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Project acronym: NanoSim

Project title: A Multiscale Simulation-Based Design Platform for Cost-Effective CO_2 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

Document ID: NanoSim-WP4-D4.1_Delivery_ParScaleCPPPOLibrary

WP N°	Del. N°	Title	Contributors	Version	Lead beneficiary	Nature	Dissemin. level	Delivery date from Annex I	Actual delivery date dd/mm/yyyy
1	D4.1	Libraries “ParScale” and “CPPPO” (including documentation and standard reaction parameters)	Author: Stefan Radl, Thomas Forgber, Federico Municchi Checked by: Christoph Kloss (DCS)	1	TUG	Other	PU	31/12/2014	31/12/2014

1 Introduction

This document summarizes the developments (i.e., code, documentation, test cases, standard parameters) for

(i) software tools that aim on simulating intra-particle reactive transport processes (name of the core library: "ParScale"), as well as

(ii) software tools that aim on filtering data from detailed CFD simulations (name of the core library: "CPPPO")

1.1 Document identification

Document Identification	**PARSCALECPPPO-LIB (ParScale and CPPPO Libraries)**
Author(s)	Stefan Radl, Thomas Forgber, Federico Municchi
Reviewers	DCS
Manager	Stefan Radl (TUG)
Version of the Product	0.1
Version of "ParScale"	1.0.1
Version of "CPPPO"	1.0.1

1.2 Scope

New simulation and data analysis tools that complete the multi-scale simulation platform are a critical part of the NanoSim project. Specifically, two tools have been identified pre-NanoSim that need to be developed in order to guarantee the success of the project

- a generic simulation tool that is able to model reactive transport processes within a porous particle and that is coupled to CFD-DEM simulators. This tool should be called »ParScale«
- a filtering tool that is able to process large amounts of data from detail CFD simulations on the fly. This tool should be called »CPPPO«

As specified in Tasks 4.1 and 4.3 of the DOW, these tools have been designed, implemented, documented and tested within the NanoSim project. These tools are fully integrated with the existing tool "CFDEMcoupling" to form the open-source co-simulation platform "COSI". Both tools are designed to interact with NanoSim's scale-bridging tool "Porto".

1.3 References

Acronym	Name
CPPPO	Compilation of Fluid-Particle Post Processing routines
DOW	Description of Work (Work Package 4)
EUC	External Use Cases (GitHub: https://github.com/NanoSim/Porto/blob/master/doc/specification/umlExternalCode/)
OPH-PRIV	Online Project Hosting – Private (available to the consortium only)
OPH-PU	Online Project Hosting – Public (https://github.com/CFDEMproject/ParScale-PUBLIC for ParScale and https://github.com/CFDEMproject/CFDEMcoupling-PUBLIC for CPPPO)
ParScale	Compilation of Particle Scale Models
TGA	Thermo-gravimetric analysis

1.4 System Overview

The tools “ParScale” and “CPPPO” are embedded into the NanoSim project as shown in Figure 1. As can be seen, there exist connections to kinetic data investigated in WP3, experimental data investigated in WP7, as well as WP5 (i.e., Euler-Euler simulations focusing on picturing clustering effects). Within WP4, as well as for the interfaces WPs, the tool “Porto” will be used to convey information for offline linking of different simulation tools.

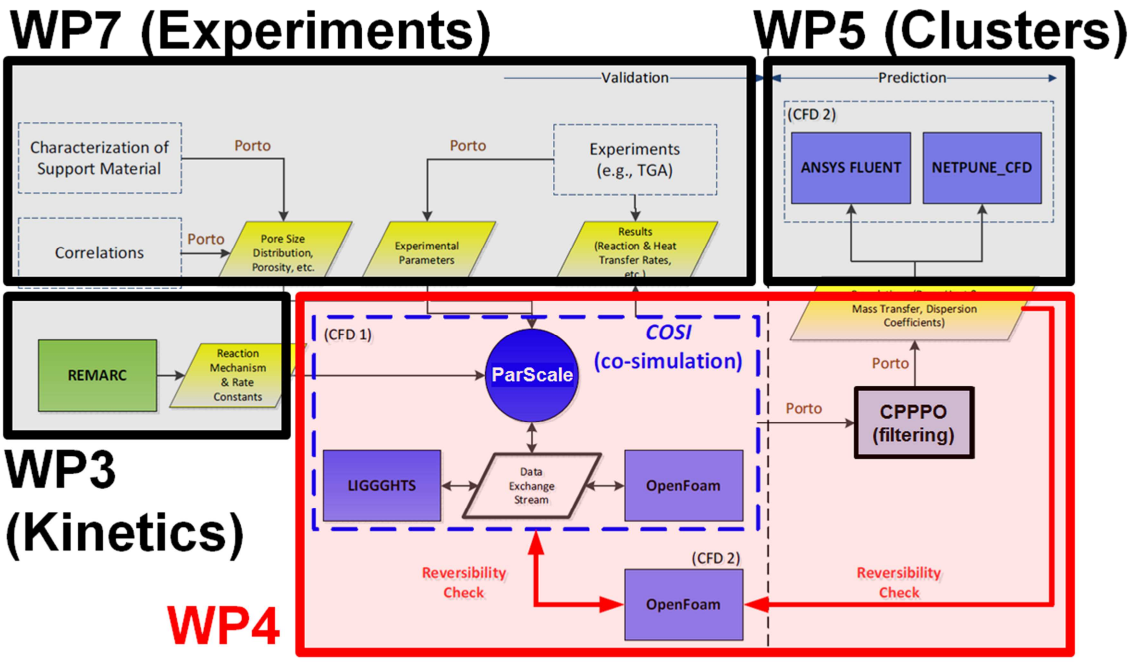

Figure 1. Overview of work packages interfacing with the tools “ParScale” and “CPPPO” developed in WP 4.

1.5 Key Features of ParScale and CPPPO

Key features of the software tools have been identified based on Use Cases, which are hosted on the EUC of NanoSim. An overview of relevant Use Cases is given in Table 1 and Table 2 (for the specifications of the variables, e.g., PASCAL_EXAMPLE_DIR, see the ‘README.md’ file in OPH-PU). Example cases illustrating these Use Cases are hosted on OPH-PU. Additional Use Cases, not designed for public release, are hosted on OPH-PRIV prior to their public release. It is planned to make more Use Cases available to the public and the consortium via OPH-PU and OPH-PRIV step-by-step during the project.

Use Case	Key Feature	Example
1 - Simulate Thermogravimetric Analysis (TGA) Experiment	Temperature and concentration distribution in a porous particle	$(PASCAL_EXAMPLE_DIR)/ testCases/ continuumSolidReactNonIsoThermal and $(PASCAL_EXAMPLE_DIR)/ testCases/ shrinkingCore
2 - Graphic Visualization of Particle Properties	Graphic visualization of particle properties in a coupled simulation	$(LIGGGHTS_EXAMPLE_DIR)/ heatTransferBed_paScal
3 - Interface with CHEMKIN-II data format, in order to interface with REMARK	Load thermophysical data and report to screen	$(PASCAL_EXAMPLE_DIR)/ testCases/ chemistryReader
4 - Prediction of the temperature distribution within particles	Analyze temperature distribution within particles for changing environmental conditions (e.g., in a TGA experiment)	$(PASCAL_EXAMPLE_DIR)/verificationCases/ heatConductionTransientBC
5 - Review of Intra-Particle Model Details	Users can understand the underlying model equations, model parameters, and the spatial discretization using within ParScale	$(PASCAL_SRC_DIR)/doc/ pdf

Table 1. Overview of Use Cases and Key Features of ParScale.

Use Case	Key Feature	Example
1 - Use the ParScale and CPPPO library in an ANSYS Fluent and NEPTUNE_CFD simulation	CPPPO capabilities with any simulator capable of csv data output	$(C3PO_ EXAMPLE _DIR)/ csvTest/
2 - Perform a CFDEM simulation of a Fixed Bed	Online filtering, sampling and binning operations on Eulerian and Lagrangian fields	$(C3PO_ EXAMPLE _DIR)/ cfdemSolverIBScalar_c3po/cfdemIBPeriodicCubicalBoxScalar/; and $(C3PO_ EXAMPLE _DIR)/ filterTest

Table 2. Overview of Use Cases and Key Features of CPPPO.

1.6 Organization and Responsibilities

TUG was responsible for implementation, testing, and analysis work, while DCS contributed with respect to the code architecture.

1.7 Software Development Workflow

The following workflow was followed during the development process:

- Definition of Functional Requirements based on Use Cases.
- Definition of Interfaces to COSI.
- Documentation of the theoretical framework.
- Implementation of the libraries, as well as standalone applications in order fulfill requirements as specified in the DOW.
- Unit testing of libraries and standalone applications.
- Setup of Use Cases, including analytical solutions, in order to benchmark »ParScal« and »CPPPO«.
- Test runs involving individual Use Cases
- Establishment of user documentation

Note, that the integration into the test harness (to be done in WP2) is planned to be completed by the end of Month 14 (i.e., February 2015).

2 Details of the "ParScale" Library

The particle scale simulation tool "ParScale" was implemented with interface capabilities to LIGGGHTS, and OpenFOAM, as well as to the reaction modelling tool REMARC. The latter is done via the CHEMKIN-II file format and a suitable parser. An interface to NEPTUNE_CFD and FLUENT was not explicitly implemented, since it was not specified as a Use Case at the beginning of the project. However, coupling to NEPTUNE_CFD and FLUENT can be realized with a CSV data interface that will be available in the LIGGGHTS simulator soon. ParScale can run in stand-alone mode to enable efficient testing and offline usage (e.g., to simulate temperatures profiles within a single particle in a TGA experiment). ParScale is equipped with general particle-scale models (i.e., "ModelEqn1DSpherical" and "ModelEqnShrinkingCore") that can be used to study complex networks of heterogeneous reactions (currently, the multi-reaction scheme is only available in OPH-PRIV, while a single-reaction scheme is available publicly). For example, particle-scale models can be used to study complex reaction-diffusion problems, as well as drying or devolatilization processes.

More details, including a comprehensive documentation of the library, as well as background information related to ParScale can be found in the README.md file, as well as in the release notes in OPH-PU.

2.1 Examples – ParScale

An overview of ParScale's standalone examples is provided in Table 1. A typical example of a ParScale simulation output (from Use Case #1 from Table 1) is shown in Figure 2, demonstrating the simulation of a heterogeneous non-isothermal reaction within a particle.

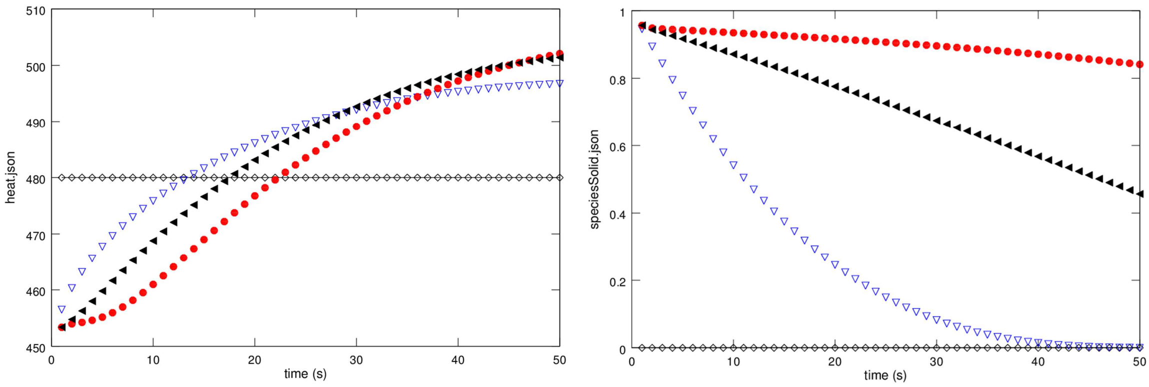

Figure 2. Typical simulation result of ParScale using a continuum particle model with a grain sub-model to picture oxidation of a solid particle (left panel: time evolution of the temperature at different locations of a particle; right panel: solid species concentration at different locations; black diamonds: ambient fluid, blue triangles: particle surface, black triangles: mid between surface and center, red dots: particle center).

Note, that ParScale is fully integrated with LIGGGHTS, i.e., the user can run coupled simulations of particle flow and intra-particle transport processes as demonstrated in ParScale Use Case #2 (see Table 1).

3 Details of the “CPPPO” Library

The filtering tool “CPPPO” was implemented with interface capabilities to LIGGGHTS, and OpenFOAM, as well as to the offline coupling software “Porto”. Specifically, CPPPO is part of the “CFDEMcoupling-NanoSim” package available via OPH-PU. An interface to NEPTUNE_CFD and FLUENT is available via a CSV data reader.

CPPPO is a library, which is split into (i) a “core” module that contains the logic for the filtering operations, as well as (ii) interface modules that can be compiled as a library, and subsequently called by existing simulators (e.g., within the COSI platform). In order to demonstrate the usage of these interface libraries, CPPPO also contains several sample applications.

CPPPO core can be run in stand-alone mode for testing, however, its main use is as part of the interface modules. CPPPO is equipped with generic filtering, sampling, and binning functionality, which is are called “operations” within CPPPO. Most important, all operations are designed to be run in parallel. These features make it easy for user to (i) analyze simulation data without coding new routines, as well as (ii) access a new level of data analysis and fidelity by filtering large simulations runs on the fly.

More details, including a comprehensive documentation of the library, as well as some background information related to CPPPO can be found in the README.md file, as well as in the release notes in OPH-PU.

3.1 Examples – CPPPO

An application of CPPPO 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, as well as derive meaningful statistics from this data via the sampling and binning applications available in CPPPO core. An example of a filtered velocity field is shown in Figure 3, 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.

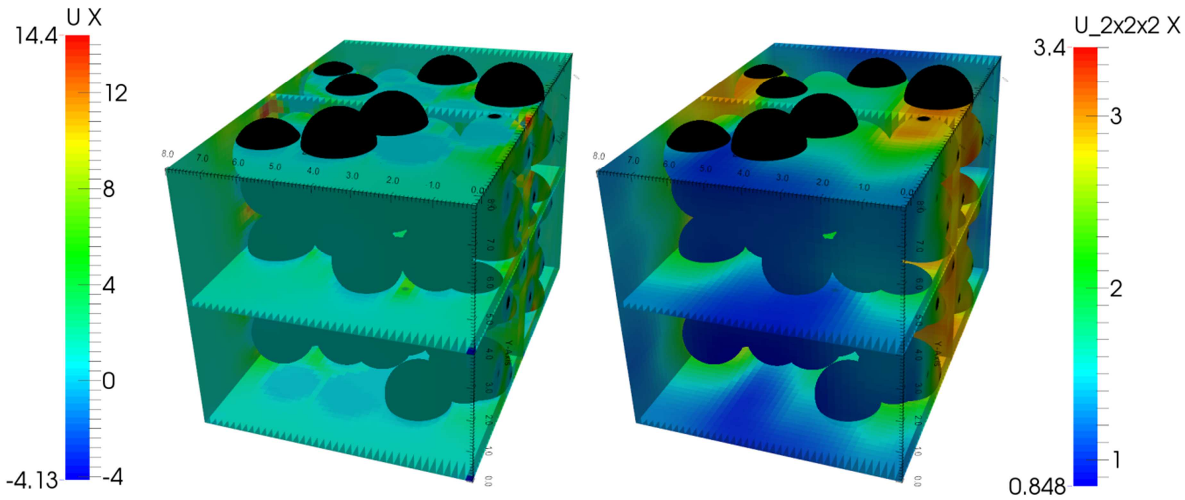

Figure 3. Streamwise (i.e., x-) component of the original (unfiltered) velocity field (left panel), as well as the filtered velocity field (right panel; a filter size equal to the particle diameter was used; a so-called Favre-averaging has been performed, which takes into account the phase fraction for averaging).

4 Appendix

4.1 Glossary

See List of definitions and abbreviations in Section 1.3

4.2 Document Change Log

Date	Description	Author(s)	Comments
18.12.2014	Initial version	Stefan Radl Thomas Forgber Federico Municchi	
19.12.2014	Review	Christoph Kloss	