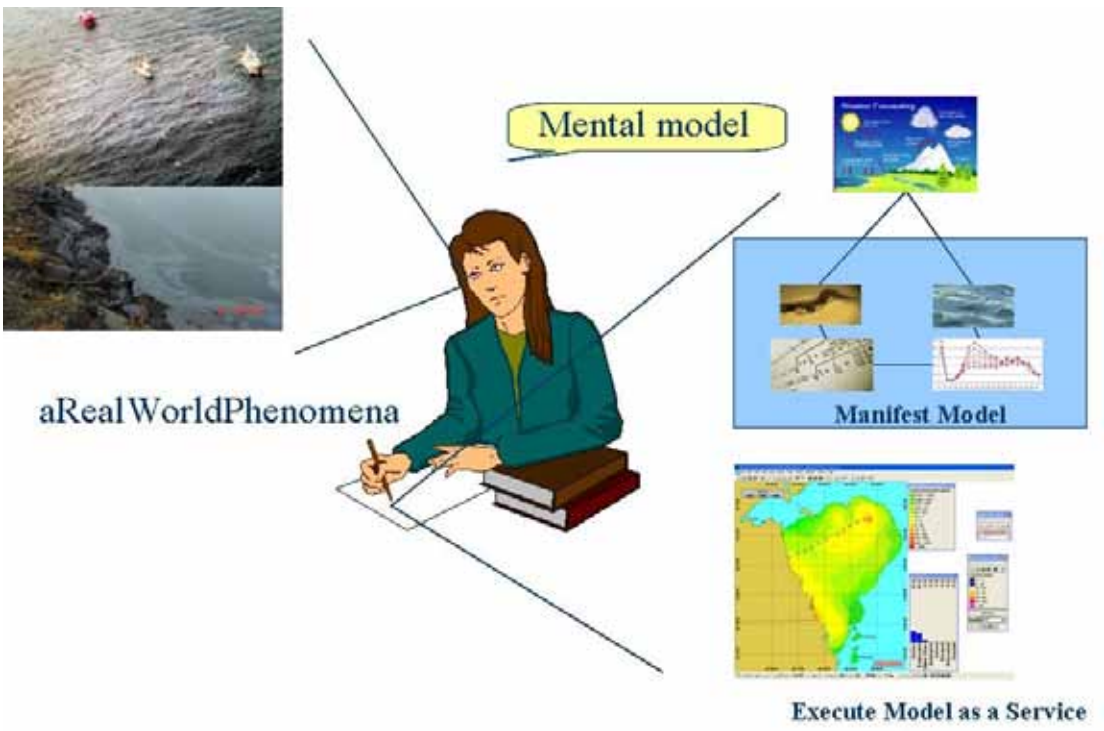


Figure 1: SiSaS model as a Service approach

- expanding the notions of computational models (visualized and/or simulated) to be much more of interactive models directly communicating with and manipulated by users.

However, in this short presentation we only present one on-going project: The SINTEF Scientific Software as a Service (SiSaS) project, which is lead by CTS but with several other SINTEF departments involved that develop scientific software as main tasks in their research activities. SiSaS focuses in particular in delivering scientific software as a service (SaaS). That is, users interact with the software not as program running on a physical machine or infrastructure at the user site, but as a virtual service transparent available on the cloud (i.e., over the intra- or internet).

The goal of the project is to provide an innovative integrated development environment, methodologies and a service oriented platform for developing and executing scientific software as services, and thereby be recognized to be a leading actor in developing and offering high quality scientific software as a natural part of our research. Hence, distribution, access and use of scientific software will have a potential to increase by many magnitudes compared with the many software package strategies and licensing policies applied to such software in the market today.

The integrated development environment will support the transformation of a real world phenomenon into software based computational models that can be executed as a service. This is exemplified in Figure 1, illustrating how a real world phenomenon (the real world phenomenon here is oil spill and the illustration is based on one of the SiSaS pilots provided by SINTEF Materials and Chemistry) is mapped into a computational model such that the distribution of an oil spill can be simulated/predicted.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

We envision the following possible contributions to and collaborations with a future CSE centre:

- Providing methods and tools for developing scientific software according to state-of-the-art principles in software engineering and as described above, also including the SaaS approaches.
- Also CSE based systems becomes more complex due to distribution of resources and the increased number functions and users depending on such systems. One hot research topic for handling such complexity and provide sufficient computational power for the user is the paradigm of cloud computing. Currently, we are engaged in several European FP7 projects where cloud computing is a main research topic.
- Education for instance related to University courses or supervising students are tightly coupled to our research projects, which are the main source for extending course material and defining new research topics adequate for student projects.
- We provide mainly two kind infrastructures, one dealing with the actual methods and tools for developing software, e.g.., a workbench approach, and one dealing with collaborative efforts though a living lab based social media.

SINTEF Materials and Chemistry

Department of Applied Mechanics and Corrosion

GENERAL OVERVIEW

The Applied Mechanics and Corrosion department focuses on characterisation and reliable use of materials under demanding conditions. We study the mechanisms of damage, fracture and degradation in materials, and develop versatile computational tools that represent the observed phenomena. In our approaches we combine state-of-the art numerical methods (non-linear Finite Element and Particle methods) with mechanical, micromechanical and environmental models. The resulting technologies enable our industrial customers to (e.g.) tailor materials and/or to design safe, robust and cost-efficient production processes, components and structures.

Our most important customers are material producers, energy industries and the automotive industry. The department works closely with the Norwegian University of Science and Technology (NTNU) and other SINTEF institutes.

The department has 42 employees divided into 3 research teams.

The Fracture Mechanics and joining team is developing models for fracture, both brittle and ductile, and tools for integrity assessment. The team also works with different joining technologies, with a strong focus on hyperbaric welding.

The core activity of the Structural Mechanics team is development of constitutive models - including damage and fracture criteria - numerical implementation in non-linear computer programs, combined with small and large-scale validation. The team are central in the CRI SIMLab (see separate presentation).

The Corrosion and surface protection team studies degradation phenomena caused by harsh environments and mechanical contact, e.g. general corrosion, hydrogen embrittlement, H2S stress corrosion cracking, mechanical wear and tribo-corrosion. Predictive tools based on FE and/or particle methods and linked with environmental models are under development.

Within our department/institute, and the associated NTNU departments, we have unique laboratory facilities that cover nano to structural length scales.

Teaching activities; the department continuously supervise a number of MSc and PhD students. Personnel from the department regularly teach at NTNU and three members of our staff holds Professor II positions at NTNU. Topics taught include: Non-linear Finite Element modelling, solid mechanics modelling, welding and joining technologies, corrosion and surface protection.

RESEARCH CHALLENGES

Our general objective is to understand and model degradation and damage mechanisms arising due to mechanical deformation and/or under the influence of environment and time. Our ambition is to have a strong position in solid mechanics modelling in general, and to be in a world-leading position in some prioritised market segments of particular importance to Norway and the Norwegian industry. We have activities within different material classes; metals, polymers, concrete and composites. Particularly important market segments are:

- Pipeline integrity
- Ligthweight materials, in particular aluminium.
- Renewable energies (Silicon and wafer technology, Offshore wind, geothermal energy)

To reach the stated overall objective, consideration has to be given to the micro-structural features of engineering materials, i.e. we face challenges that require a multiscale approach. Resolving the relevant scales and physical/chemical phenomena result in a number of computational challenges. Topics such as homogenization between scales, optimization, meshing technology, heterogeneous computing/HPC and software design and maintenance as areas where we see challenges that needs to be addressed. We further

search integration of the engineering tools used for alloy, process and product design.

CSE RELEVANT ACTIVITIES

Examples of modelling activities within the department and on different length scale are:

Atomistic modelling; Brittle fracture phenomena in steel and Silicon materials are addressed with atomistic modelling approaches in collaboration with NTNU and international partners.

Mesoscale modelling;

A generic crystal mechanics modelling technology is under development for FCC and BCC crystal structures.

Continuum scale modelling; We have twenty years of experience in continuum scale modelling of metals.

Structural modelling; Pipeline, forming/formability and structural impact modelling.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Our contributions to a CSE centre would include:

- physical testing of solid materials.
- unique competences on physical behaviour and modelling of engineering materials like metals, polymers, concrete and composites.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

The envisioned benefit from a CSE centre is;

- a meeting place for inspiration and creation of new collaborative multi-disciplinary projects between the participants (KMB/JIP/SFI/SFF).
- education of highly skilled engineers and scientists within practical numerical modelling and software design (MSc/PhD/post graduate).

A basic curriculum should be developed within the centre so that all students from NTNU will have a world class basis for doing practical numerical modelling. It is increasingly difficult to recruit qualified Norwegian candidates for such jobs in our field, and should be considered a national priority.

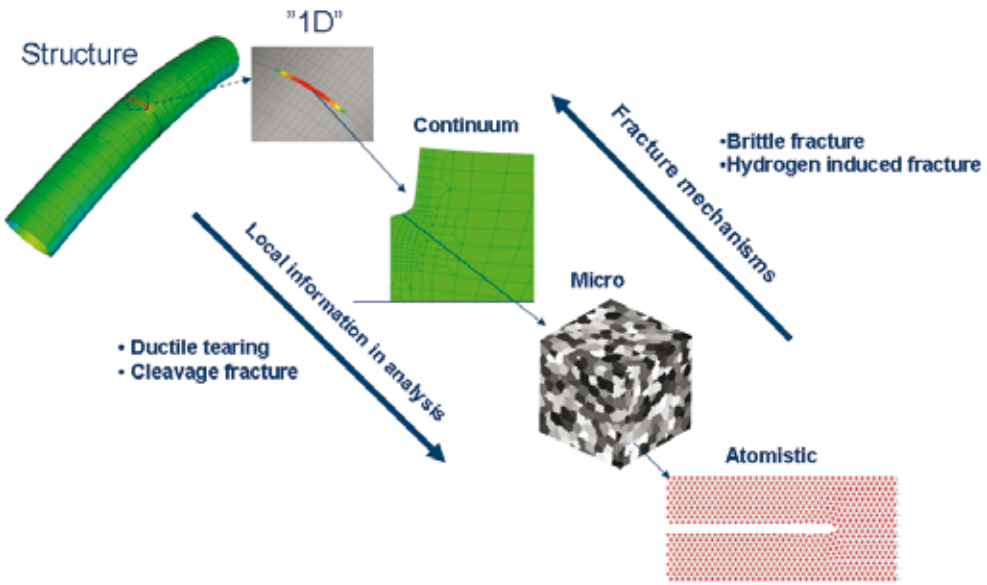


Figure 1: A multiscale approach to modelling of fracture in steel from atomistic to continuum scale. Proposed research collaboration between NTNU and SINTEF in the application for a "Research driven centre for innovation" denoted CSE-Multiscale.

SINTEF Materials and Chemistry

Department of Hydrocarbon Process Chemistry

GENERAL OVERVIEW

The department of Hydrocarbon Process Chemistry has the following main competence areas:

- Synthesis and preparation of oxides, porous materials, supported catalysts and metal complexes
- Advanced characterization
- Testing and screening of catalysts and adsorbents; fluidized and fixed bed reactors
- Combinatorial chemistry or parallel technology directed towards catalysts and adsorbents
- Molecular modelling
- New heterogeneous catalysts

While SINTEF is not a degree-granting institution, SINTEF scientists are involved in supervision of MSc students, PhD students, and postdoctoral fellows. For the time being, four postdocs are part of the Dept. of hydrocarbon process chemistry. Three of these work on molecular and atomistic materials modeling

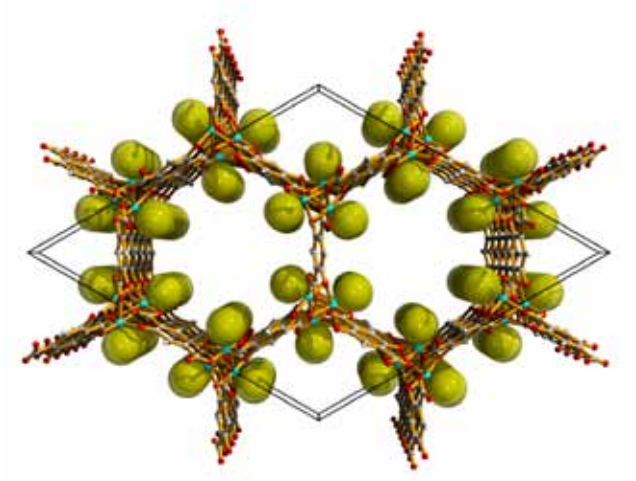


Figure 1: Crystal structure of the metal-organic framework (MOF) CPO-27. MOFs are microporous crystalline materials built from metal atoms and organic linker molecules. Potential applications include adsorption of gases; in the picture, we see CO2 molecules in the pores of the material.

RESEARCH CHALLENGES

Many catalyst systems are extremely complex, making experimental characterization difficult. This is one of the reasons why molecular modeling is part of the department's strategy. We note a clear increase in our markets' demand for fundamental understanding; a general awareness that the classic empirical *modus operandi* of catalysis research has limitations that may be overcome by improved models on the atomic and molecular scale. More specifically, challenges in our fields include accurate prediction of reaction mechanisms on surfaces and developing deterministic models for prediction of synthesis of microporous materials. From a modeling point of view, these goals are being incrementally met by improvements in methodology and available computer power. A major breakthrough, as opposed to the gradual development mentioned above, would require method development on a broader scale, coupling molecular modeling with kinetic modeling, statistical thermodynamics, and modeling of mass and heat transfer. Internationally, there have been at least two attempts at such a large-scale integration.[1] Such large-scale collaboration including industry, academic groups has produced useful multiscale modeling results for phenomena like crystallization, polymer flow, and others.

CSE RELEVANT ACTIVITIES

Present computational research includes a wide range of quantum mechanics based methods for the study of molecules and solids. For the time being, one scientist and three postdocs pursue different research avenues. More specifically:

1. Alkane activation with organometallic gold complexes. Here, quantum chemical methods are used to screen different gold complexes for stability and catalytic activity. The activity is part of a larger project financed by the GASSMAKS program of the Norwegian research council (NFR).

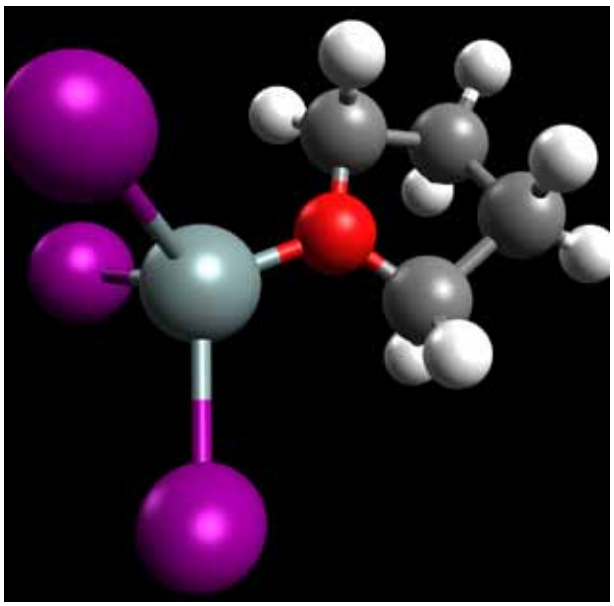


Figure 2: Molecular structure of an intermediate in silicon purification.

2. Reactions of carbon dioxide on a combined nickel/magnesium oxide system. A supported metal catalyst is investigated using band structure methods and a slab model. This is a project under the KOSK program of the NFR.
3. Selective sorption of dinitrogen oxide on mixed oxides. Another slab model study, motivated by environmental concerns and financed jointly by Norwegian industry and NFR.
4. Smaller efforts as part of running projects. This is an important part of the modeling activity: The existence of a low-threshold offer makes it easy to take it into use in an *ad hoc* manner.

In 2008, a theoretical physicist specializing in band structure calculations (Ole Martin Løvvik) was hired at the neighbouring dept. of Synthesis and Properties. We have already begun to utilize the synergistic potential offered by having partly overlapping computational competence represented in both departments.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Applied molecular modeling and quantum mechanics based materials modeling are becoming steadily more important in many areas of chemistry and materials science. Within these fields, we offer competence that is complementary to molecular modeling oriented activities at the NTNU and other Norwegian universities. Ongoing projects are described in the previous section.

Specific contributions to a CSE centre would typically include the use of molecular and atomistic modeling as part of a larger scheme. Multiscale modeling comes to mind; see “research challenges” above.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

It is our experience that computational methods are most useful when they are used in conjunction with other, experimental methods. Further, many experimentalists are not aware of the great progress that is being made in computational science. We envision that an important function of the CSE centre will be to integrate computational studies into large and multidisciplinary projects, disseminating knowledge about the possibilities offered by numerical modeling. To contribute to this goal, we can offer a broad range of capabilities within molecular and solid state modeling. Naturally, our contributions to a future CSE centre would mainly be within the areas of catalysis, surface science, and industrial chemistry.

1 OCTA project: http://octa.jp/ ;
MSC: http://www.wag.caltech.edu/

SINTEF Materials and Chemistry

Department of Marine Environmental Technology

GENERAL OVERVIEW

Research activities

SINTEF MET performs experimental, monitoring and modelling studies connected with both acute and regular releases of oil and chemicals to the marine and terrestrial environment.

Researchers at SINTEF MET study the fate and effects of pollutants on the environment, and also investigate various response methods.

Laboratory and meso-scale experiments are carried out at modern research facilities at SINTEF Sealab in Trondheim. Field experiments are designed according to research goals. For instance, in May 2009 we performed the largest oil release experiment ever done under arctic conditions.

Teaching activities

SINTEF MET supervises MSc and PhD candidates within ecotoxicology and microbiology.

Recently, SINTEF MET and Statoil jointly initiated a master's degree programme at NTNU called "Environmental Toxicology and Chemistry"[1]. The programme started in autumn 2009. Seven of our staff are involved in teaching this programme.

Department staff are involved in a wide range of teaching activities in science and engineering. Examples include an adjunct professor position at the

Figure 1: Real oil spills.

Figure 2: Experimental oil spills.

University Centre in Svalbard, NORAD courses for students from Angola, and the examination of computer science students at NTNU.

RESEARCH CHALLENGES

Unsolved problems and bottlenecks

As an integrated part of our research, SINTEF MET is developing numerical models addressing oil and chemical releases at sea. This work started in the 1970s, and throughout the 1980s and 1990s these models evolved into advanced PC-based simulation tools.

Our modelling domain consists of four sub-domains. As these sub-domains are closely interrelated, this poses a particular challenge for modelling.

As oil production and oil transport move into more vulnerable areas (ice-infested waters; near-shore), the need for scientifically sound risk analysis tools is growing. Incorporating ice and shores in the models *increases complexity*, and also requires *multiscale modelling*. Spill models can no longer operate only on regional scales (1–100 km), but must also resolve more detailed local scales on the order of 10–1000 m.

Moreover, there is a growing demand for models to *inter-operate* with external data sources and models for a broader and more holistic view of risks and effects. The "Model Web" concept denotes an infrastructure for ecological modelling, much like the World Wide Web.The Model Web would be a system of inter-operable computer models and databases communicating primarily via web services.

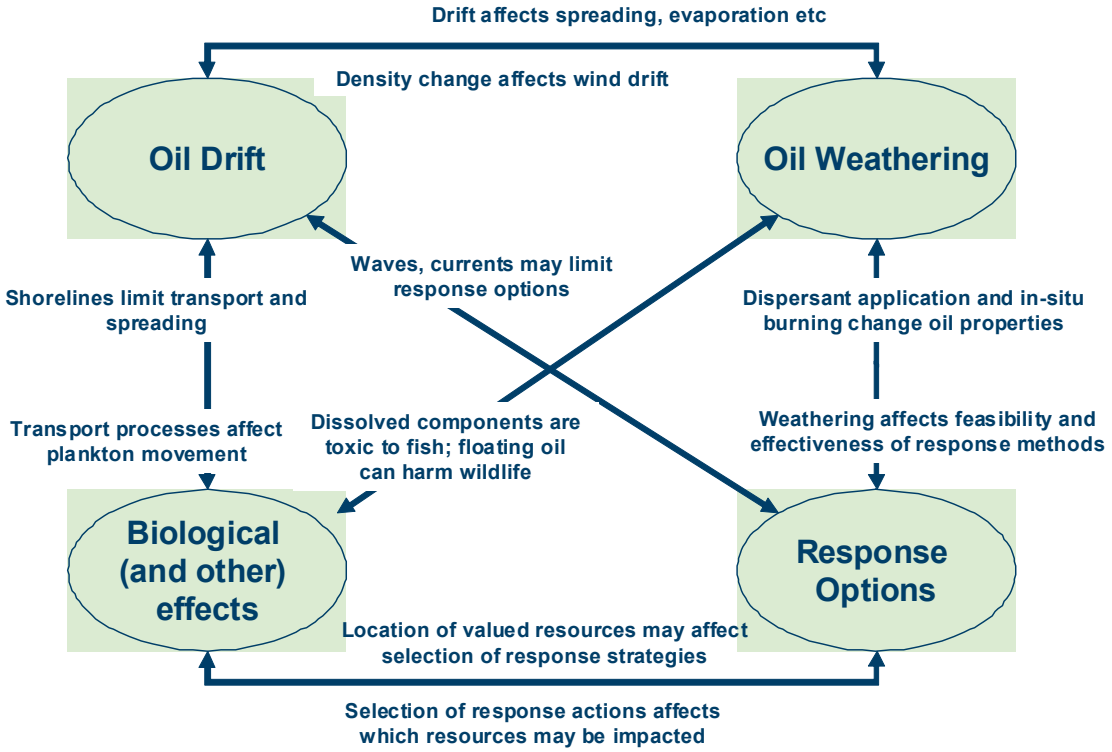


Figure 3: Oil spill modelling domain and its sub-domains

We also see a growing need for *optimization*. For instance, in order to design a contingency plan for potential oil spills, the tools should be able to run a range of scenarios and determine the "best" response strategy with respect to time, cost, risk etc., based on specific decision criteria.

Finally, there is a trend towards using the models in more *operational* and *interactive* contexts. This may be in real spill situations or in simulations. For operational use, models need to be able to *assimilate measured data* from in-situ sensors (e.g. buoys) or remote sensing platforms (e.g. satellites).

In summary, key challenges include:
- Increased complexity
- Multi-scale modelling
- Interoperability
- Operational and interactive applications
- Optimization
- Data assimilation

Needless to say, all this requires *massive computing* power.

Vision and ambitions

Based on SINTEF's overall vision, we derive the following vision for SINTEF MET:

"Oil spill technology for a better society"

Our numerical models are essential elements of this technology. SINTEF MET's modelling ambition is:

To develop the best and most versatile oil spill models in the world

Here, we mean "best" in terms of reliability, speed, and stability, and "versatile" in terms of interoperability and applicability (geography, usage types etc).

Need for computational methods

Model-level computational needs

SINTEF MET's models require numerical solvers for ordinary (ODE) and partial differential equations (PDE). Moreover, there is a need to support spatio-temporal calculations -- particle-based or grid-based. Also, there is a need to support *data assimilation*.

Reliability is the #1 model requirement. In order to ensure reliable models, **verification** and **validation** methods are needed.

As discussed above, model **optimization** methods will be very useful.

At the end of the day, simulation results are to be perceived, interpreted and understood. To this end, powerful *4D visualization* capabilities are essential.

Computational infrastructure needs

Parallel computing capabilities are obviously needed which could be multi-core or multi-CPU. Relevant multi-CPU approaches include grid computing and cloud computing.

To speak with other systems in a "model web" fashion, web connection is needed to expose and consume web services. A *security* system will ensure appropriate access.

Obviously, *compilers* and *run-time environments* are needed for the most popular programming languages in science and engineering (C, C++, Fortran, Java).

CSE RELEVANT ACTIVITIES

Research and development

Basically, all our research is relevant for CSE, since our models essentially cover our entire research domain.

More specifically, two joint industry programmes are of particular interest: Coastal Oil Spills JIP and the

Oil-in-ice JIP. Both are comprehensive programmes including field, laboratory and modelling activities, and they both pose modelling challenges that are hard to meet with our current PC-based approach.

Also, we are participating in three IT-oriented projects. All three are coordinated by SINTEF ICT:

- **SiSaS** (SINTEF Software as as Service): Strategic programme for service-orienting scientific software developed at SINTEF. SINTEF MET's oil drift model is one of three pilot cases.
- **OSS** (Ocean Space Surveillance): Strategic programme for better sea monitoring and new applications for SINTEF models through sensor data assimilation.
- **Envision:** EU project to develop an infrastructure for discovery and chaining of environmental data and models by non ICT-skilled users.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

SINTEF MET's main contribution to a CSE Centre is our *domain expertise* in marine environmental research. There is a growing awareness of the key role that the marine environment plays in issues of sustainable development. Global warming, transportation, food production and urban development are examples of such issues.

Of course, SINTEF METs related *modelling skills* is also a possible contribution.

Ongoing research projects

The "IT-technical" projects above (SiSaS, OSS and Envision) are all candidates for CSE Centre contribution.

Planned projects

All new research projects at SINTEF MET with significant modelling activities will potentially contribute to a CSE Centre. The same goes for all new "IT-technical" projects.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research themes

All projects that study pollution in the marine environment in some form, and where modelling is a key part, are natural candidates for collaboration between a future CSE Centre and SINTEF MET.

Examples of such topics from current projects: Leakage of stored CO2 from subsea reservoirs; effects of nano-particles on marine ecosystems.

Education

SINTEF MET would like to contribute actively in CSE-oriented education activities. We can provide domain expertise within an important domain, and we can also provide modelling skills.

Of course, we would also be interested in training for our own personnel at a future CSE Centre.

Infrastructure

SINTEF MET is interested in sharing (or using) computing infrastructure with (or at) a future CSE Centre.

SINTEF Materials and Chemistry

Department of Process Technology

GENERAL OVERVIEW

The main focus of work in the Department of Process Technology is to develop and improve chemical and metallurgical processes and unit operations by combining fundamental experimental and theoretical modelling utilizing the latest in experimental and numerical research. The Department enjoys close collaboration with NTNU and other SINTEF institutes, in particular with Petroleum Research and Energy Research. Some of this collaboration is also formalized by the KinCat Gemini Centre. The Department has 65 employees divided into 4 research groups.

The CO2 group is a key player in basic research on post-combustion capture processes both nationally and internationally and together with NTNU forms the core of a large industrial thrust for developing a commercial post-combustion capture process.

The flow technology group is working on multiphase flow modelling. Major activities include metallurgical furnaces and development of a new generation of multiphase flow simulator for oil and gas pipelines.

The chemical engineering group is a key player in new technology developments for enabling long distance transport of natural gas hydrates and wax in multiphase oil and gas pipelines, and is recognized for its strong modelling work on process optimization in e.g. LNG systems, GTL and polyolefin reactor systems. The group is also a key player in development of new Lagrangian/mesh free simulation methods within chemical engineering and material processing.

The catalysis group works closely with NTNU and Statoil on the development and testing of catalysts for gas to liquid processes (GTL). Octane and sulphur removal processes are also important area of research, covering the range from nanoscale to plant scale.

Teaching activities; the Department has supervised a large number of MSc and PhD students. Personnel from the Department regularly teach at NTNU and one member of our staff is an adjunct professor at NTNU. Topics taught include: Atomistic modelling, thermodynamics, multiphase fluid mechanics and turbulence, and chemical engineering.

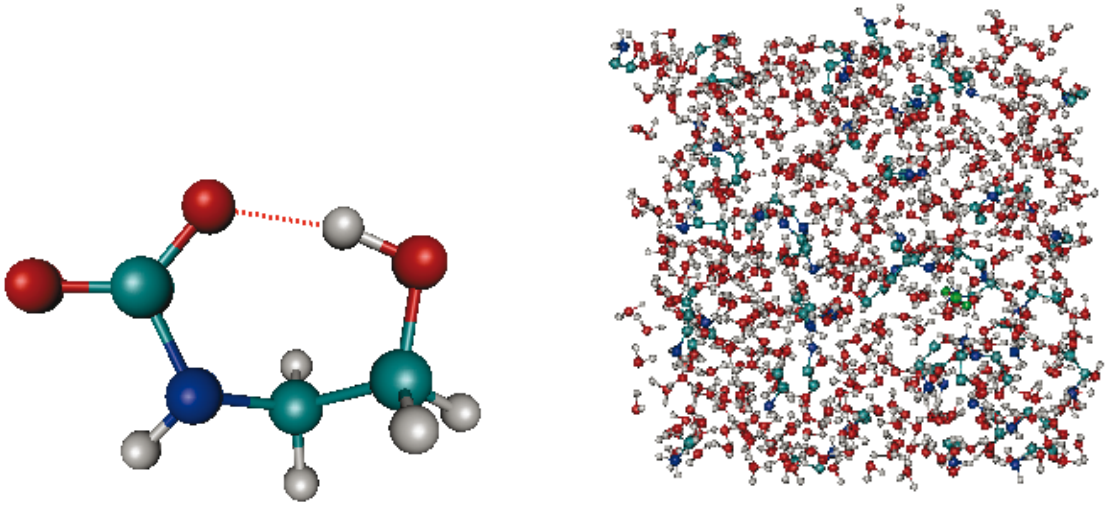


Figure 1: Molecular simulation: Left: a monoetanolamine (MEA) molecule with an absorbed CO2 molecule forming a carbamate. CO2 (upper left part of complex) absorbes to the amine group of MEA. Right: (Oxygen=red, carbon=green, nitrogen=blue, hydrogen=grey). Eirik F. da Silva and Hallvard F. Svendsen Ind. Eng. Chem. Res. 2004, 43, 3413-3418*

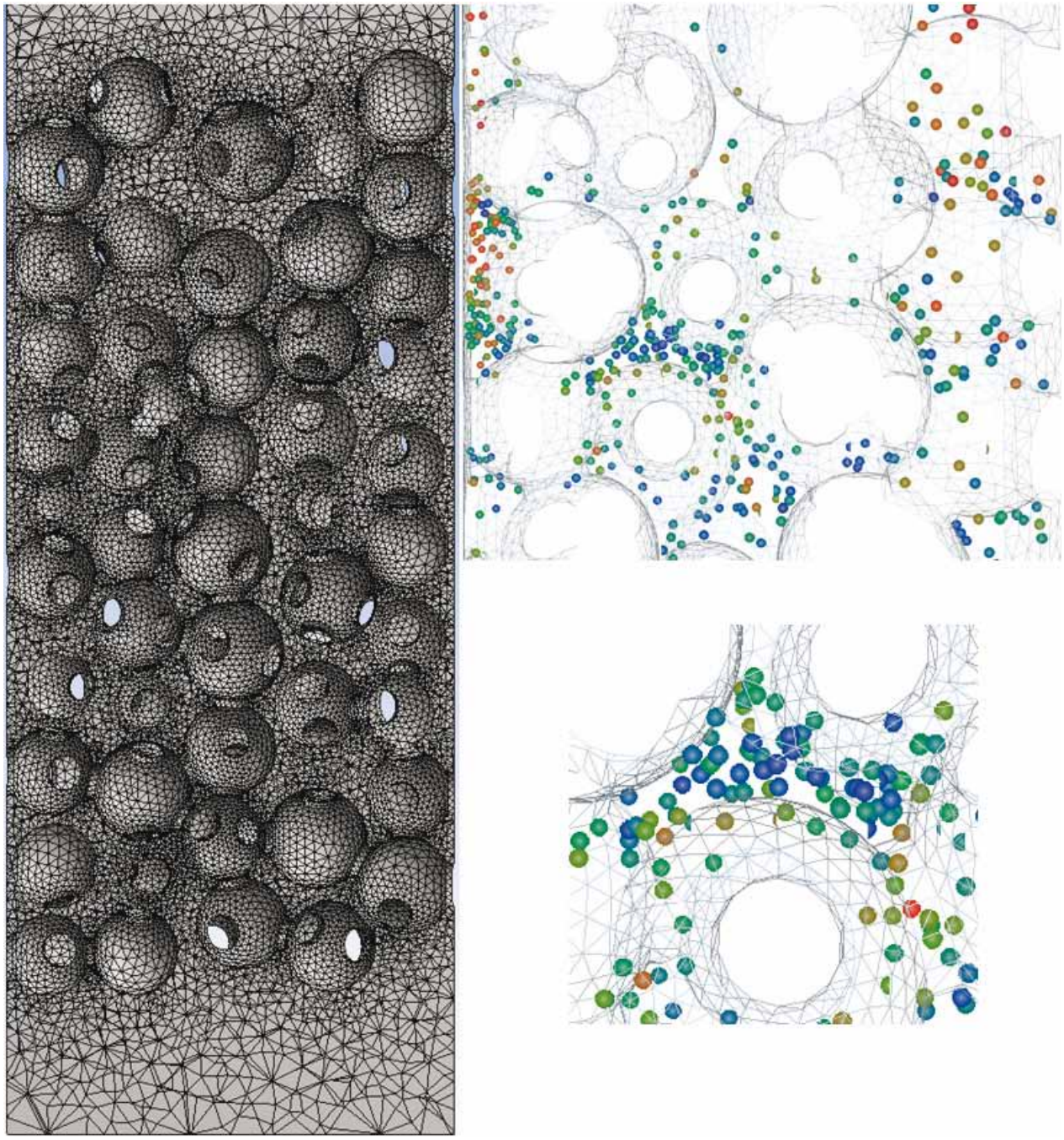


Figure 2: Hierarchical modelling of a packed bed combining continuum based (CFD) and particle based (DEM) methods to study fines migration in gas-solid flows. W. Yang et al. in preparation. Particles are coloured by velocity magnitude (red=1m/s, green 0.5m/s and blue low to zero velocity).

RESEARCH CHALLENGES

As a department we are involved in projects spanning the entire scale from atomistic to plant wide processes. Thus we continuously face challenges that contain a mixture of physical and chemical phenomena that manifest themselves at different scales.

Resolving the relevant scales and physical/chemical phenomena result in a number of computational challenges including: optimization, thermodynamics, chemical reactions and turbulent (multiphase) fluid flow. Thus topics such as homogenization between scales, optimization, ensemble averaging, stiff systems of equations, meshing technology, heterogeneous computing/HPC and software design and maintenance are areas where we see significant research challenges that need to be addressed.

Four strategic goals in the Department are related to CSE:

1. become the leading group in Europe on development of absorbents for CO_2 capture and modelling of post-combustion capture processes.
2. become a preferred international supplier of simulation tools for reactive multiphase transport problems in industry
3. our competence in process modelling and optimization should be considered to be internationally leading
4. our work on particle based methods should build on collaboration with leading international groups and early deployment of new technological advancements and be a driving force behind cross disciplinary collaboration in SINTEF.

CSE RELEVANT ACTIVITIES

The modelling activity in the department can be divided as follows based on the length scale:

Atomistic modelling: Computational chemistry is used to improve the understanding of the chemistry of CO_2 absorption in amine-water systems. Molecular simulation can also be used for predicting the performance of new solvents. Such predictive models are intended to facilitate the screening for new solvents. Other examples include calculations of flow inside carbon nanotubes and transport in membrane materials.

Coarse grained atomistic modelling: Understanding deposition and adsorption of nanoparticles on solid surfaces is of key importance in many processes. In the oil industry understanding how surfactants and demulsifiers influence interface stability and dynamics is the key to understanding water in oil separation. Dissipative particle dynamics is used as tool to study surfactant and demulsifier dynamics in such applications.

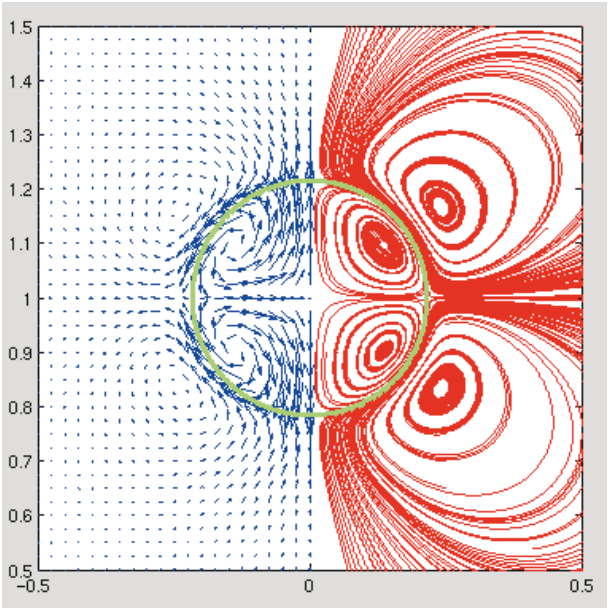


Figure 3: Phase field simulation of deformation and internal circulation in a liquid droplet in an external electric field. Such simulations are used to study coalescence in emulsions, and to investigate the effect of surfactants and demulsifiers on the dynamics of droplets. Y Lin et al. in preparation.

Mesoscale modelling: The microstructure of a fluid (bubbles, droplets and dispersed particles) or solid material (grain structure, distribution of inclusions) influence fluid and material properties (stress-strain response) or heat and mass transfer as well as bulk handling properties. Methods such as phase field, discrete element method, smoothed particle hydrodynamics, and fibre dynamics are used (particle based methods). In addition ODE, PDE and DAE solvers are used to study heat and mass transfer in detail.

Macroscale modelling: The preceding methods are often used to provide input to computational fluid dynamics (CFD) or finite element models (FEM) of unit operations. In addition, CFD models are coupled to thermodynamic models when studying reacting systems or systems including phase transitions.

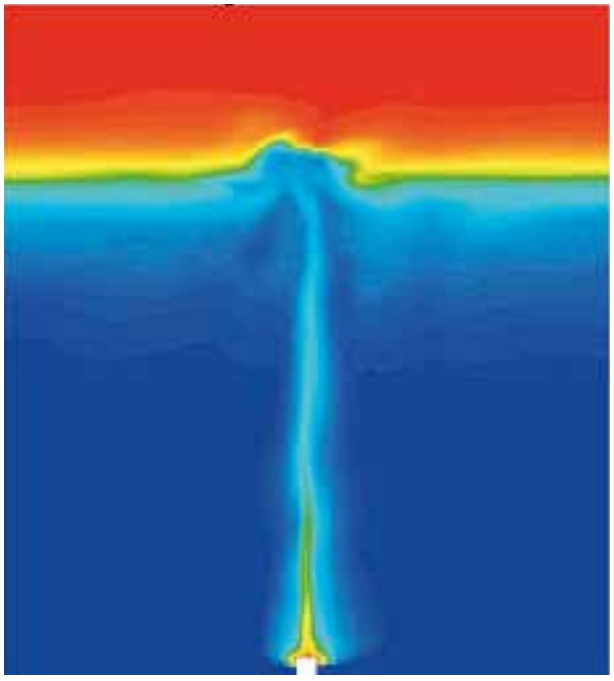


Figure 4: Large eddy simulation of a gas plume in a rectangular vessel. Such simulations build on drag, heat and mass transfer correlations developed using detailed simulations on the relevant scales. P. Skjetne et al. in preparation.

Process/system modelling: At the process level the Department utilizes both commercial software and in-house codes often integrating the two. System optimization coupled with flow sheet simulators are a speciality. Major developments that include hierarchical modelling at several scales include LEDA, CO_2-Sim, SiSIM and Hipersol.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The Department spans a wide range of problems of great importance to both society (e.g. CO_2 capture) and industry (reacting flows with multiphase mass, heat and momentum transfer in reactors and pipelines, as well as system optimization).

Our contributions to a CSE Centre would include unique competence on physical modelling ranging from atomistic to plant scale supported by experimental facilities and/or data for validation. The experience from large software development projects such as LEDA, SiSIM, SOFT, and CO_2-Sim would also be useful contributions.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

The envisioned benefits from a CSE Centre are:

- a meeting place for inspiration and creation of new collaborative multi-disciplinary projects between the participants (KMB/JIP/SFI/SFF).
- education of highly skilled engineers and scientists within practical numerical modelling and software design (MSc/PhD/post graduate).

A basic curriculum should be developed within the Centre so that all students from NTNU will have a world class basis for doing practical numerical modelling. It is increasingly difficult to recruit qualified Norwegian candidates for such jobs in our field, and should be considered a national priority.

SINTEF Materials and Chemistry

Department of Synthesis and Properties

GENERAL OVERVIEW

The main focus within SINTEF's Department of Synthesis and Properties is to develop and improve materials and products with tailored chemical and physical properties by combining fundamental materials research with applied research. Advanced analytical instruments are used often in combination with modelling. The Department has close collaboration with NTNU and the University of Oslo (UiO) and contributes to university education as several employees have a part-time associated professorship at one of the universities. Some of this collaboration is also formalized by the TEM Gemini Centre. The department has 56 employees divided into 5 research groups, serving important customers in the Norwegian and international metallurgical, polymer and oil industries as well as producers of fine chemicals.

RESEARCH CHALLENGES

Our research group Materials Physics has extensive computational modelling activity in numerous fields, some of which are listed below:

- Fundamental understanding of precipitation in Al 6xxx alloys – directly relevant for alloy development within the Al industry and reduced energy consumption during industrial heat treatment.
- Modelling and characterization of interfaces, thin films and defects in solar cell structures – relevant to solar-grade silicon industry as well as the solar cell industry, of vital importance for renewable energy and electricity contributions.
- Microstructure modelling (homogenization, precipitation, recrystallization, work hardening...) in Al alloys – directly relevant for alloy development and processing within the Al industry and reduced energy consumption.
- High temperature corrosion and catalysis – directly relevant for syngas refinement in the oil and gas industry.
- Electronic structure studies with ab initio modelling and electron spectroscopy – directly relevant for the catalysis and PV industry, both areas are of great importance for renewable energy contributions.

In order to contribute to general knowledge and value generation as well as enhance our customers competitiveness, a common long-term ambition and challenge within these areas related to the modelling activity, is to bring in predictive power that is relevant for a large range of applications. In most cases this requires first principle methods in order to correctly catch and describe the determining underlying physical phenomena. However, the very limited time and size scales that can be reached by first principles requires multi-scale modelling with all its challenges of communication between models and correctly understanding the meaning of the different parameters within the different levels.

Our research group Polymer and Composite Materials frequently uses commercial CFD and solid mechanics codes to model moulding processes and the mechanical response of finished products, often in close collaboration with various industrial partners. The group has limited focus on the development of its own specialized code but works with several issues where this is of great interest. The most central unsolved problems here are:

- Reliable 3D prediction of orientation of fillers and fibres in moulding processes. Commercial codes perform this fast and efficiently. However, the models employed are very simple and do not describe several important mechanisms such as fibre – fibre interactions.
- Moulding processes including friction and flow on both micro- and macroscales requiring different constitutive models and different focus on heat transfer. This has been addressed by multi-scale modelling.
- The solid state mechanical response of products made of filled thermoplastics relies on mechanical behaviour on several length scales and the spatial orientation and distribution of fillers. Multi-scale modelling is required to model this beyond the linear elastic region.

CSE RELEVANT ACTIVITIES

The modelling activity within the Department is in several areas:

The activity within atomistic modelling is manifold, including collaboration with IFE for development of band structure calculations of KNO_3; investigations of the interfaces in Si-based thin-film solar cells, combining DFT calculations and thin film processing (see Figure 1); DFT modelling linked to synthesis and the characterization of Pd based membranes for hydrogen separation; collaboration with UiO on the modelling of oxides for fuel cells and collaboration with NTNU on the modelling of early precipitation of metastable hardening phases in Al alloys. The Department is also coordinating the upcoming European Commission project Hipersol, where the contacting and passivating interfaces in commercial Si-based solar cells will be modelled using a multi-scale framework, including density functional theory (DFT) on the atomistic level, via empirical molecular dynamics to finite element modelling (FEM) on the macroscopic level. The project also involves SINTEF's Department of Process Technology, where most of the FEM modelling will be done.

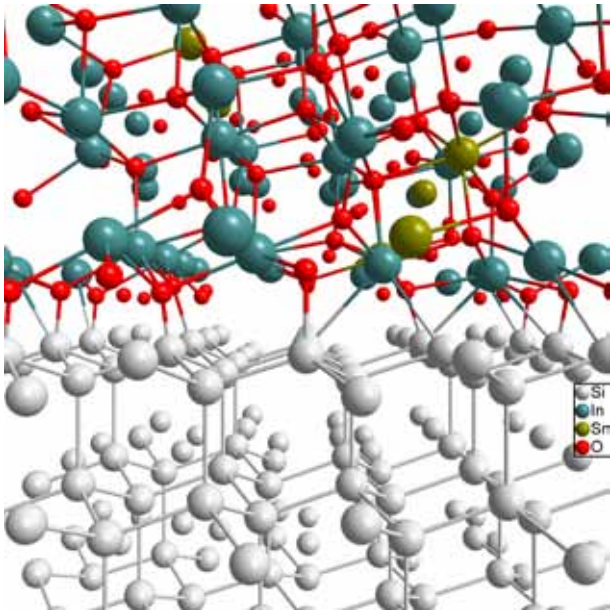


Figure 1: An atomistic model of an interface between Si (grey atoms) and the transparent conducting oxide ITO (indium tin oxide). This is being studied in a SEP on solar cell interfaces.

The activity within microstructure modelling of aluminium alloys is in close collaboration with NTNU and Hydro Aluminium. An important project for driving this activity is the MoReAl KMB, with focus on homogenization, softening and work hardening. Another Al-related modelling activity includes the Hydro's fund project mentioned below as well as thermodynamical and diffusion modelling of paste-based diffusion coating of Al alloys.

The process modelling for polymer and composites is focused on modelling the relationship between production processes, morphology and/or structure formation and end properties, where the material parameters needed in constitutive equations often have to be obtained thorough inverse modelling.

Regarding teaching activities, several MSc and PhD students are supervised by personal from the Department. In addition, Ole Martin Løvvik gives the course Quantum Nano Physics at UiO, where a central part is devoted to density functional theory (DFT) calculations.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The atomistic and microstructure modelling activities in the Department of Synthesis and Properties are usually closely linked with advanced characterization like X-ray photoelectron spectroscopy and high-resolution transmission electron microscopy. This is a crucial part of the modelling effort, since it gives valuable input related to the geometric structure on the atomistic level, as well as electronic structure. Similarly, the calculations give important information about experimental results, in addition to predicting proper-

ties of hypothetical materials. Thus, the combined efforts of atomistic modelling, microstructure modelling and advanced characterization will be a powerful and unique contribution to this Centre.

Another specific contribution to the Centre might be through the competence and tools we are building in the Hydro fund project Next Generation Simulation Tool for a Better Process Description: Through Process Modelling together with the Department of Metallurgy and Applied Mechanics and Corrosion. In this project there is a need for meshing simulated 3D grain structures, so that they can be used as input to grain resolved crystal plasticity finite element modelling. Such a volume mesh-generation tool could also be a valuable contribution to the CSE Centre.

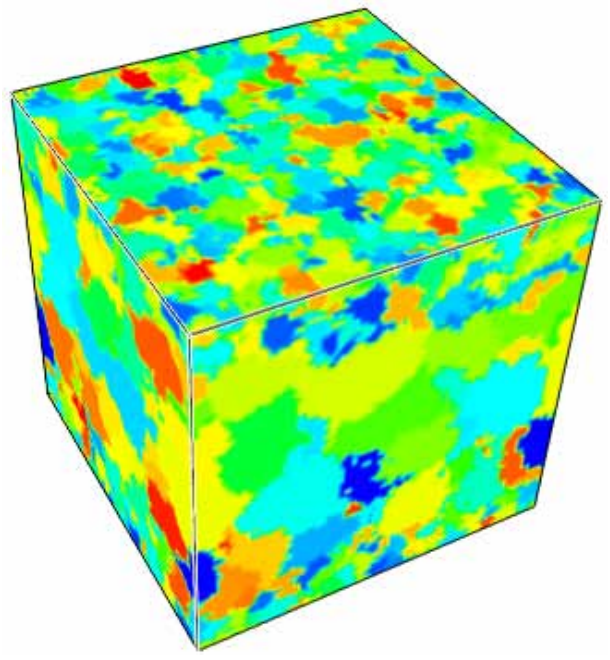


Figure 2: A generated 3D grain structure of Al with small grains at the top and bottom surfaces. Such a structure is difficult to measure experimentally, but is needed as input to crystal plasticity FEM. The meshing of such grain structures is a major challenge in a Hydro's fund project.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

The principal envisioned benefit from a CSE Centre is the creation of new, large collaborative multidisciplinary projects, where we believe we could contribute through our key areas – see above. In addition, we see it as a place to find help for solving specific numerical problems and the development of problem specific flexible codes that do not dependent on commercial (black box) software.

For instance, concerning atomistic modelling, the main tools used in Synthesis and Properties are density functional band-structure calculations, using periodicity to build extended structures (bulk materials, surfaces, interfaces, polymers, etc.). Bringing this together with the complementary modelling activity at Hydrocarbon Process Chemistry, with their primary focus on molecular codes (for molecules and clusters), has proven to give new insight into nanostructured materials. Hence, we are hoping to extend the collaboration between our groups when addressing new, ambitious projects related to nanotechnology.

Another field where collaboration within the CSE Centre could be fruitful is flow modelling of melted polymers with focus on interactions between polymer fluid and solid particles (filler, glass fibres, etc.) and the resulting orientation, segregation and viscoelastic properties of the final polymer. Such simulations can be used in projects in materials and process development.

Finally, collaboration with a future CSE Centre would also be natural when it comes to development of tools for quantitative analysis and data extraction from advanced characterization in materials physics. This includes image processing, spectral analysis and 3D reconstruction from electron tomography.

SINTEF MARINTEK

Department of Offshore Hydrodynamics

GENERAL OVERVIEW

The Department of Offshore Hydrodynamics has long served the offshore oil and ship industry, by means of model testing, theoretical developments and software development.

The Department has the following main areas of expertise:

- Analysis of mooring systems, risers, offshore vehicles and platforms, hydrodynamic analysis and simulation of marine operation
- Model scale testing of mooring systems, risers, offshore vehicles, platforms and marine operation
- Analysis of wave and wave-platform interaction
- Measurement of vehicle and platform loads under wave, wind and current
- Model scale testing and numerical simulation of Dynamical Position Systems

RESEARCH CHALLENGES

As a result of Hurricane Katrina we have noted a significant increase in our markets' demand for analysis and testing loads under extreme environment conditions which are complex, such as effect of viscosity, extremely non-linear waves and wave-current interaction. This demands new analytic tools and new numerical simulation methods.

The joint simulation of high winds and waves in our test facilities is not achievable.

Thus we need to couple model test with numerical simulation in real time. This places exacting requirements on computing performance.

Complex interactions between structure-and water such as hydroelasticity problems demand multidisciplinary approaches such as offshore wind turbines and wave energy converters.

Increasing water depth approaches make it more difficult to simulate mooring systems in the ocean basin laboratory. Developing an active truncating system where the lower part of the mooring system is modelled numerically can increase the accuracy of the model test and can open new markets for MARINTEK.

Figure 1: Experiments for water impact studies

Increasing activity in the Arctic results in challenges to model the ice load of offshore vehicles and platforms.

Access to high performance computing expertise also makes it possible to compute the structural response under water impact loads including wave slamming and tank sloshing, "ringing" and "springing" response of platforms under wave loads.

CSE RELEVANT ACTIVITIES

Present computational research includes a wide range of computational fluid dynamics methods for the study of wave loads under extreme conditions. Both commercial software and tailored software developed in-house are used.

The Department of Offshore Hydrodynamics is part of a group of SINTEF departments which are developing a numerical model based on Smoothed Particle Hydrodynamics method for multiphysical applications.

New numerical software, based on hydrodynamics potential theory is under development, to model wave-current interaction.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The Department has specialist competence in the design and accomplishment of complex model tests such as marine operation with several models of offshore vessel and platform, design and realization of extreme environment specification.

The Department has built a scientific network between European Universities as a participant in the HYDRA III project, supported by the European Commission.

Department staff are engaged in lecturing and supervision to students on topics such as BEM, the modelling of stochastic processes and other probabilistic methods, CFD and wave theory.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

MARINTEK and the Department of Offshore Hydrodynamics in particular have excellent connections with industries that provide us with technical challenges and the funding to solve them.

It would be relevant for the Department of Offshore Hydrodynamics to collaborate with a future CSE Centre as this will enable us to address the research challenges mentioned above.

The Department of Offshore Hydrodynamics already uses heterogeneous computing, but can gain from collaborating with experts on this subject.

SINTEF MARINTEK

Department of Structural Engineering

GENERAL OVERVIEW

The Department of Structural Engineering has long served the offshore oil and ship industry, by means of laboratory testing, theoretical developments and software development.

The Department of Structural Engineering has the following main competence areas:

- Analysis of riser, umbilical and marine power cable systems, global response analysis and local stress analysis
- Full scale mechanical testing of riser pipes, cables and umbilicals
- Fatigue testing of component materials
- Analysis of pipeline installation operations, monitoring
- On-bottom stability of pipelines under wave loads and thermal expansion
- Structural response of platforms and ships under wave loads

Many of the Department's employees have studied at the Institute of Marine Technology (in the same building) and remain in close collaboration with the academic staff, for example on issues including material testing, computation of vortex induced vibrations (VIV) and computation of flexible pipelines and umbilicals. Over the years, the Department has provided co-supervision to a number of MSc and PhD candidates at the Institute. The structural laboratory is run jointly by the Department and the Institute.

RESEARCH CHALLENGES

Heavier numerical models, including increasingly realistic models of umbilicals providing electric and electric power, and information to subsea installations push us from direct solvers on sequential computer architectures towards iterative solvers on heterogeneous architecture.

Merging measurement data into FEM models by a technique known as inverse FEM (to get better insight into laboratory test results or field data) creates large optimization problems. These, and the modeling of friction between the components of flexible risers push us towards the solution of very large non-symmetric problems, and indefinite (saddle point) problems.

Our software SIMLA for the simulation of pipeline installation on uneven seabed has recently been adapted to run in real time on the installation vessel's bridge.

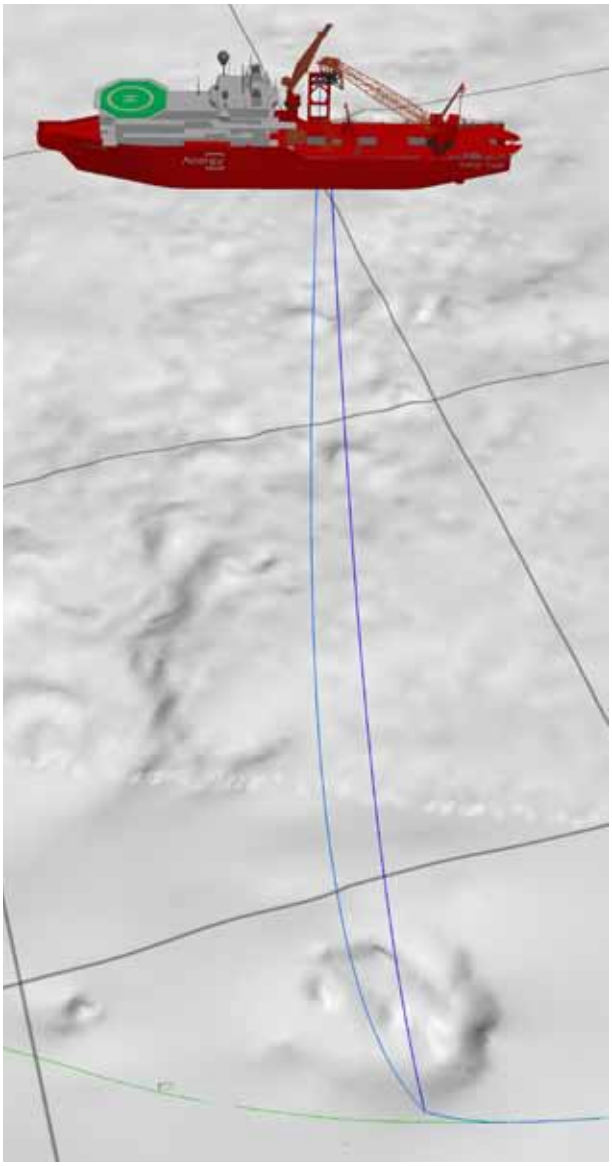


Figure 1: Analysis of pipe laying operations on uneven seabeds with SIMLA

Real-time computing will increasingly become relevant to simulate on-going operations, or to separate tests in a physical and a numerical part.

The "Lifeboat" project, aiming at increasing the safety of lifeboats allowing to evacuate offshore installations highlighted the need for better modeling of "hydroelastic" interaction between structural deformation and fluid behavior. Another problem that requires "multiphysic" solutions is the modeling of the dynamic behavior of offshore wind mills.

Fatigue of metals under oscillating load is a severe problem for all offshore industries. Yet in spite of massive amounts of testing, existing fatigue models for engineering use are very simple. There is no way to predict (without new tests) the fatigue strength of a new alloy, or the effect of corrosive environments, essentially because what happens at the crack tip is not understood. Clearly, a deeper understanding would require simultaneous modeling at the atomic level (dislocation movements and atom diffusion), and larger scales (crack and void coalescence, crack tip deformation and remote stress field).

Access to competence in high performance computing would also open up possibilities for the computation of structural response under water impact loads including wave slamming and tank sloshing, and "ringing" and "springing" response of platforms under wave loads.

CSE RELEVANT ACTIVITIES

All of the challenges described above require high performance computing. The Collaboration with CSE is seen as a way to improve the Department's ability to use high performance computing.

Solving each of the above challenges involves 3 steps

a) The mathematical modelling of physical phenomena
b) The transformation of the above models in a discrete numerical form (FEM, time steps, SPH, Lagrange multipliers etc…)
c) The solution of the above numerical problem on non-homogeneous computer architectures (Newton Raphson, Krylov methods, Gauss Seydel, etc…)

We foresee the possibility to collaborate with CSE on all 3 points, and seek in particular the CSE competence on b) and c).

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

The Department has specialist competence on the modeling of offshore structures, pipelines and umbilicals in particular.

Department employees would be competent to provide lecturing and supervision to students on issues including FEM, modeling of stochastic processes and other probabilistic methods, structural dynamics, inverse FEM and optimisation, with a good ability to connect theory to industrial challenges.

The facilities at the Structural laboratory could be used to validate fatigue models or other material models developed by CSE.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

MARINTEK, and the Department of Structural Engineering in particular, has an excellent connection to industries that provide us with technical challenges and the finances to solve them.

For some of these challenges, it would be relevant for Structural Engineering to get into an alliance with CSE to meet the above mentioned challenges.

Structural Engineering could for example be a user of heterogeneous computing, and require new developments in that field, but would not make such developments itself, as they are outside the department's core business area.

SINTEF Petroleum Research

GENERAL OVERVIEW

SINTEF Petroleum Research (SPR) focuses its research activities on technologies for the exploration and production of petroleum resources. The institute develops solutions for exploration, field development, production and carbon storage. SPR has a clear international profile in its project portfolio, and has offices in Stavanger, Bergen, Trondheim and Houston.

SINTEF Petroleum Research comprises the following departments:

- Seismic and Reservoir Technology
- Production Technology
- Formation Physics
- Wellstream Technology
- Basin Modeling
- Drilling and Well Construction

SINTEF Petroleum Research has the ambition of being one of the most acknowledged contract research institutes worldwide within exploration technology and reservoir characterization, drilling and efficient well construction, and long distance multiphase flow.

In SINTEF Petroleum Research there is a long and successful tradition for combining theoretical models, laboratory measurements, and numeric simulations. In addition models and theories are tested out on full size field cases in close collaboration with oil companies. SPF has throughout the years developed many software tools for the oil and gas sector. Some of these are commercialized, others are tools or support programs for researchers both in the industry and in SINTEF.

With respect to scaling our models cover everything from micrometer pore size to many kilometer reservoirs, and from quick events as fracturing to slow processes developing over geological time.

Both this typical modus operandi and the wide span in space and time fits well with the basic principles of CSE multiscale.

RESEARCH CHALLENGES

Based on the background and strategy of SINTEF Petroleum Research, the research challenges for software development involve several factors:

- Combining existing and new software to larger and more user friendly systems
- Increasing computing speed
- Market launching of some selected software systems
- Finding and developing new numerical methods for solving problems where more traditional numerical tools fail (DEM and SPH are examples)
- Integrating our present knowledge on different length scales into common models and software tools, i.e. multiscaling (from pore to core and reservoirs).

CSE RELEVANT ACTIVITIES

Many of our research activities might be relevant for a multiscale approach, here are some examples.

Research and Development

Multiphase flow in pipelines represent physics on a wide range of scales, e.g. from the thickness of a fluid-fluid interface or the size of a sand grain, up to the dimensions of the pipe itself. Physics-based prediction and analysis of the physical behaviour will require advanced experiments and combining powerful numerical methods (e.g. CFD, DEM and SPH).

Reservoir multiphase flow, including CO2 flow: from pore scale to near-well area to reservoir. Coupling different scales is a challenge that should be addressed in order to enable realistic predictions of reservoir and wellbore flow.

Natural fracture networks and fault systems in the Earth crust are typical structures that exist at several scales. Natural fracture networks largely control hydrocarbon production in carbonate reservoirs. Fault systems control barriers for the reservoir flow and af-

fect stability of production wells and stress dynamics caused by depletion.

Rock fracturing and microseismic activity: Several scales are involved in propagation of induced fractures in rocks and materials. Multiscale approach is required in order to capture e.g. fluid-driven fracture growth and fine details of the fracture front advancement.

Teaching activities:
Teaching and supervision of MSc and PhD candidates on topics mentioned above.

POSSIBLE CONTRIBUTIONS TO A CSE CENTRE

Ongoing activities:

- Validation experiments on multiphase flow and sand transport at SINTEF multiphase flow laboratories located at Tiller.
- Competence on reservoir flow.

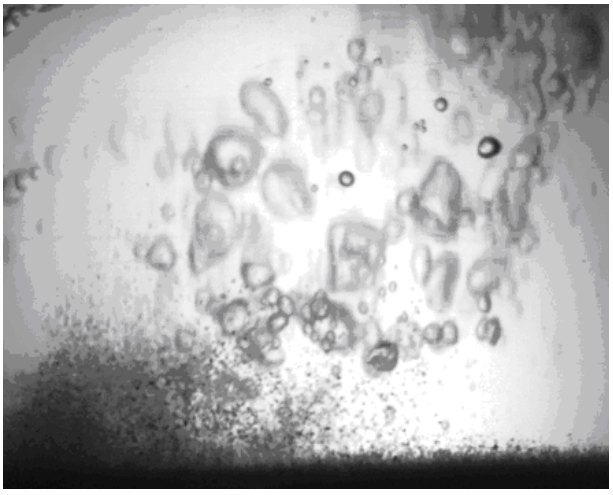


Figure 1: Sand transport in horizontal air-water slug flow showing entrainment of sand in the middle of a slug body. Sand particle diameter was 280 µm. Pipe diameter was 67.2 mm (Reference: experiment be03122 of SINTEF Petroleum Research project 32103200).

- Competence on thermo-hydro-mechanically coupled phenomena in hydrocarbon reservoirs.
- Competence on particle methods and development of particle codes.

Planned activities:
Prediction of well and pipeline sand transport in multiphase flow and/or in the present of a particle bed phase is of interest for the petroleum industry. Recirculation (back-flow) of fluids and particles in inclined wells and wetting effects on particles may greatly affect the transport properties.

Mudloss modeling as applied to drilling problems represents one of the many multiscale challenges in petroleum industry. The use of multiscale methods would enable improved design of drilling fluids and would improve on the environmental impact of drilling.

ENVISIONED COLLABORATION WITH A FUTURE CSE CENTRE

Research topics:
Numerical algorithms for fluid flow modeling and geomechanics.

Heterogeneous computing – implementation of advanced algorithms and simulators on GPU in order to facilitate scenario analysis and history matching in reservoir simulation.

Education:
Joint supervision of master and Ph.D. students by scientists from SINTEF Petroleum Research and NTNU.

ABBREVIATIONS

DEM: Discrete Element Method
SPH: Smoothed Particle Hydrodynamics
CFD: Computational Fluid Dynamics
GPU: Graphics Processing Unit

Norwegian Centre of Excellence

CeSOS
– Centre for Ships and Ocean Structures (a Norwegian Centre of Excellence 2003–2013)

Introduction

The overall aim of CeSOS is to contribute new knowledge for sustainable, economic and safe use of the oceans as a means of transport, and as a source of food, energy, hydrocarbons and minerals. Our research focus will be on generic information that can serve as a basis for the future development of marine technologies, and for industries engaged in similar activities. Engineering research carried out at the Centre is inspired by the technology outlook over a 20-25 years perspective.

VISION

... to establish a world-leading centre for developing fundamental knowledge about the behaviour of ships and ocean structures and chaotic seas, by integrating theoretical and experimental research in marine hydrodynamics, structural mechanics and automatic control.

... to contribute to the international competitiveness of the Norwegian marine industries, as well as to the safety and protection of the marine environment.

Future development of the marine industries and infrastructure requires new structures and facilities, such as high-speed transport, deep-water operations and fish farms in more exposed sites than at present. Challenges in marine technology have hitherto been associated with surface transport, fisheries and the petroleum industry. But aquaculture and the harvesting of natural bio-resources in Norwegian waters are envisaged to increase ten-fold in the next two decades. Shipping and oil and gas operations in harsher environments, including the arctic, are expected to increase, as are demands for renewable energy from ocean wind, wave and current.

A thorough understanding of the behaviour of ships and ocean structures and their operation is required to meet the challenges of new and existing marine industries. The Centre will address the operation and behaviour of surface vessels, platforms and facilities in the ocean environment (Figure 1), by improving present-day technologies and initiating new design concepts and operational procedures.

An important aspect of engineering science is to envisage potential new devices or processes, together with the need to document serviceability and safety. Risk and reliability methodology, taking account of the effect of human factors, are vital in structural design and in planning marine operations.

The aims of CeSOS

The principal objective of the Centre is to gain new fundamental and physical insight into the behaviour of ships and ocean structures, to establish a basis for their design and operation. Our strategy is to integrate three disciplines – hydrodynamics, structural mechanics and automatic control – and to apply theoretical, numerical and experimental methods to those research challenges.

This is achieved by developing:

- Hydrodynamic models to deal with strongly nonlinear free surface-body interaction, considering green water loading, water impact, sloshing in 3D

Figure 1: Selected ships and ocean structures employed in different types of marine technology.

containers, run-up on platform legs, finite amplitude wave-induced motions and structural loads. Attention will also be given to manoeuvring and sea-keeping during marine operations, including interaction between ships.

- Nonlinear controller and observer designs for ships, ocean structures and underwater vehicles based on close integration of control theory, hydrodynamics and structural mechanics.
- Methods for predicting extreme and cyclic effects of hydrodynamic loads on ships, ocean structures, risers and pipelines and positioning systems, considering the stochastic and nonlinear character of the loads and possible hydroelastic effects, taking account of the effect of automatic control and human intervention.
- New methods for quantifying the risk and reliability of facilities and operations in the ocean, considering natural hazards and operational issues.

The focus is on generic knowledge that can serve as a basis for the future development of marine technologies, and for other industries engaged in similar activities.

Project plan

CeSOS research projects improve our understanding of physical phenomena, establish or improve mathematical models, and analyse the behaviour of floating ocean structures, to estimate motions, internal forces and the interaction between a possible automatic control system and human operators, with the ultimate goal of assessing the serviceability and safety of the system. There is no universal method available today for this purpose. With the diversity of structures and associated wave/body phenomena, our strategy is to improve models and gradually obtain more unified approaches.

Currently the research in CeSOS is organised in 24 project themes, reflecting both the main scientific disciplines and the technological applications. Research is organised and managed to ensure an interdisciplinary process, and cross-fertilisation between projects.

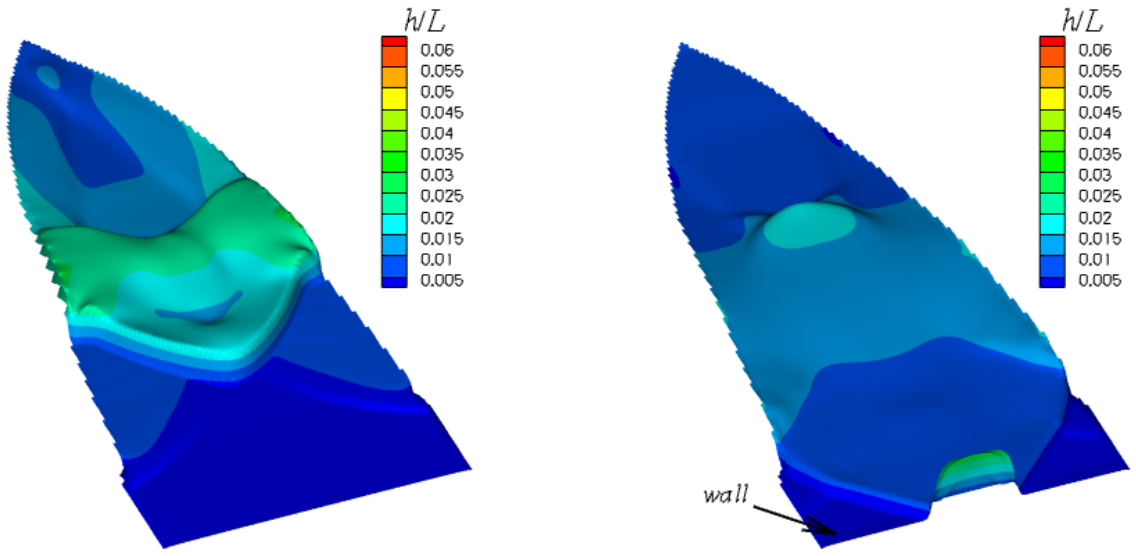


Figure 2: Water-on-deck event: 3D view of the numerical water-level (h) evolution. Time from top to bottom: 0.46T and 0.67T. T=0 after the beginning of water on the deck. Regular incoming waves long λ=2□/k=L and steep kA=0.25. L is the ship length, A and T are the incoming-wave amplitude and period.

This involves engaging highly qualified researchers with relevant competence, using theoretical methods, powerful computers and unique experimental facilities. Access to full-scale data is available through our industrial partners.

Computational mechanics

The ultimate goal of CeSOS is to make numerical predictions of the behaviour of strongly nonlinear phenomena in the time domain, by accounting for the probabilistic nature of the loading and system properties. To reach this goal a hierarchy of methods for determining hydrodynamic and ice loads as well as structural dynamic behaviour, by including the effect of automatic control, are addressed.

Reference: **http://www.cesos.ntnu.no/**

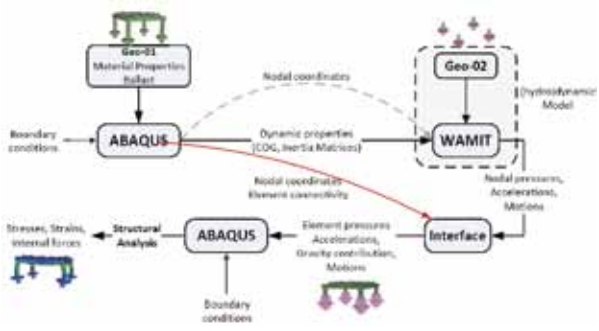


Figure 3: Flow-chart of the ABAQUS-WAMIT-ABAQUS interface

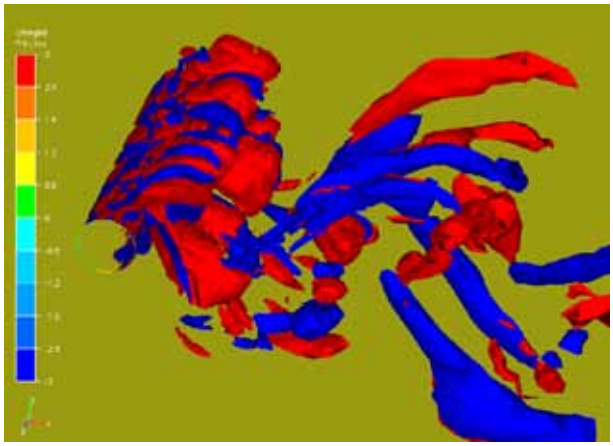


Figure 4: Predicted three-dimensional vorticity structures along the span of a beam

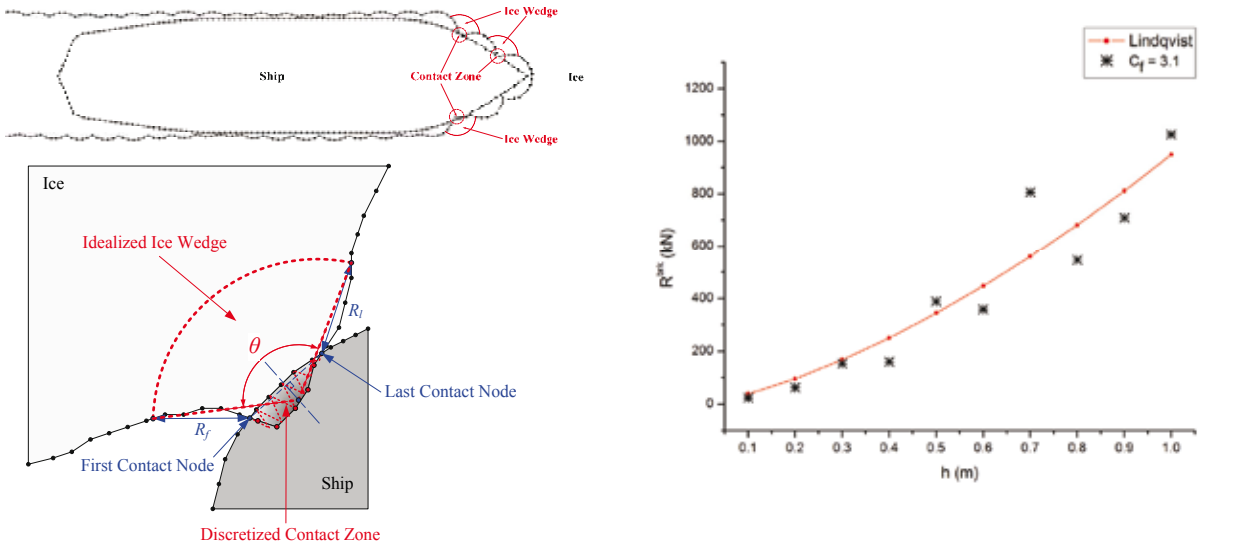


Figure 5: Discretization of ship hull and ice edge as well as comparison of the predicted and measured mean resistance on icebreaker Tor Viking II in level ice.

Norwegian Centre of Excellence

CREATE

Centre for Research-based Innovation in Aquaculture Technology

Introduction

The main objective of CREATE is to combine world-leading companies that supply aquaculture equipment and technology with prominent scientific research institutions into a centre with a common focus to innovate technology, products and solutions specifically to improve the grow-out phase of marine fish culture.

CREATE (Centre for Research-based Innovation in Aquaculture Technology) conducts research to assist in the innovation of technology, products and solutions specifically to improve the grow-out phase of marine fish culture. SINTEF Fiskeri og havbruk AS are the host institution for the centre. The three Norwegian industry partners involved in the centre, AKVA group AS, Egersund Net AS and Erling Haug AS, are all word-leading suppliers of equipment and technology in their respective market segments. Five internationally recognized research institutions are active research partners within the centre: NOFIMA Marin, the Institute of Marine Research (IMR), Centre for Ships and Ocean Structures (Centre of Excellence), the Department of Engineering Cybernetics at the Norwegian University of Science and Technology, and SINTEF Information and Communication Technology. The centre also has research collaborations with the Open Ocean Aquaculture (OOA) Engineering group at the University of New Hampshire, USA (UNH).

RESEARCH AND PROJECTS

CREATE focuses research and development within the following three main research pillars and aims to integrate knowledge between them:

Equipment and constructions

The physical equipment used to farm fish.

Operation and handling

The process of executing and carrying out operations necessary to farm fish.

Farming intelligence

Control of the total process of farming by understanding the integrated use of equipment and the process of operations and combining this with knowledge of biological issues and the physical environment.

Currently seven main projects are running within CREATE and six PhD students and two post-doctoral

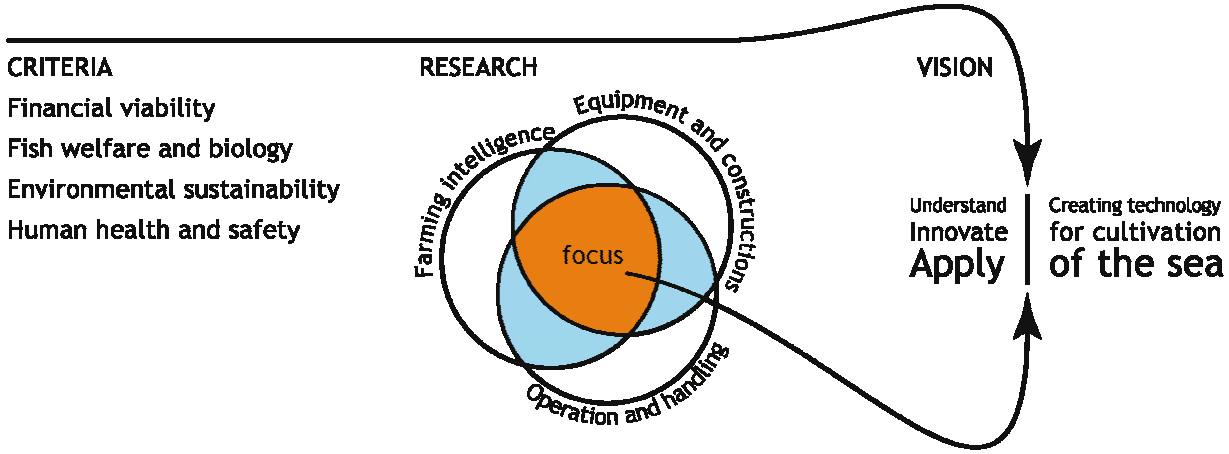


Figure 1: Vision and research pillars for CREATE.

researchers are engaged at the centre. The projects and PhD topics and their relation to the three research pillars of CREATE are shown in Figure 2.

Cage environment

The objective is to develop improved standards for oxygen management in marine net cages to secure fish welfare and efficient production.

Biostatistical analysis

The main objective is to develop a cage-by-cage analytical tool capable, by applying standard and relevant statistical procedures, of identifying main explanatory factors involved in the differential performance of fish populations in cages.

Submergible cage farming and technology

The dual objectives of this project are to: 1) improve the reliability of cage sinking and floating processes by means of process control, automation and remote controlling; and 2) to understand the tolerances of fish in submerged cage culture.

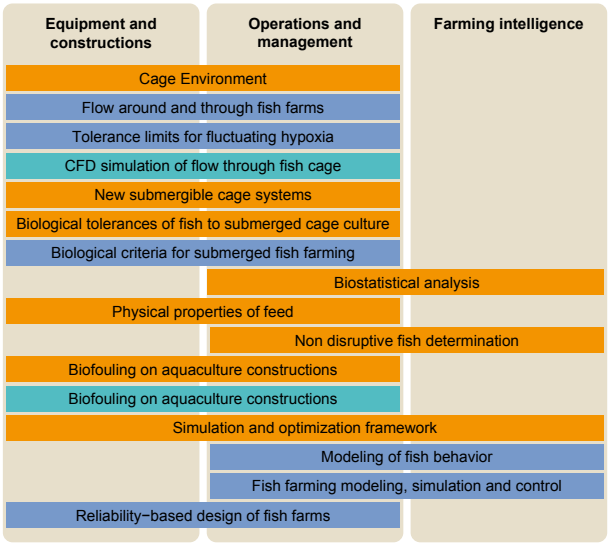


Figure 2: Overview of projects, PhD and post.doc topics and demonstrators within CREATE.

Biofouling on net constructions and solutions for antifouling control

Develop a knowledge-fundament, capacities and solutions on biofouling, biofouling control, biofouling loads and biofouling sensors dedicated to net constructions.

Non disruptive fish weight determination and video surveillance

Assess and demonstrate the feasibility of automatic analysis and estimation of fish weight distribution based on images obtained from the AkvaGroup VICASS system.

Physical properties of feed, hardness and durability

Development of feedback systems to minimize physical damage of feed during transport in feed systems.

SimFrame – CREATE Simulation and Optimization Framework

Development of a framework for simulation, optimization and monitoring of all aspects of modern fish farming.

SIMLab

– Centre for Research-based Innovation at NTNU 2007–2014

Introduction

The Norwegian Research Council has defined SIMLab (Structural Impact Laboratory) at the Department of Structural Engineering in cooperation with the Department of Materials Technology and SINTEF as a Centre for Research-based Innovation (CRI) for the period 2007-2014. The objective of the CRI scheme is to strengthen Norwegian research groups that work in close collaboration with industry in order to support long-term research that promotes innovation and value creation. The present industrial partners in the Centre are Hydro Aluminium, StatoilHydro, SSAB Swedish Steel, Plastal, AUDI, Renault, the Norwegian Public Roads Administration and the Norwegian Defence Estates Agency.

VISION

To establish SIMLab as a world-leading research centre on design of
Crashworthy and Protective Structures

Objective

Within the field of structural impact SIMLab is concentrating on research areas that are of common interest to the industrial partners. Hence, a link is created between Norwegian industry and some of the major actors in the global market, i.e. the automotive industry. In order to meet the requirement for innovation and value creation in an international market, Norwegian industry continuously has to adopt new and original knowledge in product development. Here, *computational mechanics* with an efficient modelling of the whole process chain, through process modelling, is a key requirement for success. The key feature is a strong coupling between materials, product forms, production process and the structural behaviour. In order to meet the future challenges in product development foreseen by the industrial partners, a multidisciplinary approach is needed where researchers from the partners and academia contribute. This is only achievable through activities at a centre with long-term objectives and funding. Thus, the main objective of the Centre is

To provide a technology platform for development of safe and cost effective structures using advances in experimental testing techniques and computational mechanics.

Research areas

The technology platform, see figure, is developed through advances in the following basic research areas:

Materials: Development of identification methods and improved quantitative constitutive models and failure criteria for large-scale analyses as well as identification methods.

Solution techniques: Establishment of accurate and robust solution techniques for the simulation of impact problems.

Structures: Investigation of fundamental response mechanisms of generic components and structures as well as the behaviour and modelling of joints.

This research area 'Structures' is serving as a link between 'Materials', 'Solution techniques' and a Demonstrator activity. The selection of demonstrators is carried out in close cooperation with the industrial partners. The interaction between the activities denoted 'Basic Research' and 'Demonstrators' is crucial with respect to validation and possible refinement of the technology developed at the Centre.

SIMLab is dealing with aluminium extrusions, plates, and castings, high-strength steels and polymers.

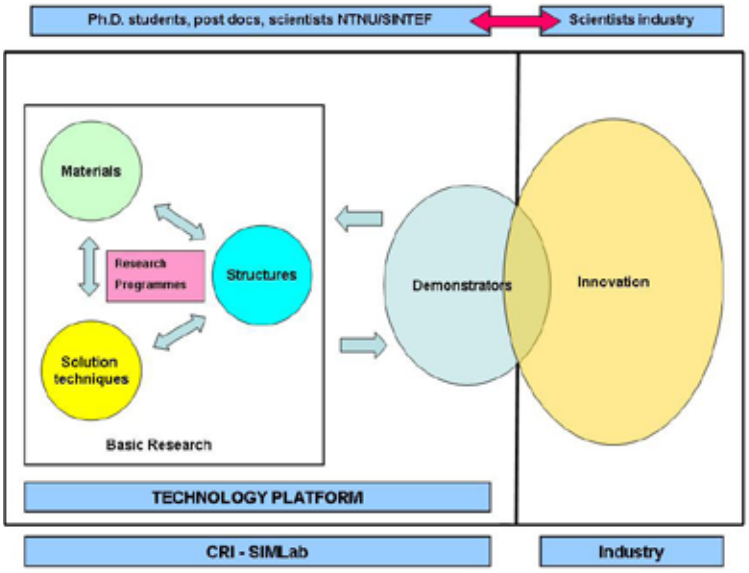


Figure 1: Research areas.

The basic research areas **Materials**, **Solution techniques** and **Structures** are linked by **Research programmes**. The number of research programmes and the content in each programme (research projects) can vary dependent on the interest of the partners. The following research programmes are defined:

Fracture and Crack Propagation (F&CP): Validated models for fracture and crack propagation in ductile materials including rolled and extruded aluminium alloys, high strength steels, cast aluminium and magnesium and polymers will be developed. Formulations for shell structures and solid bodies will be established and implemented in LS-DYNA for verification and validation. Accuracy, robustness and efficiency are the major success criteria for the F&CP models.

Connectors and Joints (C&J): Information about the behaviour and modelling of self piercing rivet connections subjected to static and dynamic loading condi-

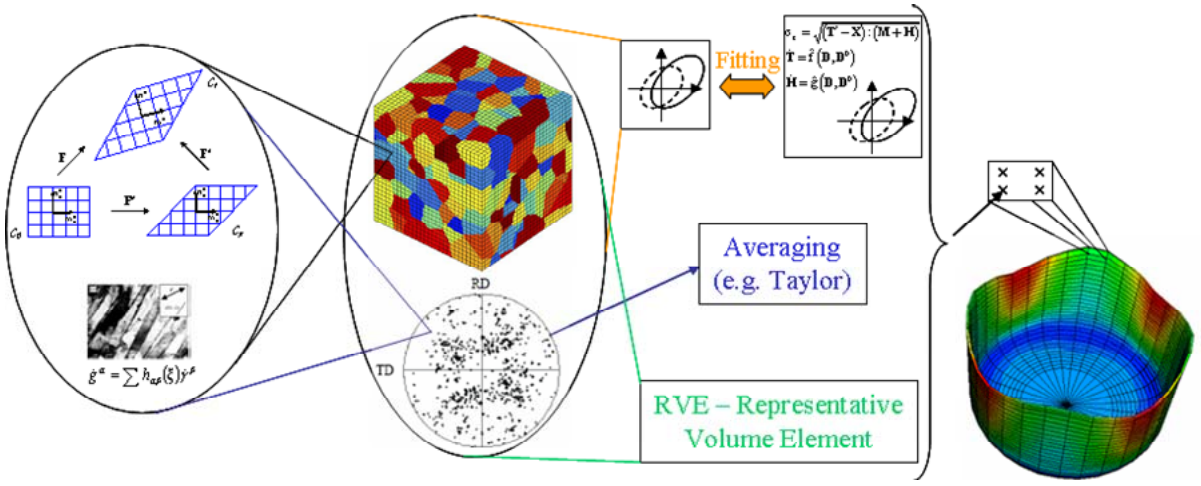


Figure 2: Multiscale approaches.

tions will be obtained. Focus is put on the establishment of a model for large scale shell analyses as well as the behaviour of joints using dissimilar materials.

Polymers (Poly): Validated models for polymers subjected to impact loading conditions will be developed. An important prerequisite is to establish a set of test methods for material characterization and generate an impact test database. The programme is for the time being limited to thermoplastics.

Multi-scale Modelling of Metallic Materials (M4): Phenomenological constitutive models of metals are available in commercial FE codes, but they do not provide any information about the physical mechanisms responsible for the material response. Thus, in this programme the material response is described by the elementary mechanisms governing the macroscopically observed phenomena. This is required for the design of optimized process chains, for the development of next generation phenomenological models, and for reducing material characterization costs.

Optimal Energy Absorption and Protection (OptiPro): A basis for the design of safer, more cost effective and more lightweight protective structures for both civilian and military applications subjected to impact and blast loading will be developed. This also includes road restraint systems as well as submerged pipelines subjected to impact from fishing gear.

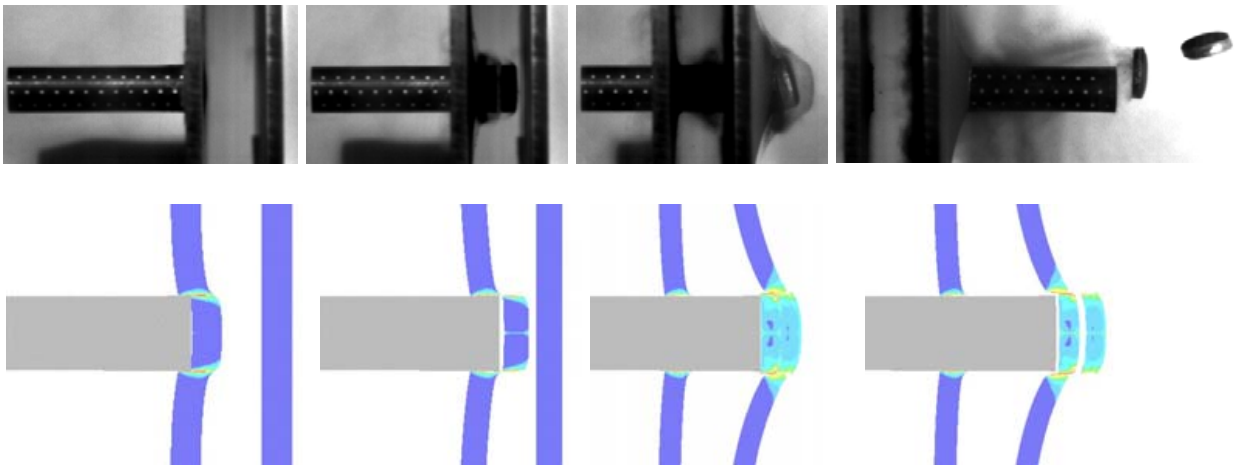


Figure 3: Experimental test versus LS-DYNA simulation of the perforation process of a 2x6 mm thick double-layered steel plate spaced.

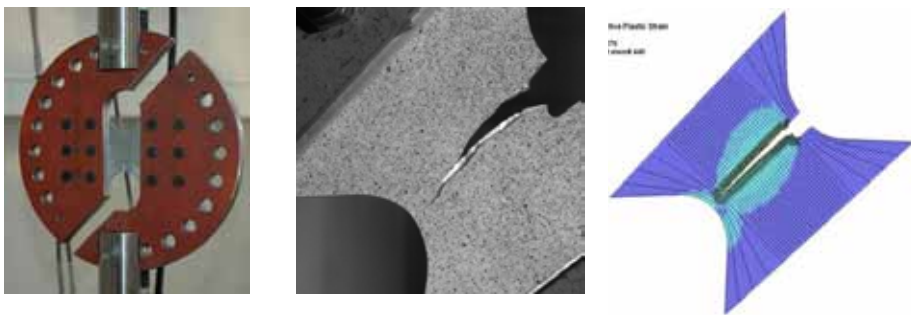


Figure 4: Arcan test set-up in the laboratory (left) and crack propagation in test (middle) and simulation (left) for 45° load angle. Damage-driven adaptivity is used in the simulation.

NTNU – Trondheim
Norwegian University of
Science and Technology

The Norwegian University of Science and Technology (NTNU) in Trondheim represents academic eminence in technology and the natural sciences as well as in other academic disciplines ranging from the social sciences, the arts, medicine, architecture to fine arts. Cross-disciplinary cooperation results in ideas no one else has thought of, and creative solutions that change our daily lives.

SINTEF

SINTEF is the largest independent research organisation in Scandinavia. We create value through knowledge generation, research and innovation, and develop technological solutions that are brought into practical use.

SINTEF is a broadly based, multidisciplinary research concern with international top-level expertise in technology, medicine and the social sciences. Our aim is to become the most renowned research institution in Europe. SINTEF is a non-commercial organisation. The profits of our contract research projects are invested in new research, scientific equipment and competence development.