



NanoSim



NanoSim - A Multi-scale Simulation-Based Design Platform for Cost-Effective CO₂ Capture Processes using Nano-Structured Materials

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 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**.

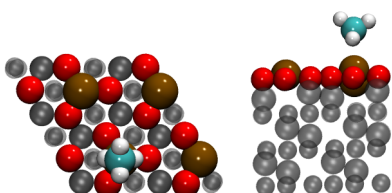
The NanoSim project will demonstrate the capabilities of this multi-scale software platform to custom design an industrial scale reactor/process in a way that most effectively leverages the superior reactivity and tailored selectivity of any specific nano-structured material.

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 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

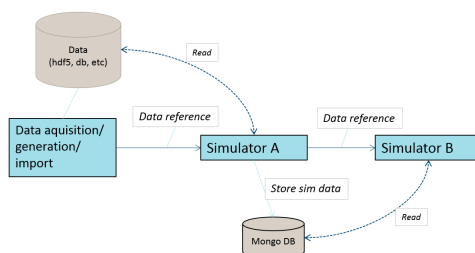


Atomistic calculations for the design of nano-structured materials: UCL is performing calculations on the reaction mechanisms underlying chemical looping reforming on metal oxide surfaces. Advanced quantum mechanical simulations, using Density Functional Theory to treat atoms explicitly, are being used to understand the binding and dissociation of CH₄ 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

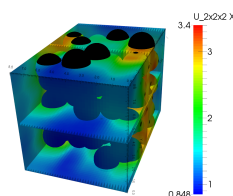
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The consortium: The [NanoSim consortium](#) consists of SINTEF (coordinator), TU Graz, DCS Computing, UC London, NTNU, Andritz, INP Toulouse and University of Coimbra.



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 PrOcessing", 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.



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