Towards resolved intra particle temperature predictions in coupled simulations

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Key Question

How can we predict intra particle transport phenomena (temperature, reactions) in a fluid-particle systems?

Figure 1: Basic concept of Chemical Loop Combustion
Key Question

- Periodic box ($H/d_p = 15$). \[^{[1]}\]
- Upper wall $T^* = 1$, lower wall $T^* = 0$.
- Combination of Biot and Peclet number as key non-dimensional influence parameters.

$$Pr = \frac{(0.5 \, D_p)^2}{K/(\rho_p \, c_p)} \quad Bi = \frac{D_p \, \alpha_p}{K}$$

- Matching results for small $Bi$ with. \[^{[2]}\]
- Intra particle temperature profiles should be considered at higher $Bi$.
- Influence the prediction of the heat transfer rate.

Content

1. The “NanoSim” project
2. PaScal
3. Test Drive
4. Conclusion and Outlook
NanoSim Project

Title

Goals
• Open source multi-scale software platform (CFDEMcoupling, OpenFOAM, LIGGGHTS, and PaScal, C3PO as core tools).
• Facilitate rational design of second generation gas-particle CO₂ capture techniques based on nano materials, CLC.
• Highly generic for general gas-particle contacting processes (e.g., biomass gasification/combustion).

Figure 4: Vector plot of the flow field (flow into the positive x-direction, x = 4 dp).
NanoSim Project

Key Facts

• Consortium: SINTEF, TUG, UCL, INPT, NTNU, DCS, ANDRITZ, UCOIMBRA

• Scientific coupling of relevant phenomena on different scales, fully automatic, LGPL License

• PaScal (particle scale simulation) and C3PO (online post-processing utility)

• C/C++ environment, interface capabilities to LIGGGHTS, OpenFOAM, FLUENT, NEPTUNE_CFD, Stande-alone mode

• Variety of particle scale models to solve reaction-diffusion models incl. heterogeneous reactions

Figure 5: Temperature of the gas (top panel) and inside coal particles (bottom panel) in a 2D setup (Schmidt and Nikrityuk, 2012).
Figure 6: Part of the Porto Information Flow
**PaScal**

**Key Facts**

- C/C++ environment, **Particle Scale** tool for calculating transient Intra Particle Properties, LGPL Licence.
- Development started in February 2014, hosted in CFDEMcoupling Github Repository.
- Public availability planned.

![Figure 7: Current Github repository of PaScal](image)
Base classes (Error, Input, Output,..), Accessible base classes.

**Modular system**, easy to extend and understand (documentation).

Designed for spherical particles, **1D discretization** with fixed number of mesh points.

Standard integrator **CVODE** (variable-order, variable-step multistep method, 1-5 order, BDF, robust for stiff systems).
Figure 10: Test case of transient boundary conditions inside PaScaI/examples/

- **Input script “in.convective”**.
- **“0/”** folder for internal conditions, **“settings/”** for model constants.
- **“Allrun”/”Allclean”** scripts, **“README.md”** (Markdown) for problem description, **“plotMe.m”** for plotting functionality.
- **HDF5, JSON** data format available for output, both can be post-processed with Octave.
- Run.config for DCS test harness.
Conclusion

- Novel simulation tool called **PaScal**.
- **general framework** for coupled system of PDEs (spherical coordinates).
- Sub-time stepping by CVODE.
- Capable of temperature, species profiles, stiff ODE systems (reactive systems).
- Standalone or Library.

Outlook

- Library to be coupled to **LIGGGHTS** and **CFDEMcoupling** (& other **OpenFOAM** solvers).
- Public release in December 2014 (planned).
- Current activity: Interfaces, Coupling, Multiple reactions, Documentation.
One timestep

**LIGGGHTS** (fix_pascal_couple)

- Fix_shellTemperature
- Fix_shellHeatFlux
- PaScal called at end_of_step in LIGGGHTS

**Initialisation**

**PaScal object**

- Initialisation from latest time step.
- Inner loops for all particles, temperature, species, chemistry.
- Calculation of intra particle properties, relevant properties for LIGGGHTS.

**Parameters to LIGGGHTS for next timestep**

- Runs as Slave Program.
- Serial Init, than Parallel Run.
- No interaction to Master during runtime.
- Automatic Sub-time stepping through CVODE (needed for chemistry).

Figure 11: Timestep in LIGGGHTS/PaScal coupling
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Thank you!