Towards resolved intra particle temperature predictions in coupled simulations

Graz University of Technology

Thomas Forgber

Stefan Radl

DCS Computing

Christoph Kloss

Key Question

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

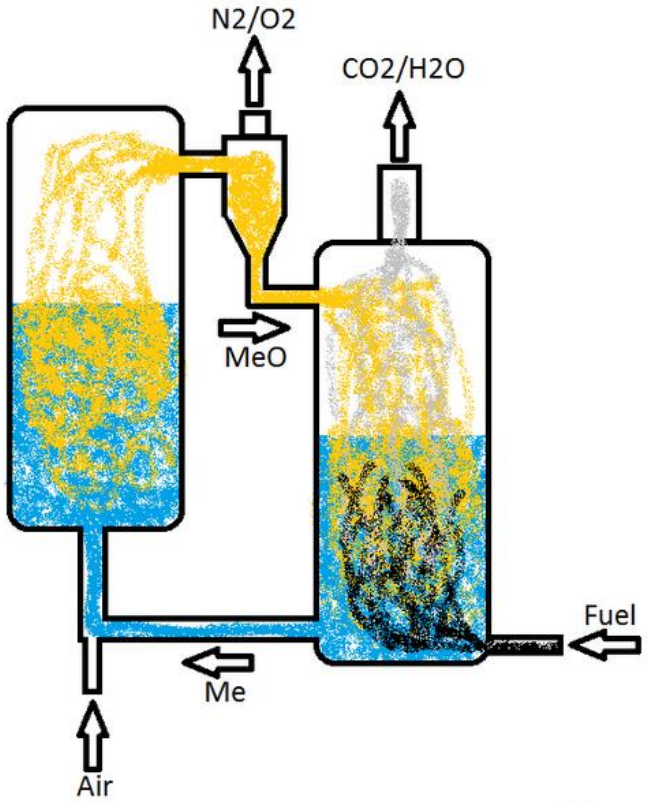


Figure 1: Basic concept of Chemical Loop Combustion

Key Question

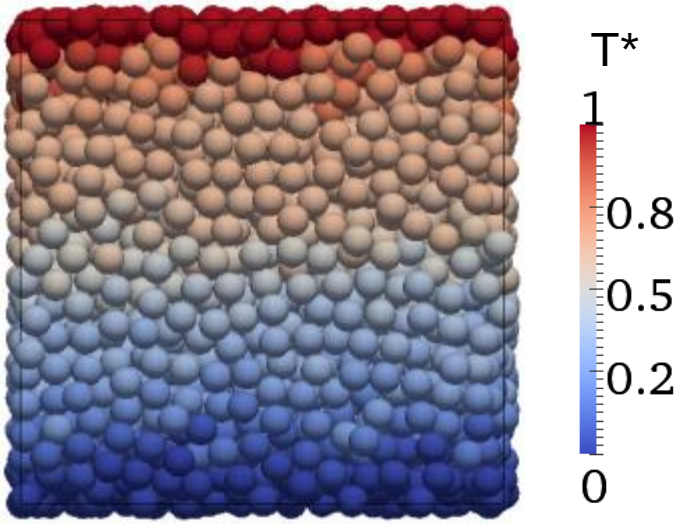


Figure 2: Sheared particle bed

- 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.

$$Pr = \frac{(0{,}5\ D_P)^2}{K/(\rho_P\ c_P)} \qquad Bi = \frac{D_P\ \alpha_P}{K}$$

- Matching results for small Bi with. [2]
- Intra particle temperature profiles should be considered at higher Bi.
- Infulence the prediction of the heat transfer rate.

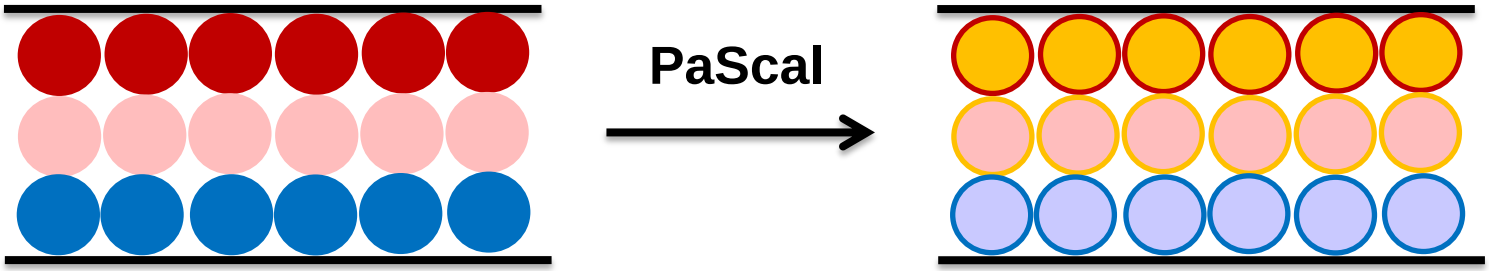


Figure 3: Basic scope of PaScal

[1] Lees and Edwards, *Journal of Physics C: Solid State Physics* (1972)
[2] Bhageshvar, Kloss, Radl, Khinstast, Powder Technology (2014)

Content

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

NanoSim Project

Title

Multiscale Simulation-Based Design Platform for Cost-Effective CO_2 Capture Process by Nano-Structured Materials.

Goals

- Open source multi-scale software platform (**CFDEMcoupling**, **OpenFOAM, LIGGGHTS**, and **PaScal, C3PO** as core tools).
- Facilitate rational design of second generation gas-particle CO_2 capture techniques based on nano materials, CLC.
- Highly generic for general gas-particle contacting processes (e.g., biomass gasification/combustion).

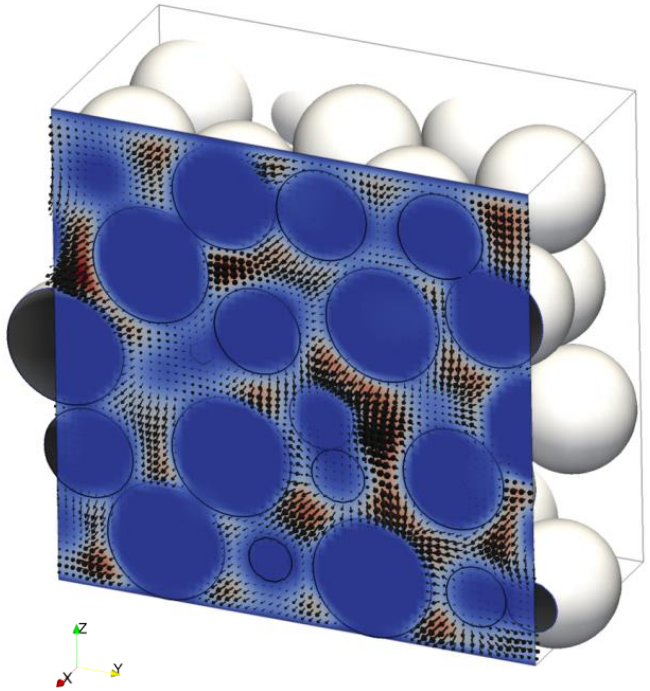


Figure 4: Vector plot of the flow field (flow into the positive x-direction, x = 4 dp).

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

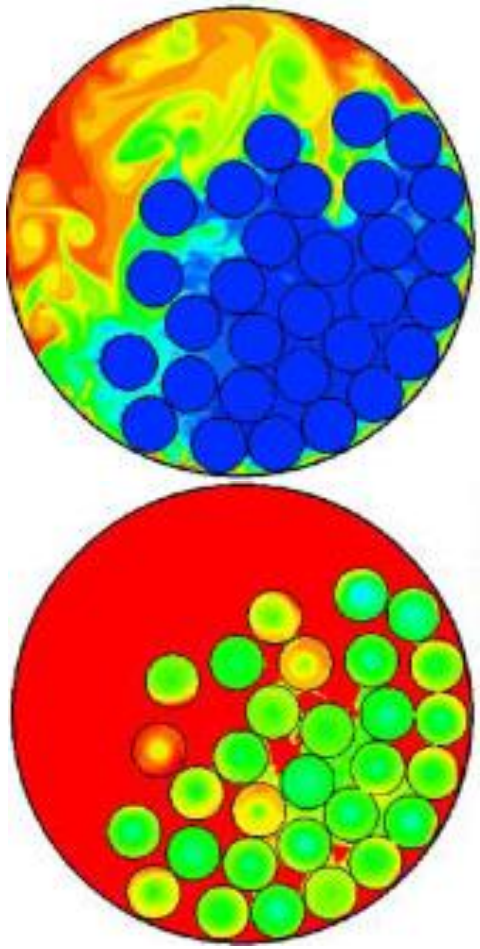


Figure 5: Temperature of the gas (top panel) and inside coal particles (bottom panel) in a 2D setup (Schmidt and Nikrityuk, 2012).

NanoSim Project

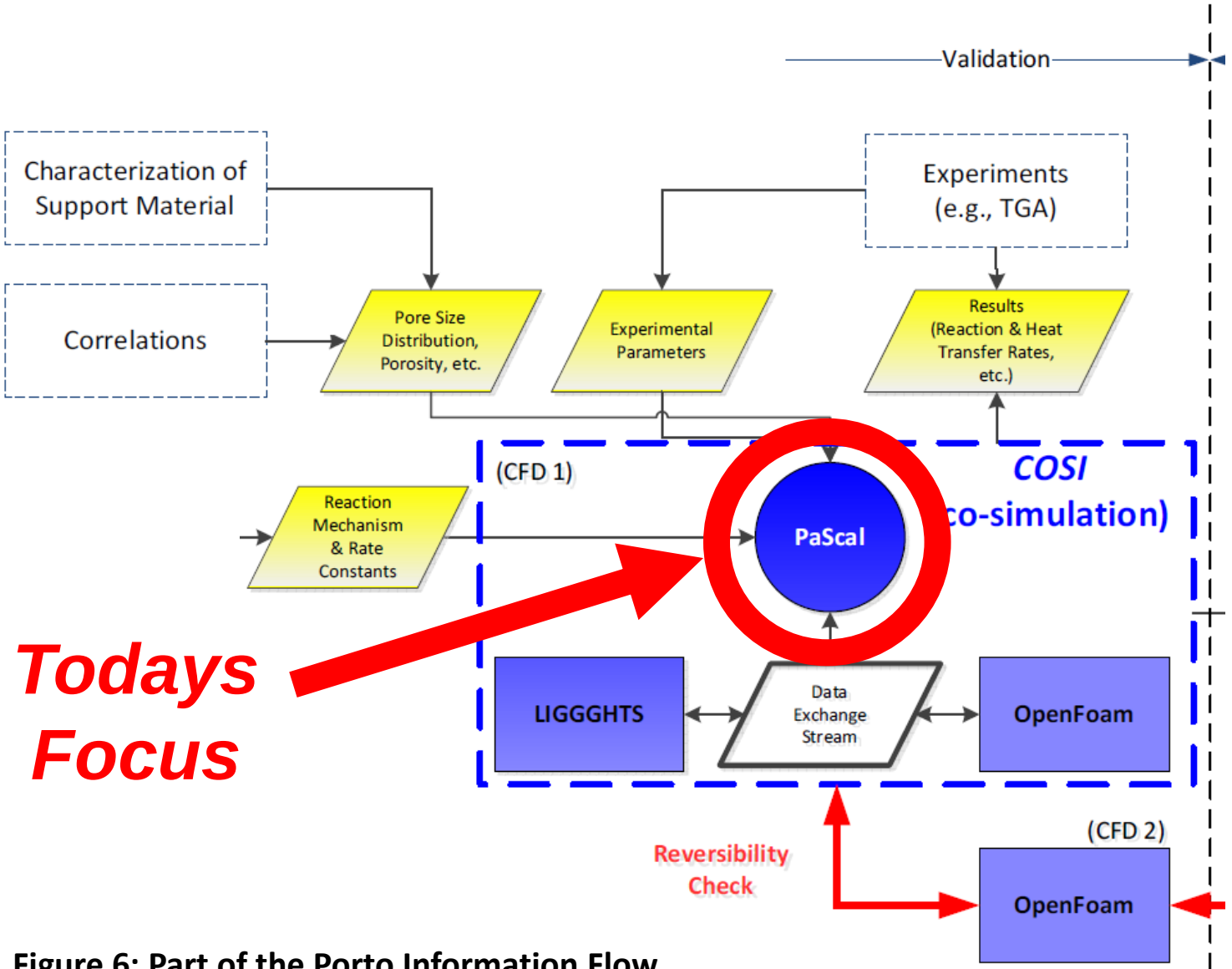


Figure 6: Part of the Porto Information Flow

PaScal

Key Facts

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

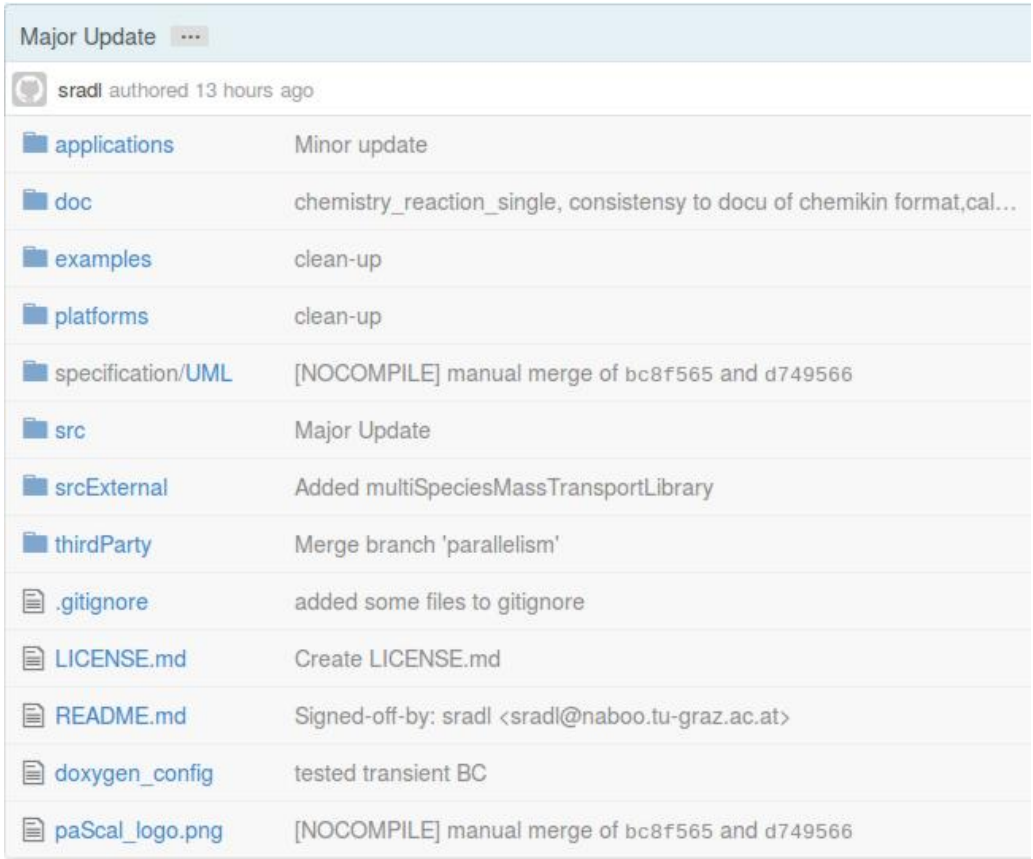


Figure 7: Current Github repository of PaScal

PaScal

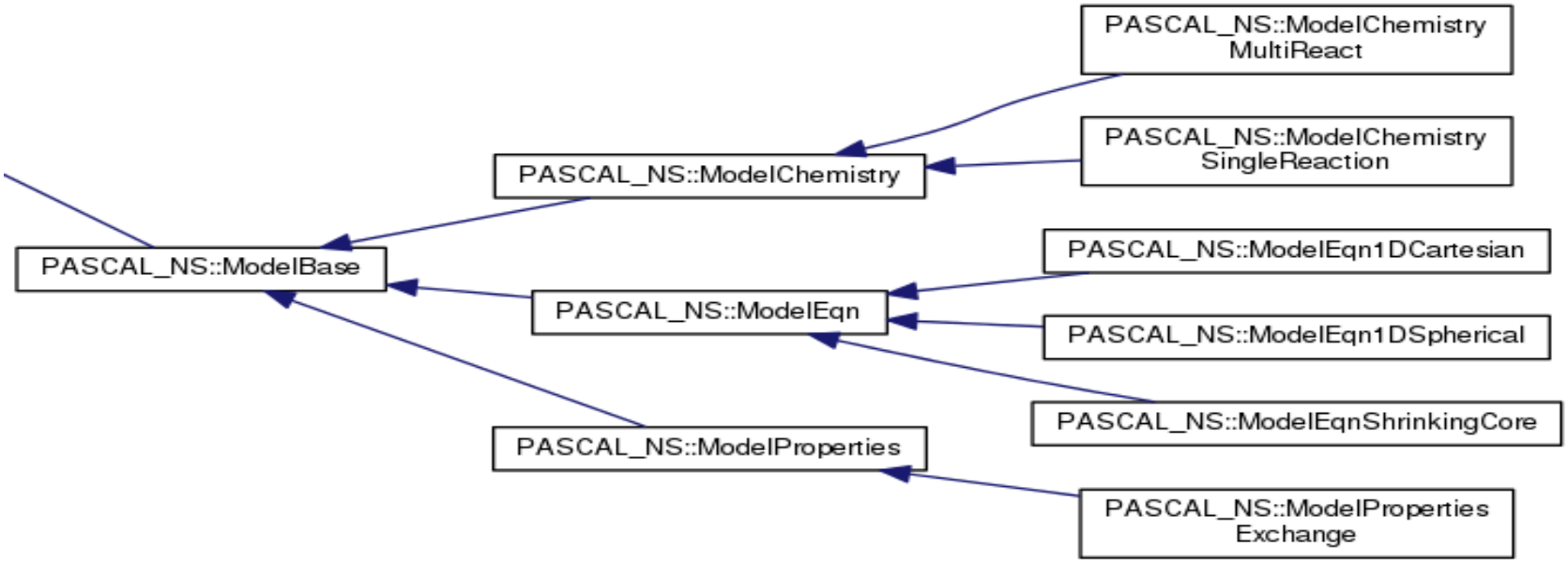
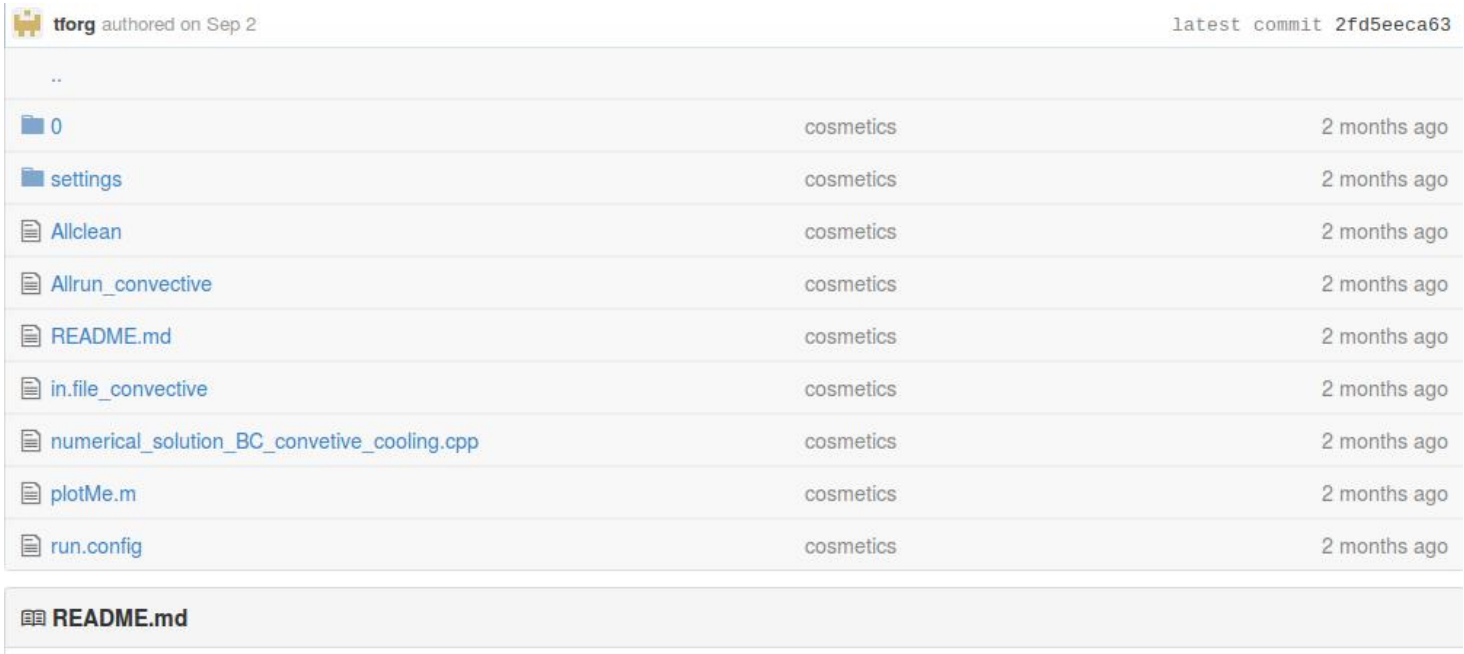


Figure 9: PaScal Model Base Class diagram

- 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).

Test Drive



tforg authored on Sep 2 — latest commit 2fd5eeca63

..		
0	cosmetics	2 months ago
settings	cosmetics	2 months ago
Allclean	cosmetics	2 months ago
Allrun_convective	cosmetics	2 months ago
README.md	cosmetics	2 months ago
in.file_convective	cosmetics	2 months ago
numerical_solution_BC_convetive_cooling.cpp	cosmetics	2 months ago
plotMe.m	cosmetics	2 months ago
run.config	cosmetics	2 months ago

README.md

Figure 10: Test case of transient boundary conditions inside *PaScal/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 and Outlook

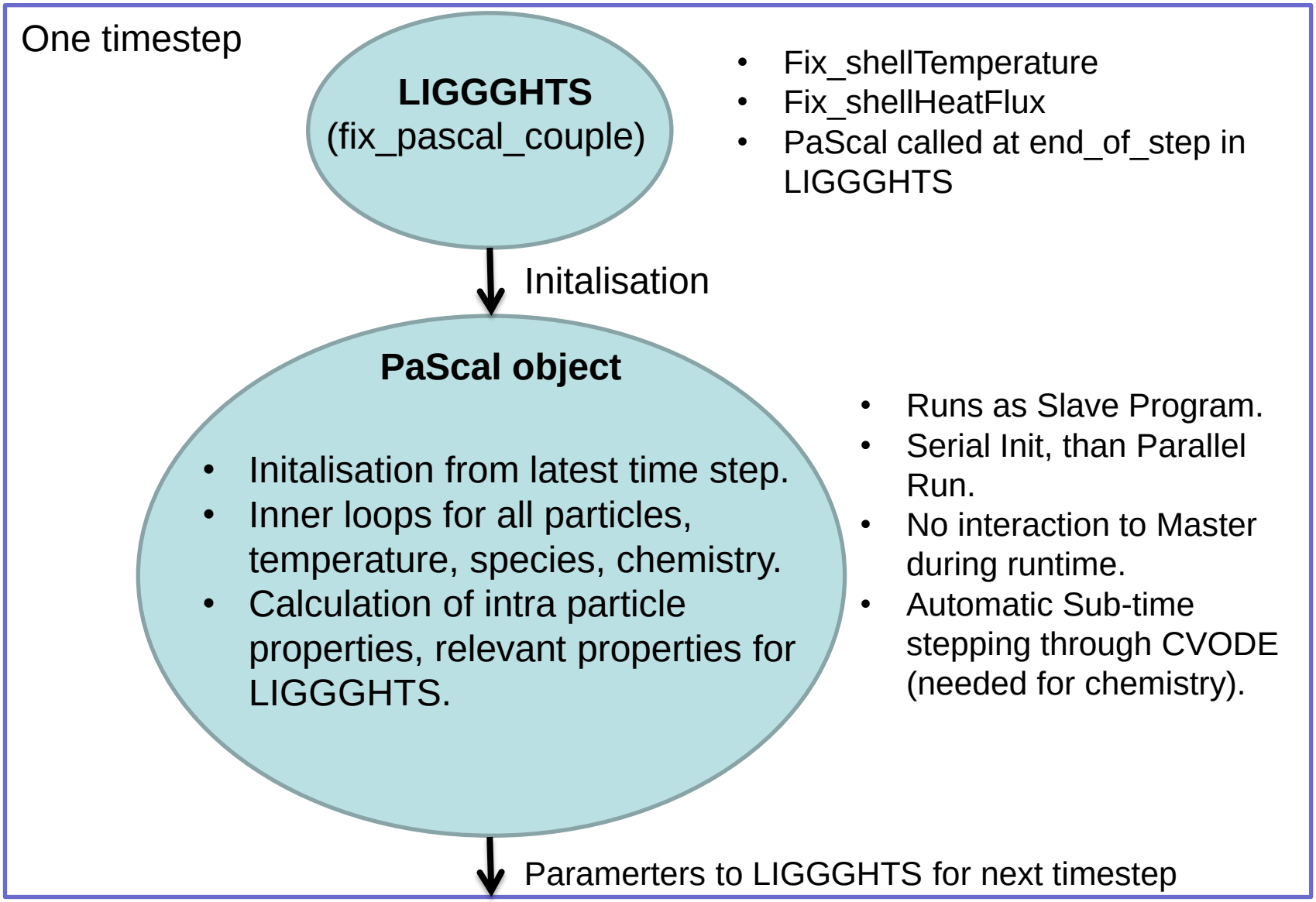
Conclusion

- 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.

Conclusion and Outlook



- Fix_shellTemperature
- Fix_shellHeatFlux
- PaScal called at end_of_step in LIGGGHTS

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

- 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

Towards resolved intra particle temperature predictions in coupled simulations

Graz University of Technology

Thomas Forgber

Stefan Radl

DCS Computing

Christoph Kloss

Thank you!