



**Grant Agreement No.:** 604656

**Project acronym:** NanoSim

**Project title:** A Multiscale Simulation-Based Design Platform for Cost-Effective CO<sub>2</sub> 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:** 1<sup>st</sup> of January , 2014

**Duration:** 48 months

WP N°	Del. N°	Title	Contributors	Version	Lead beneficiary	Nature	Dissemination level	Delivery date from Annex I	Actual delivery date dd/mm/yyyy
9	1	Dissemination Report	Christoph Kloss Shahriar Amini	0	SINTEF	Report	PU	31/06/2014	31/06/2014

## 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<sup>®</sup> 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 CO<sub>2</sub> 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

1. Forgber, T.; Tolchard, J.; Zaabout, A.; Dahl, P. I.; Radl, S.: Optimal Particle Parameters for CLC and CLR Processes - Predictions by Intra-Particle Transport Models and Experimental Validation. - in: IV International Conference on Particle-based Methods (2015) In Press; 2015
2. Radl, S.; Forgber, T.; Aigner, A.; Kloss, C.: ParScale - an Open-Source Library for the Simulation of Intra-Particle Heat and Mass Transport Processes in Coupled Simulations. - in: IV International Conference on Particle-based Methods. (2015) In Press; 2015
3. CFD-DEM predictions of heat transfer in packed beds using commercial and open source codes, Arpit Singhal, Schalk Cloete, Federico Municchi, Stefan Radl and Shahriar Amini - in: IV International Conference on Particle-based Methods. (2015) In Press; 2015
4. Goniva, C., Pirker, S. & Kloss, C. (2014): Open Source CFD-DEM and DEM Simulation Technology – an application driven development. Talk at the 1st Austrian Partikelforum, Vienna
5. Christoph Kloss (2014) , Open source DEM and CFD-DEM: A variety of applications across industries and fields of science, WCPT7, Beijing, 2014
6. T. Hagelien, S. Radl, C. Kloss, C. Goniva, P.I. Dahl, S. M. Nazir, P.Fede, S. Amini - Porto: A framework for information interchange and multi-scale fluid mechanics simulations, 3rd EUMMC Workshop, Jyväskylä, Finland, 2015
7. S. Mohd Nazir, S. Cloete, S. Amini, O. Bolland (2015): Thermodynamic Analysis of Reforming Processes, 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage (TCCS8), 16-18th June 2015.

### Publications - Lecture or presentation

1. P. Fede, L. Bennani, H. Neau, C. Baudry, J. Lavieville, Z. Hamidouche, E. Masi, O. Simonin. High parallel computing of reactive particulate flows in complex geometries
2. Radl, S.; Municchi, F.; Forgber, T.: Perspectives for Modeling Reactive Particulate Systems using Open-Source Tools. - in: 2nd Austrian Particle Forum. BOKU Vienna am: 15.04.2015
3. Forgber, T.; Radl, S.; Kloss, C. .: Towards resolved intra particle temperature predictions in coupled simulations. - in: PFAU 9.0. Linz am: 03.11.2014
4. Open Source CFD-DEM Modelling for Particle-Based Processes, Christoph Goniva\*, Bruno Blais † and Christoph Kloss \*, CFD 2015 Melbourne
5. Application-Driven Development of CFD-DEM Modelling for Particle-Based Processes (2015) Christoph Goniva\*, Bruno Blais † and Christoph Kloss, Int. Conference on Particle-based Methods, Barcelona 2015
6. Application-Driven Development of Discrete Element Method Modelling for Reactive Particle-Based Processes (2015), Christoph Kloss\*, Stefan Radl † and Christoph Goniva\*, Int. Conference on Particle-based Methods, Barcelona 2015

## 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](http://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](http://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](http://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://ss.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](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 28<sup>th</sup>-29<sup>th</sup> 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<sup>®</sup>project & Open source community(DCS): As commercial supporter of the CFDEM<sup>®</sup>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<sup>®</sup>project community and the Molecular Dynamics (MD) community, since LIGGGHTS<sup>®</sup> is an offspring of LAMMPS, one of the standard MD engines. Naturally, there is also a very strong link to the OpenFOAM<sup>®</sup> CFD community, since CFDEM<sup>®</sup>coupling is based on OpenFOAM<sup>®</sup> 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 stake holders:

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



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## The NanoSim Project

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 develops 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 the existing CFD-DEM and DEM codes LIGGGHTS® and CFDEM®coupling. The resulting open source software platform will be used to facilitate the rational design of second generation gas-particle CO<sub>2</sub> 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.

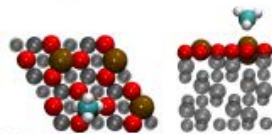
The NanoSim project will demonstrate the capabilities of this multi-scale software platform to custom design an industrial scale reactor/process in a way that most effectively leverages the superior reactivity and tailored selectivity of any specific nano-structured material.

Some snapshots from the first year of research within the NanoSim projects are highlighted below. We wish you a pleasant reading. Feel free to contact us!

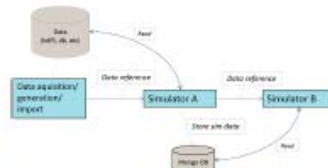


A new open source simulation engine is born: ParScale stands for "Particle Scale Models". ParScale is a new, stand-alone simulation engine, and can predict intra-particle transport processes such as heat or mass transfer and reactions. It will be publicly available in December 2015 via [www.cfdem.com](http://www.cfdem.com) and its [github account](#).

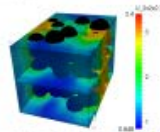
ParScale can currently be coupled to the soft-sphere DEM simulation engine LIGGGHTS®, and a coupling to the CFD-DEM engine CFDEM®coupling will be available soon. This will then allow full handling of reactions in gas-solid systems: For example, the rate of oxidation of porous metal particles suspended by a hot gas stream can be predicted directly by ParScale. ParScale is the last tool that completes the multi-physics co-simulation platform "COSI" within the NanoSim project. COSI is the first open-source simulation platform that is able to perform fully-coupled parallel simulations of reactive fluid-particles systems with sophisticated intra-particle transport models



Atomistic calculations for the design of nano-structured materials: UCL is performing calculations on the reaction mechanisms underlying chemical looping reforming on metal oxide surfaces. Advanced quantum mechanical simulations, using Density Functional Theory to treat atoms explicitly, are being used to understand the binding and dissociation of CH<sub>4</sub> molecules in order to determine the thermodynamics and kinetics of the reaction. In the Figure, the binding geometry of methane to the (0001) surface of haematite iron oxide is shown. Furthermore the change in electronic density, reflecting the formation of chemical bonds, shows that there is a significant charge transfer to the methane. This data is useful for parameterisation and optimisation of materials and multiscale models



Porto is connecting different simulators and scales. The novelty of the Porto framework lies in the offline data-centric code-coupling strategy. Due to the complexity of (correctly, safely and maintainable) sharing data between multiple in-house and commercial tools (proprietary and open) the new approach to the problem is building a database of meta-data that describes the data (and models) in terms of entities and relationships. This meta-data can be used for various things such as validating type correctness (avoid confusion about types, units, dimensions etc), automatic configuration of generic file import/export filters, it can be used for code generation (metaprogramming of classes and structures) and even generation of source code that can be used to extend software such as OpenFOAM, Octave/MatLab and ANSYS Fluent. The Porto framework is made available for download [here](#) with a brief tutorial that teaches the key features of the scripting environment



A new post-processing tool for particle simulations is born: CPPPO stands for "Compilation for Fluid-Particle Data Post Pr-Ocessing", and will be publicly available by December 2015 [here](#). CPPPO is designed as a generic tool for the post-processing - especially filtering - of flow data, as well as heat and concentration data from parallel multiphase CFD simulations. An application is the extraction of velocity and force statistics to characterize two-phase flows. For example, CPPPO is able to compute a filtered (i.e., spatially-averaged) fluid velocity field during a simulation run (i.e., "on the fly"), as well as derive meaningful statistics from this data. An example of a filtered velocity field is shown in Figure 1, in which the filtered fluid velocity from a test case (i.e., flow through an array of particles) is compared with the original fluid velocity.



The consortium: The [NanoSim consortium](#) consists of SINTEF (coordinator), TU Graz, DCS Computing, UC London, NTNU, Andritz, INP Toulouse and University of Coimbra.



The [NanoSim project](#) is running from January 2014 to December 2017. NanoSim is funded from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no. 604656.

Figure 1: 12 Month Newsletter to disseminate the project progress

<p><b>IS-Multi-Scale Modelling of Reactive Particle-Based Processes</b>  Invited Session organized by Christoph Kloss, Stefan Radl, Christoph Goniva, Thomas Hagelien and Shahriar Amini</p>	<p><b>WeE02</b>  Room: VS217  Chair: Christoph Kloss  Co-Chair: Christoph Goniva and Stefan Radl</p>
<p><b>Application-driven development of CFD-DEM modelling for particle-based processes</b>  C. Goniva*, B. Blais and C. Kloss</p>	



**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**

KER 1 - Title	COSI (Simulation Platform) extension of existing parts - main developer: DCS short description	COSI (Simulation Platform) new parts / ParScale - main developer: TUG short description	PORTO (Simulation Workflow) main developer: SINTEF short description
<b>Description of the Result</b>	<p>A Computer Aided Engineering (CAE) software that can simulate what happens with particulate material during transport, storage and flow processes, such as conveying, discharge, heat transfer. Typical materials can e.g. be biomass, coal, pharmaceutical tablets, chemical powder.</p> <p>Simulation software to predict behavior of particles and fluids in multi-phase systems with CFD-DEM technique (resolved and unresolved)</p>	<p>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.</p> <p>Technical details: 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)</p>	<p>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</p>
<b>Innovativeness introduced compared to already existing Products/Services</b>	<p>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.</p> <p>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.</p> <p>First open source CFD-DEM offering with customer-driven development, full commercial support, quality control</p>	<p>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.</p> <p>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.</p> <p>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.</p>	<p>Exchange of Formal Metadata Schemas for use in dataexchange between dataformat-agnostic - instead of relying on external APIs or file formats applications or wrappers.</p>
<b>Unique Selling Point</b>	<p>Low investment (just in-kind costs) costs for customer to test the software</p> <p>Software can be customized (Open source),, and can handle different levels of complexity</p> <p>Software is transparent (Open Source)</p> <p>Full customizability &amp; scalability (computational and harnessability), fast time to market, new innovative models (first on the market)</p>	<p>Low investment (just in-kind costs) costs for customer to test the software</p> <p>Software can be customized (Open source),, and can handle different levels of complexity</p> <p>Software is transparent (Open Source)</p> <p>Linking to existing established open source CAE eco-system</p> <p>100% more reliable; 100% more applicable; 100% more support</p>	<p>Enabling technology for multi-scale, multi- physics applications. Potential for bridging data warehouses with domain applications and workflows.</p>
<b>Product/Service</b>	Difficult to assess.	Academic segment: 200-1000	Porto is framework for software

<b>Market Size</b>	Probably between 1-10 million USD per year on the long run	research groups Industrial segment: 5-100 companies with strong R&D focus in energy, pharma, chemical, life science Comment Andritz: In technology supply: potential of at least 20 companies	development tightly connected to research, and is not intended as a standalone product
<b>Market Trends/Public Acceptance</b>	Models in the relevant fields become increasingly complex, and hence modularization of software is key.	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	There are several initiatives to standardize platforms of interoperability. Efforts from Porto are currently part of the EU Cluster Multiscale Materials Modelling
<b>Product/Service Positioning</b>	Mixture of consultancy, research, software access & support (freemium model), and training	Exclusive product (high price), since simulation and modeling market is specific. B2B market for R&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	The current strategy is standardizing the formal schema for metadata interchange.
<b>Legal or normative or ethical requirements (need for authorisations, compliance to standards, norms, etc.)</b>	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 foreseen	Since the product is licensed under LGPL, there are no foreseeable legal hurdles for linking to existing simulators.  Software standards and quality assurance need to be in place. Scientific validation needs to be ensured  No ethical hurdles foreseen	
<b>Competitors</b>	There is a large number of competitors, including software houses, universities and consultancy companies. The number of competing consulting companies is steadily increasing.	Other universities, research companies (bioenergy 2020+, SINTEF), software providers, consultants, freelancers.	No direct competitors. Many potential collaborators/influencers
<b>Prospects/Customers</b>	(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	(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	Porto is framework for software development tightly connected to research, and is not intended as a standalone product

<b>Cost of implementation - bringing product/service to the "market" (before Exploitation)</b>	The product is already on the market	The product is already on the market ("base version"), initial invest: ca. 150k; premium version with GUI and support infrastructure: 80k	Porto is framework for software development tightly connected to research, and is not intended as a standalone product
<b>Time to market</b>	6 - 18 month depending on size of project	For consulting projects: 6 - 18 month depending on size of customer.	Porto is framework for software development tightly connected to research, and is not intended to be a standalone product
<b>Foreseen Product/Service Price</b>	For consulting/support: typical cost around 120 €/hr. A typical training is between 440 and 840 €/participant.	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: >= 10k€	? Porto is framework for software development tightly connected to research, and is not intended to be a standalone product
<b>Adequateness of Consortium Staff</b>	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	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.	-
<b>External Experts/Partners to be involved</b>		KIT (Prof. Deutschmann) is currently testing the "base" version of the software, maybe partner for GUI development	
<b>Status of IPR: Background (type and partner owner)</b>	IPR is jointly held by DCS Computing, JKU Linz, TU Graz and a large number of other contributors	little background code-wise, there was a FORTRAN code available which was public but not documented at all (partner owner) Copyright for parts of ParScale DCS and JKU Linz	
<b>Status of IPR: Foreground (type and partner owner)</b>	Copyright is held by DCS and TUG. Agreement on future exploitation of IPR is ongoing.	Copyright is held by TUG (majority) and DCS. Agreement on future exploitation of IPR is ongoing.	
<b>Status of IPR: Exploitation Forms (type and partner owner) e.g. direct industrial use, patenting, technology transfer, license agreement, publications, standards, etc.</b>	Trademark: registration partially completed, partially ongoing freemium model established; direct industrial use via consulting; publications	Trademark (planned); some models might be kept as company secret via non-disclosure agreement; direct industrial use via consulting; publications	
<b>Partner/s involved expectations</b>	TUG: increase number of publications; acquire future research projects; acquire future consulting projects. DCS: marketing of results (increasing visibility), acquire future research projects; acquire future consulting projects	TUG: increase number and impact of publications; acquire future research projects; acquire future consulting projects. DCS: include ParScale into COSI platform, foster industrial usage, marketing of results (increasing visibility), acquire future research projects; acquire future consulting projects,	Porto is expected to be an enabler for interoperability and provide support for connectivity workflows
<b>Sources of financing foreseen after the end of the project</b>	public and industrial funding; collaborative agreements	public and industrial funding; collaborative agreements Knowledge transfer and long-term sustainability will need continued funding until market size and penetration is large enough for self-sustainability H2020	The technology is developed as Free and Open Source as is part of a larger portfolio of products and projects with different funding models.

Table 2: Excerpt of preliminary exploitation result of Exploitation Strategy Seminar