PRACE 2.0 for Austria

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Abstract

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Contents

1 Background

[PRACE]

2 Benefits Gained

3 Contributions Required

Potential PRACE 2.0 Projects

A Synthesis of Microscopic Models for the Design of Improved Multiphase Flow Systems

Proposer

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Topic

Understanding the flow behavior of disperse multiphase systems, i.e., fluid or solid particles dispersed in a continuous fluid phase, is of key importance in various scientific disciplines, such as medicine (e.g., blood flow) or chemical engineering (e.g., particle separation or mixing). In addition to flow, often the transport of dissolved species (e.g., oxygen dissolved in our blood), as well as chemical reactions are critical factors that impact the overall system dynamics.

Unfortunately, there are significant gaps in our current understanding of these multiphase flow systems, and questions like:

- *How fast do particles exchange heat and mass with the surrounding fluid?*
- *How should we operate a chemical reactor such that the output of the desired product is a maximum ?* , or
- *How can we separate, or mix, spherical and non-spherical particles in a suspension most efficient?*

still require tedious experimental studies, or excessive computer simulations. Indeed, the above questions have been addressed by many researchers, with the conclusion that a so-called *Multiscale modeling strategy* is the most promising approach. Such a strategy aims on connecting the *micro scale* (i.e., that of individual particles), the *meso scale* (i.e., that of an ensemble of particles), and the *macro scale* (i.e., that of the largest scales, i.e., a chemical reactor). [**VanderHoef2008**, **Deen2004**]. The proposed project focusses on the smallest scales, for which still elementary models are missing, especially for (i) reactive systems, as well as (ii) systems made up by irregular non-spherical particles, and (iii) systems with complex particle-particle interaction forces. Connection of scales will be realized by filtering high-fidelity simulation data, subsequent data analysis, and model synthesis.

Previous Work

Bubble Swarms and Reactive Mass Transfer at Dynamic Interfaces This project (duration 2008-2011, FWF-funded) focussed on the simulation of mass transfer and (bio-)chemical reactions in bubbly flows. The work consisted of (i) model and code development, (ii) application of the models to study various multiphase systems, and to (iii) experimentally confirm selected simulation results [**Radl2007**, **Radl2007a**, **Radl2008**, **Radl2010d**, **Radl2010e**, **Radl2010f**, **Radl2010g**, **Gruber2013**].

Infrastructure Used: ccluster.tugraz.at (cluster with ca. 90 CPUs, hosted by TU Graz).

Code Used: In-house FORTRAN code coupled to PETSC (http://www.mcs.anl.gov/petsc/).

Accelerated Multiphase Flow Predictions This project (duration 2010-2012, FWF-funded) developed a code for the simulations of cohesive gas-particle systems on graphic processing units (GPUs). The work consisted of (i) code development, (ii) development of data filtering routines, and (iii) model development to accelerate multiphase flow predictions using a so-called "filtered" simulation approach. [**Radeke2009**, **Radl2011**, **Radl2012b**, **Sundaresan2013**]

Infrastructure Used: GPU-Workstations and GPU-Servers (hosted by the IPPT and TU Graz)

Codes Used: In-house GPU code *r2d2* (using CUDA programming languange), as well as OpenFOAM (http://www.openfoam.com/).

Comprehensive Investigation of Wet Powder Blending This project (duration 2012-2015, FWF-funded) is currently on the way to simulate liquid transport in flowing granular materials. The work consists of (i) development of a numerical strategy to simulate wet agglomerates, (ii) experimental validation, (iii) apply the methodology to relevant systems, and (iv) couple the numerical strategy to simulations on the next larger scale. [**Radl2010c**, **Siraj2011a**, **Siraj2011b**, **Radl2012a**, **MohanBhageshvar2014**].

Infrastructure Used: dcluster.tugraz.at and icluster.tugraz.at (clusters with in total ca. 2600 CPUs, hosted by TU Graz, sponsored by NAWI Graz)

Codes Used: OpenFOAM (http://www.openfoam.com/), LIGGGHTS and CFDEM (http://www.cfdem.com/).

aiBAT - advanced industrial-scale Bioreactor Analysis Tool This project (duration 2013-2016, FFG-funded) focusses on the development of an improved tool to optimize large-scale reactors for the anti-infectives production. The project connects to previous work that focussed on the development of a Lattice-Boltzmann code to simulate multiphase stirred tank bio-reactors. [**Sungkorn2011**, **Sungkorn2011a**, **Sungkorn2011b**].

Infrastructure Used: dcluster.tugraz.at (a cluster with ca. 1900 CPUs, hosted by TU Graz, sponsored by NAWI Graz) and a local GPU-Servers (hosted by the IPPT and TU Graz)

Codes Used: Latticle-Boltzmann Code (FORTRAN using MPI for parallelization, as well as CUDA GPU code).

FLIPPR - Future Lignin and Pulp Processing Research This project (duration 2013-2017, FFG-funded) is currently ongoing, with a consortium consisting of key players in the Austrian pulp and paper industry, as well as three academic partners (http://www.flippr.at/). The IPPT is focussing on fibre fractionation technology, for which simulations are used to better understand the flow and motion of suspended particles. Specifically, the IPPT (i) is currently developing a fibre model, as well as (ii) is performing simulation of flow in (structured) channels to understand the separation process. The work connects to previous work on flow in micro-channels [**Vigolo2013**, **Vigolo2014**].

Infrastructure Used: dcluster.tugraz.at and icluster.tugraz.at (clusters with in total ca. 2600 CPUs, hosted by TU Graz, sponsored by NAWI Graz)

Codes Used: LIGGGHTS and CFDEM (http://www.cfdem.com/).

NanoSim - A Multi-scale Simulation-Based Design Platform This project (duration 2014-2017, EU FP7-funded) is currently ongoing under the lead of Stiftelsen SINTEF (Norway, http://www.sintef.no/NanoSim/. The IPPT is leading the second-largest Work Package in the project (i.e., Lagrangian Modelling), which aims on developing two new open-source libraries to (i) simulate mass transfer and reactions on a sub-particle scale, as well as to (ii) filter data of high-fidelity simulations on various scales and using various codes. The work connects to previous work at our institute, which focussed on the development of particle-scale models for catalyst preparation, combustion and gas-cleaning processes [**Lekhal2001a**, **Wurzenberger2002**, **Liu2012**], as well as direct numerical simulation of reactive flows and data filtering [**Radl2008**, **Radl2012b**, **Radl2014**].

Infrastructure Used: dcluster.tugraz.at and icluster.tugraz.at (clusters with in total ca. 2600 CPUs, hosted by TU Graz, sponsored by NAWI Graz)

Codes Used: LIGGGHTS and CFDEM (http://www.cfdem.com/), as well as the in-house developments *PaScal* and *C3PO*.

Planned PRACE Activites and Infrastructure Access

The IPPT is planning to contribute to PRACE 2.0 by writing proposals for preparatory access within (A) the ongoing NanoSim project, as well as (B) a possible follow-up project focussing on three-phase flow systems.

(A) NanoSim - Probing the Scalability of COSI The newly development libraries *PaScal*, as well as *C3PO* will be integrated into the first fully open-source co-simulation platform *COSI*, which bill be based on CFDEM http://www.cfdem.com/ to simulate reactive fluid-particle systems. Preparatory access to PRACE would enable benchmarking of *COSI* beyond the current resources available at TU Graz or VSC. Specifically, we would like to assess the scalability of the platform that performs a coupled integration

at three length and time scales: (i) integration of the Navier-Stokes equations to model fluid flow, (ii) solution of Newton's equation of motion to describe particle motion, as well as (iii) solution of heat and mass particles of reacting porous particles. Clearly, these simulations are extremely demanding, and an optimal (i) domain decomposition, as well as (ii) parallelization of the individual integrators for each sub problem is key. Despite individual parts of COSI have demonstrated excellent scalability on PRACE Tier-0 systems (see the recently published OpenFOAM [**Culpo**] benchmark), or other HPC systems (e.g., see http://lammps.sandia.gov/bench.html), the coupling of individual components of COSI is still a bottleneck, and is currently untested beyond 128 CPUs. We are planning to run COSI on up to ca. 5k cores to identify bottlenecks in message passing, as well as to fine-tune the domain-decomposition and parallelization strategy used in COSI. Also, the performance of data filtering operations across multiple CPUs to be developed needs to be assessed. Finally, the computationally costly modelling of certain particle properties (e.g., non-sphericity, or cohesive forces) will be attempted. Acceptable scalability of COSI would enable studies of reactive particulate systems with a meaningful size, such that models on the next level (characterized by larger length and time scales) can be developed. Currently model development is clearly limited to unreactive systems and several model assumptions, that might be unrealistic in some situations (e.g., in case heat conduction within individual particles is limiting, or cohesive particle-particle interaction forces exist). PRACE 2.0 could help in removing some of these model assumptions, and lead to a break-through in the modelling of realistic reactive particulate systems involving non-spherical, cohesive, or porous particles that undergo fast chemical reactions.

Infrastructure Required: Preparatory access to a PRACE system to allow parallel computation on up to 5k CPUs. In case scalability is demonstrated, a follow-up request for project access will be prepared.

(B) Three-Phase Simulations of Gas-Particle-Solid Systems Our previous projects clearly identified that effects of (i) suspended particles in bubbly flows [**Raffensberger2010**], as well as (ii) liquid droplets in a gas-particle suspension are extremely hard to model [**MohanBhageshvar2014**]. Consequently, often an over-simplified simulation approach to study these three-phase systems must be chosen. Within the ongoing project "Comprehensive Investigation of Wet Powder Blending", we have already developed the basic methodology to directly simulate three-phase systems. Unfortunately, these direct simulations are limited to a few particles, which is clearly too small to derive closures for certain phenomena that required tracking of (at least) a few thousand particles. Within this future project we will run the developed code on a larger cluster to assess scalability, as well as push the limit on the maximal system size that can be simulated in order to gather meaningful data on, e.g., clustering phenomena observed in wet granular flows, or attachment of suspended particles to gas bubbles.

Infrastructure Required: Preparatory access to a PRACE system to allow parallel computation on up to 5k CPUs. In case scalability is demonstrated, a follow-up request for project access will be prepared.