**Grant Agreement No.:** 604656

**Project acronym:** NanoSim

**Project title:** A Multiscale Simulation-Based Design Platform for Cost-Effective CO₂ Capture Processes using Nano-Structured Materials (NanoSim)

**Funding scheme:** Collaborative Project

**Thematic Priority:** NMP

**THEME:** [NMP.2013.1.4-1] Development of an integrated multi-scale modelling environment for nanomaterials and systems by design

**Starting date of project:** 1st of January, 2014

**Duration:** 48 months

<table>
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<tr>
<th>WP N°</th>
<th>Del. N°</th>
<th>Title</th>
<th>Contributors</th>
<th>Version</th>
<th>Lead beneficiary</th>
<th>Nature</th>
<th>Dissemi n. level</th>
<th>Delivery date from Annex I</th>
<th>Actual delivery date dd/mm/yyyy</th>
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<tr>
<td>9</td>
<td>1</td>
<td>Dissemination Report</td>
<td>Christoph Kloss</td>
<td>0</td>
<td>SINTEF Report</td>
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<td>31/06/2014</td>
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1 Introduction

1.1 About this report
This report consists of the plan for the dissemination of knowledge arising from the NanoSim project, a report of the activities performed in the first 24 months of the project towards the aforementioned purposes as well as a list of planned activities for the future. The NanoSim dissemination plan will be used by consortium members, but also by EC or other third parties, for acquiring a complete picture of the most important activities undertaken or scheduled on the future route to full dissemination of the knowledge. More specifically, the document includes the NanoSim dissemination strategy, describing the means of dissemination both for the software platform to be developed as well as for the other scientific results to be disseminated. It also describes the target audiences and the means for communicating with them. Furthermore, the planned and performed dissemination activities are presented, including events, conferences, scientific journals, the project website, the project fact sheet, press releases, various dissemination materials as well as any liaison activities. This report will be regularly updated to give a cumulative overview of the project’s undertaken and planned activities.

1.2 Objectives of NanoSim
The objective of the NanoSim project is to create an efficient and cost effective multi-scale simulation platform based on free and open-source codes. This platform will connect models spanning a wide range of scales from the atomic scale through the particle and cluster scales, the industrial equipment scale and the full system scale. To support the information flow and data sharing between different simulation packages, the NanoSim project will develop an open and integrated framework for numerical design called Porto to be used and distributed in terms of the GNU Lesser General Public License (LGPL). A core co-simulation platform called COSI (also licensed as LGPL) will be established based on existing CFDEM®coupling (an open source particle and continuum modelling platform). To establish this software tool, the project will develop and improve models to describe the relevant phenomena at each scale, and will then implement them on the next coarser scale. This scientific coupling between scales will be supported by sophisticated software and data management in such a way that the actual model implementation in various software packages will be fully automatic. The resulting open source software platform will be used to facilitate the rational design of second generation gas-particle CO2 capture technologies based on nano-structured materials with a particular focus on Chemical Looping Reforming (CLR). However, the final NanoSim platform will be sufficiently generic for application in a wide range of gas-particle contacting processes. Finally, the NanoSim project will demonstrate the capabilities of this multi-scale software platform to custom design an industrial scale reactor/process in a way that most effectively leverages the superior reactivity and tailored selectivity of any specific nano-structured material. Such efficient process optimization capabilities will maximize the economic benefits of nano-structured materials through process intensification.

2 Dissemination Strategy

2.1 Scientific Dissemination
NanoSim explicitly includes dissemination activities for a scientific and a general audience. The following list gives an overview over scientific publications in the first 24 months of the project
Publications: Contribution to conference (meeting, congress, workshop) proceedings

5. Christoph Kloss (2014) , Open source DEM and CFD-DEM: A variety of applications across industries and fields of science, WCPT7, Beijing, 2014

Publications - Lecture or presentation

4. Open Source CFD-DEM Modelling for Particle-Based Processes, Christoph Goniva*, Bruno Blais † and Christoph Kloss *, CFD 2015 Melbourne
2.2 Workshops

The consortium has decided to hold workshops adjacent to the following major conferences/events/congresses. The three events were carefully selected: The first one has a focus on technical interaction with dedicated scientists. The second one will have a large European-Scale networking impact. The third one will steer towards reaching European industry in the oil&gas, process, and related industries.

- **2015: Minisymposium (organization led by DCS)** in the frame of IV International Conference on Particle-based Methods - PARTICLES 2015, 28 - 30 September, 2015, Barcelona, Spain, organized by CIMNE (Barcelona), with ~400 attendants (http://congress.cimne.com/particles2015). The change to month 22 was approved by the project officer. DCS has advertised the workshop on its web platform cfdem.com which has a high visibility in the particle modelling area. Application for the MS was filed and was accepted by the conference organizers. In Table 1, the program of the workshop, entitled “Multi-Scale Modelling of Reactive Particle-Based Processes” is shown. Presentations by NanoSim Consortium members have been highlighted

  **Benefits for the NanoSim consortium**: CIMNE is one of Europe's leading research organizations in numerical modelling; CIMNE is full partner in the SIMPHONY FP7 project under the same call; the topically related T-MAPPP ITN is holding its consortium meeting adjacent to this conference; the PARTICLES conference is a hub for scientists and engineers in particle-based methods. The audience of the invited symposium was about 100 listeners from different fields. The NanoSim consortium had lots of interesting discussions with modelers and engineers, including colleagues from Univ. Grenoble, JKU Linz, TU Braunschweig, Twente University, Univ. Edinburgh, Univ. Leeds, Univ. Manchester, CIMNE, DEM Solutions, Nestle, John Deere, Procter & Gamble, ArcelorMittal, Johnson Matthey, Astec, and many others. The workshop was also used to connect to the FP7 project (ITN) T-MAPPP (www.t-mappp.eu).

- **2016: Symposium** of CECAM (Centre Européen de Calcul Atomique et Moléculaire).

  **Benefits for the NanoSim consortium**: there will be opportunity to network with FP7 projects under the same call and with the materials modelling community

- **2017: Symposium (organization to be led by SINTEF)** in the frame of 12th International Conference on Computational Fluid Dynamics In the Oil & Gas, Metallurgical and Process Industries, June 2017, to be organized by SINTEF

  **Benefits for the NanoSim consortium**: connection to industrial stake-holders.

2.3 Website and Newsletter

A **user forum and documentation** of selected features to be developed by the NanoSim consortium will be hosted. This webpage will catch the interest of large base of users, and attract partners for future collaboration projects with the consortium members. This is one critical part in the identification of future channels for the exploitation of the project outcomes. The web presence will be also used for hosting online tutorials for self-study (both for the consortium members during the project and for the public after the project has finished). DCS will use its existing www.cfdem.com platform to establish and maintain user forums. Source code (as well as code documentation and test cases) under development will be shared via a secured github account (https://github.com/NanoSim/) between consortium members. The same channel will be used to release code to the public, during and after the project has finished. The github accounts will be maintained by DCS and SINTEF.
Newsletters will be sent out in months 12, 24, 36, and 48 to disseminate the project progress.

The Newsletters (12) was assembled and successfully sent out to a group of ~130 stakeholders across Europe, including heads of laboratories and research institutes, key players in industry, as well as to members of the EMMC (European Materials Modelling Council).

A professional (yet free) newsletter service provider was used to each recipient can unsubscribe if desired. The list of recipients is stored and can be extended over time. An online version of the newsletter can be viewed here:

http://75500.seu1.cleverreach.com/m/6084941/523090-9601c7219d8a7d3672fe90109f3acdb2

Figure 1 shows a snapshot of the newsletter.

2.4 Academic Teaching and Training

DCS:

- As a full partner at the Marie Curie ITN “T-MAPPP”, DCS will considerably contribute to contribute to the training of a network of young PhD researchers in multiphase particulate processes and will disseminate NanoSim results in that frame.
- Christoph Kloss (DCS) was holding a course at JKU Linz entitled “Introduction to Particle Simulation” (https://iss.jku.at/studienhandbuch/30592?id=30592&lang=en) between April and June 2014. An introduction to particle-scale simulation technology is given there. Students elaborate on a project, which is linked to industrial application.
- Christoph Kloss and Christoph Goniva (DCS) are holding also commercial courses for particle-scale modelling of multiphase processes, which are open for external participants. The course is held 3-4 times a year, typically there are 20 participants from 5-6 countries for each course.

TUG:

- Stefan Radl (TUG) was holding the course “669.266-Design of Multiphase Flow Processes” (https://online.tugraz.at/tug_online/lv.detail?cperson_nr=56876&clvnr=176437) is ongoing with 15 participants. An introduction to LIGGGHTS and particle scale models will be provided (screencasts have been / will be prepared)
- A Master Program student (Raphael Pichler) has started and will assist in benchmarking PaScal simulations based on conjugate heat & mass transfer simulations using OpenFOAM.

2.5 Connection to other Projects and Scientific Communities

NanoSim will definitely profit from interaction with related projects and scientific communities. The NanoSim consortium has identified the hereafter mentioned actions as relevant. They are structured into 3 categories:

Connection with related EU level projects:

- 2016 workshop: The workshop in the frame of the 2016 CECAM conference will be an excellent opportunity to meet and connect with projects under the same call.
- T-MAPPP the FP7 Marie Curie ITN: DCS is full partner in this project. The role of the T-MAPPP network (16 partners) is to train a next generation of researchers who can support and
develop the emerging inter- and supra-disciplinary community of Multiscale Analysis (MA) of multi Phase Particulate Processes. The goal is to develop skills to progress the field in both academia and industry, by devising new multiscale technologies, improving existing designs and optimising dry, wet, or multiphase operating conditions. T-MAPPP is recruiting twelve Early Stage Researchers (doctoral training) and three Experienced Researchers (postdoctoral). T-MAPPP will hold its consortium meeting and dissemination events adjacent to the NanoSim workshop in the frame of the PARTICLES 2015 conference.

- EC cluster: EC-cluster workshop in Darmstadt, September 26th 2014. The 5+1 Cluster presented the different interoperability strategies and discussed needs for standardization and a common terminology.

- EC cluster: EC-cluster interoperability workshop in Jyväskylä, Finland, May 28th-29th 2015. The cluster presented applications of multiscale and multiphysics modelling in materials science, organization and storage of data, datastructures for interoperability and integrated modelling platforms. The cluster committed to define a common representation of materials, materials modelling and metadata.

- ECCOMAS Thematic Conference 2015 on CM3: Computational Multi Physics, Multi Scales and Multi Data in Transport Modeling, Simulation and Optimization; May 27–29, 2015, Jyväskylä, Finland (cluster workshop)

- EMMC (European Materials Modelling Council). kick-off meeting on 5th Nov 2014 (DCS represented NanoSim there).
  The EMMC is a networking organization. The EC is listening to the EMMC in terms of how to set up future funding schemes in the field of materials modelling.

Key persons:
Nadja Adamovic (TU Wien, Head of Management Board)
Adham Hashibon (Fraunhofer, Board, EMMC wiki)
Gerhard Goldbeck (Board).

Connection with scientific and open source communities:

- CFDEM®project & Open source community (DCS): As commercial supporter of the CFDEM®project, DCS possesses an open, vivid and widely-recognized and strong dissemination channel to the open source community. Using this channel to disseminate NanoSim results will give the NanoSim deliverables the impact they deserve. It is also worthwhile to mention that there is a strong link between the CFDEM®project community and the Molecular Dynamics (MD) community, since LIGGGHTS® is an offspring of LAMMPS, one of the standard MD engines. Naturally, there is also a very strong link to the OpenFOAM® CFD community, since CFDEM®coupling is based on OpenFOAM® technology.

- Particle Based Modelling Community (PARTICLES2015 workshop): There is now only a very weak link between a particle-based modelling community and the CFD based modelling community. Both communities can give significant inputs to the NanoSim project and as the PARTICLES conference series is one of the worldwide hubs for the particle-based modelling techniques, this is a natural chance to connect.
• CFD community (CFD 2016 workshop): The CFD 2016 conference is expected to be attended by leading engineers and scientists in the field of reactor design and numerical modelling. It will be a unique chance to connect and disseminate NanoSim results in the frame of this conference.

Connection with industrial stakeholders:

CFD Community, Oil & Gas Industry (CFD 2016 workshop). The CFD conference series has a very strong focus on industrial application of numerical methods (CFD) in the Oil & Gas, Metallurgical, Process and related industries. Researchers, scientists, decision makers and other stakeholders do participate in this series of conferences.

2.6 Exploitation

Key NanoSim results that can be subject to exploitation can be structured as follows:

• Software platform: Extension of existing COSI software parts (COSI CFDEMcoupling and LIGGGHTS)
• Software platform: Novel software parts complementing of existing COSI software parts (COSI ParSCale)
• Software platform: Porto connection between the scales
• Nano-materials

Generally, the dissemination can be subdivided into the following categories:

• Universities and other lecturers (TUG, UCL, INPT, Coimbra, DCS) strengthen their teaching and training activities and make use of the educational materials created in the NanoSim project. This process has already started. Especially TUG and DCS improved their teaching and training and incorporated aspects of NanoSim.
• Software developers and consultants (DCS, TUG) use the result to strengthen their business. There was an “Exploitation strategy seminar” by organized and held by Meta Group on 4 December in Amsterdam which focused on this aspect. NanoSim was represented there by DCS, TUG, Andritz, SINTEF, UCL. An excerpt of the preliminary result is shown in Fig. 2.
• Industrial partners use the know-how and the software to develop and market new processing technologies. Andritz (full partner of NanoSim) is intending to use the generated knowledge / software for future reactor design, both for optimization and for exploring new concepts.
Figure 1: 12 Month Newsletter to disseminate the project progress

IS-Multi-Scale Modelling of Reactive Particle-Based Processes
Invited Session organized by Christoph Kloss, Stefan Radl, Christoph Goniva, Thomas Hagelien and Shahriar Amini

Application-driven development of CFD-DEM modelling for particle-based processes
C. Goniva*, B. Blais and C. Kloss
**ParScale** - An open-source library for the simulation of intra particle heat and mass transport processes in coupled simulations
S. Radl, T. Forgber*, A. Aigner and C. Kloss

Design and validation of a robust CFD-DEM model for the investigation of viscous solid-liquid mixing in agitated vessels
B. Blais*, M. Lassaigne, C. Goniva, L. Fradette and F. Bertrand

Application-driven development of Discrete Element Method modelling for reactive particle-based processes
C. Kloss*, S. Radl and C. Goniva

Optimal particle parameters for CLC and CLR processes – predictions by intra-particle transport models and experimental validation
T. Forgber, J.R. Tolchard, A. Zaabout, P.I. Dahl and S. Radl*

DEM particle characterization by artificial neural networks and macroscopic experiments
L. Benvenuti*, C. Kloss and S. Pirker

Numerical simulation of reactive flow in granular media using a LBM approach. Application to the study of biomass torrefaction
S. Martin* and O. Bonnefoy

**Table 1: Programme of the NanoSim consortium workshop at the Particles 2015 conference**
<table>
<thead>
<tr>
<th>KER 1 - Title</th>
<th>COSI (Simulation Platform) extension of existing parts - main developer: DCS short description</th>
<th>COSI (Simulation Platform) new parts / ParScale - main developer: TUG short description</th>
<th>PORTO (Simulation Workflow) main developer: SINTEF short description</th>
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<tr>
<td><strong>Description of the Result</strong></td>
<td>A Computer Aided Engineering (CAE) software that can simulate what happens within particulate material during energy conversion and materials processing, such as combustion, or another type of chemical reaction or heat transfer. Typical materials can e.g. be biomass, coal, pharmaceutical tablets, chemical powder. Simulation software to predict reactive intra-particle transport phenomena (heat, mass) in porous particles. Code, documentation (+training material), example cases (verification). It is a prediction tool, that helps designers and operators of multiphase reactors, or dryers, or granulators (energy, chemical productions, pharma)</td>
<td>Porto is an datacentric interoperability and development platform with a technology stack consisting of a) Formal Metadata Schema b) Scripting shell with an extension framework c) Workflow runner based on an Hierarchical State Machine d) Code Generation facilities e) Lightweight Web-Service capabilities f) Architecture for developing dataformat agnostic applications g) MongoDB backend for data and metadata storage</td>
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<tr>
<td><strong>Innovativeness introduced compared to already existing Products/Services</strong></td>
<td>CAE software that will allow engineers to design processes and products involving particulate materials. It provides unique methodology to adress open industrial challenges. As open source software, the collaboration between partners and quality assurance by a world-wide community of experts is fostered. Linking of the software to existing commercial (closed-source) and open-source simulators is ensuring that the CAE software workflow has the required predictive capability. First open source CFD-DEM offering with customer-driven development, full commerical support, quality control</td>
<td>CAE software that will allow engineers to design processes and products involving particulate materials. It provides unique methodology to adress open industrial challenges. As open source software, the collaboration between partners and quality assurance by a world-wide community of experts is fostered. Linking of the software to existing commercial (closed-source) and open-source simulators is ensuring that the CAE software workflow has the required predictive capability. Current tools are often not fully predictive or robust (e.g., lack certain physics), and existing tools are less flexible and need an expert run. The final product will be more user friendly.</td>
<td>Exchange of Formal Metadata Schemas for use in dataexchange between dataformat-agnostic - instead of relying on external APIs or applications or wrappers.</td>
</tr>
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<td><strong>Unique Selling Point</strong></td>
<td>Low investment (just in-kind costs) costs for customer to test the software Software can be customized (Open source), and can handle different levels of complexity Software is transparent (Open Source) Full customizability &amp; scalability (computational and harnessability), fast time to market, new innovative models (first on the market)</td>
<td>Low investment (just in-kind costs) costs for customer to test the software Software can be customized (Open source), and can handle different levels of complexity Software is transparent (Open Source) Linking to existing established open source CAE eco-system 100% more reliable; 100% more applicable; 100% more support</td>
<td>Enabling technology for multi-scale, multi-physics applications. Potential for bridging data warehouses with domain applications and workflows.</td>
</tr>
<tr>
<td><strong>Product/Service</strong></td>
<td>Difficult to assess.</td>
<td>Academic segment: 200-1000</td>
<td>Porto is framework for software</td>
</tr>
<tr>
<td>Ice Market Size</td>
<td>Probably between 1-10 million USD per year on the long run</td>
<td>research groups</td>
<td>Probably between 1-10 million USD per year on the long run</td>
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<tr>
<td>Market Trends/Public Acceptance</td>
<td>Models in the relevant fields become increasingly complex, and hence modularization of software is key.</td>
<td>Products and their production need to become more efficient (costs), cleaner, safer, and smarter. This necessitates the use of CAE software. Public acceptance is key for industrial users to communicate internally and to customers that the technology is widely established and accepted. Waste market expanding (increase of population, regulations become more restrictive), pharma market growth (?), consulting getting more important due to flexibility reasons. Public acceptance is limited by information and awareness raising for new technologies. Cost of computing is decreasing.</td>
<td>There are several initiatives to standardize platforms of interoperability. Efforts from Porto are currently part of the EU Cluster Multiscale Materials Modelling.</td>
</tr>
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<td>Product/Service Positioning</td>
<td>Mixture of consultancy, research, software access &amp; support (freemium model), and training</td>
<td>Exclusive product (high price), since simulation and modeling market is specific. B2B market for R&amp;D companies and research institutes consulting services Secondary, the product should be made available as a “base” version in the open-source community to open channels for consulting and model improvement (“freemium model”. Third, training and related services</td>
<td>The current strategy is standardizing the formal schema for metadata interchange.</td>
</tr>
<tr>
<td>Legal or normative or ethical requirements (need for authorisation, compliance to standards, norms, etc.)</td>
<td>The product is licensed under GPL, legal boundary conditions for linking to existing simulators have to be obeyed. Software standards and quality assurance need to be in place. Scientific validation needs to be ensured. No ethical hurdles forseen.</td>
<td>Since the product is licensed under LGPL, there are no forseenable legal hurdles for linking to existing simulators. Software standards and quality assurance need to be in place. Scientific validation needs to be ensured.</td>
<td>No ethical hurdles forseen.</td>
</tr>
<tr>
<td>Competitors</td>
<td>There is a large number of competitors, including software houses, universities and consultancy companies. The number of competing consulting companies is steadily increasing.</td>
<td>Other universities, research companies (bioenergy 2020+, SINTEF), software providers, consultants, freelancers.</td>
<td>No direct competitors. Many potential collaborators/influencers.</td>
</tr>
<tr>
<td>Prospects/Customers</td>
<td>(i) industrial partners that use the software tool, (ii) industrial partners/research centers/research groups that use the product via a consulting project, (iii) students/industrial partners that receive training on the software.</td>
<td>(i) industrial partners that use the software tool (plant operators and designers), (ii) industrial partners/research centers/research groups that use the product for their research or via a consulting project, (iii) students/industrial partners that receive training on the software.</td>
<td>Porto is framework for software development tightly connected to research, and is not intended as a standalone product.</td>
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<td>Cost of implementation</td>
<td>Time to market</td>
<td>Foreseen Product/Service Price</td>
<td>Adequateness of Consortium Staff</td>
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<td>The product is already on the market</td>
<td>6 - 18 month depending on size of project</td>
<td>For consulting/support: typical cost around 120 €/hr. A typical training is between 440 and 840 €/participant.</td>
<td>consortium staff developed software product, so fully skilled with respect to the software itself. Academic and industrial partners have experience with training and consulting projects</td>
</tr>
<tr>
<td>The product is already on the market (“base version”), initial invest: ca. 150k; premium version with GUI and support infrastructure: 80k.</td>
<td>For consulting projects: 6 - 18 month depending on size of customer.</td>
<td>For consulting: typical cost between 70 and 100 €/hr. A typical training is between 440 and 840 €/participant. For software access, some support and quality control: &gt;= 10k€</td>
<td>perfect, consortium staff is highly competent to run/use/extend code, consortium would be able to bring the product on the market without help. Academic and industrial partners have experience with training and consulting projects.</td>
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Table 2: Excerpt of preliminary exploitation result of Exploitation Strategy Seminar