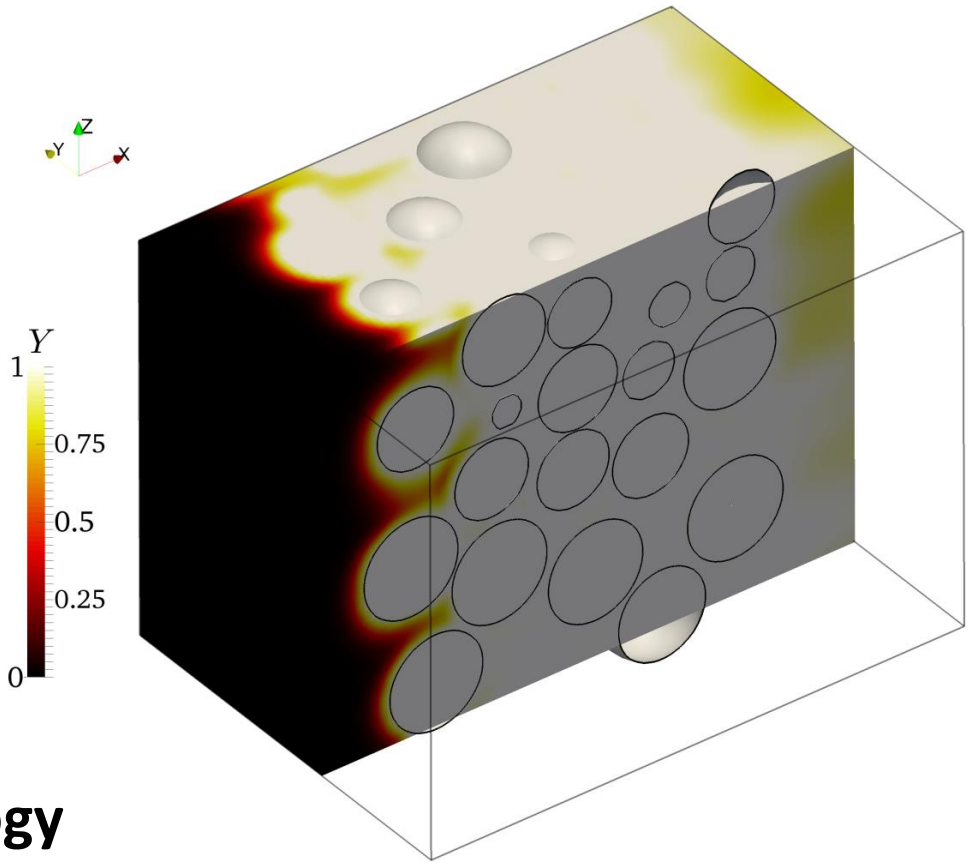
Perspectives for

Modeling Reactive Particulate Systems using Open-Source Tools

Stefan Radl,
Federico Municchi,
and Thomas Forgber



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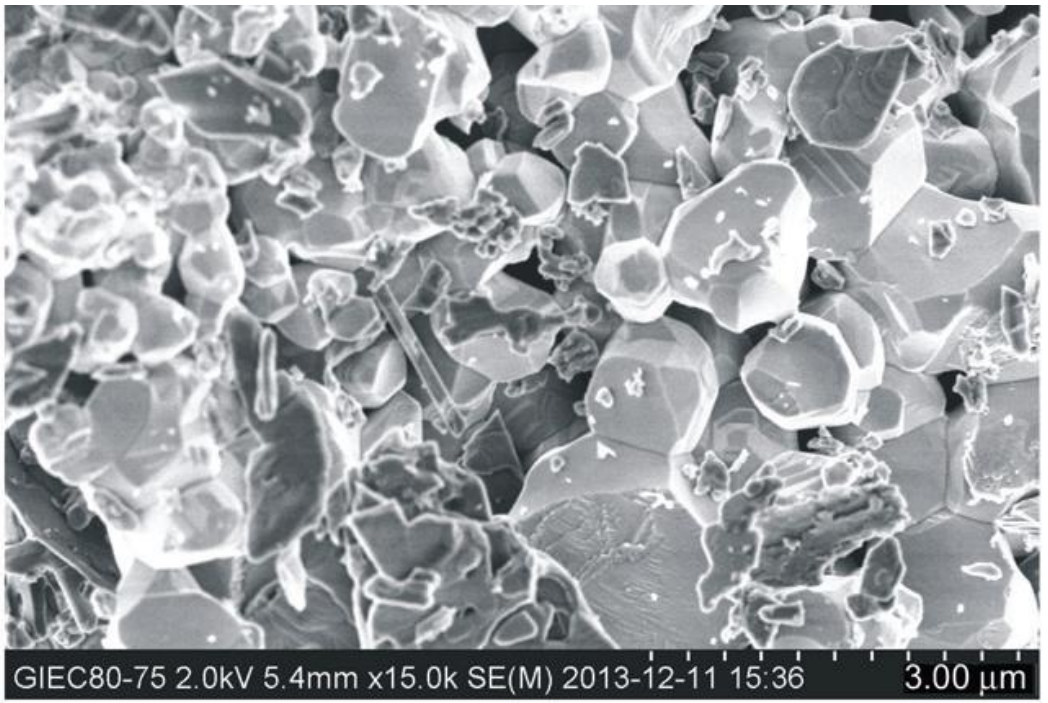
Why Modeling Reactive Flows?

1 - Next Generation Chemical Looping Processes

- Methan reforming via **partial oxidation** using solid oxygen carriers has significant economic advantages.
- **Iron-based oxygen carriers**, nano-structured and doped with a second metal, are promising.
- Rational **design** is challenging (sintering, optimal pore structure) and **requires a model**.

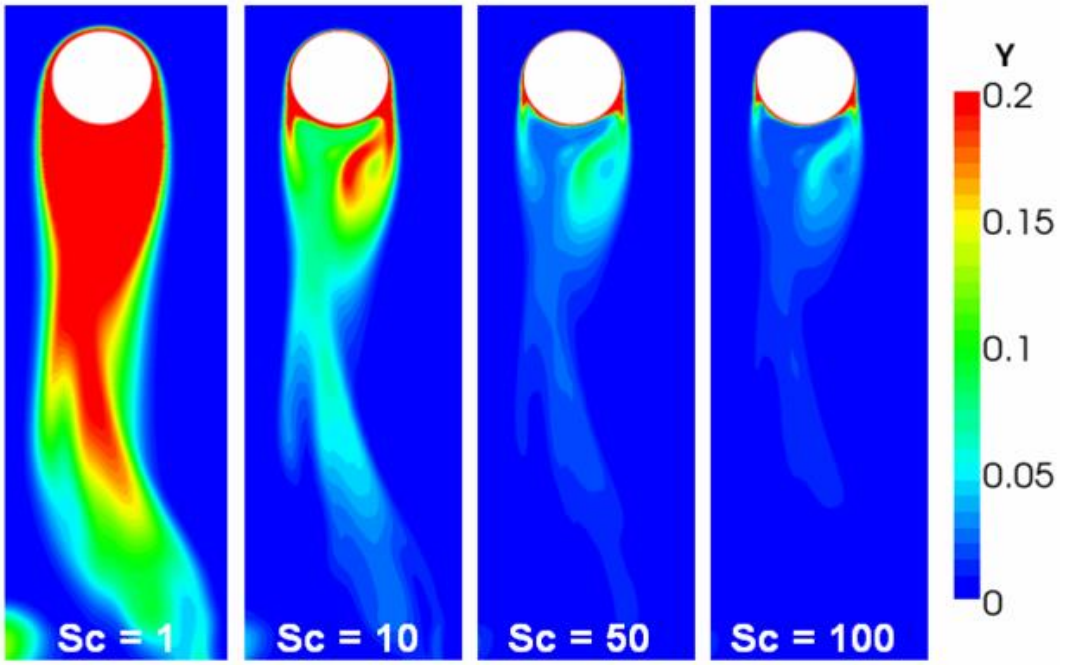


SEM image of a typical nano-structured Ni-modified Fe_2O_3/Al_2O_3 oxygen carrier (Wei et al., 2014).

Why Modeling Reactive Flows?

2 - Scientific Curiosity

- Resolution of **flow, concentration, and temperature** field by solving the relevant transport equations.
- **Detailed information** allows (i) profound process **understanding**, and (ii) is the basis for **coarse-grained** models (e.g., DNS → LES)

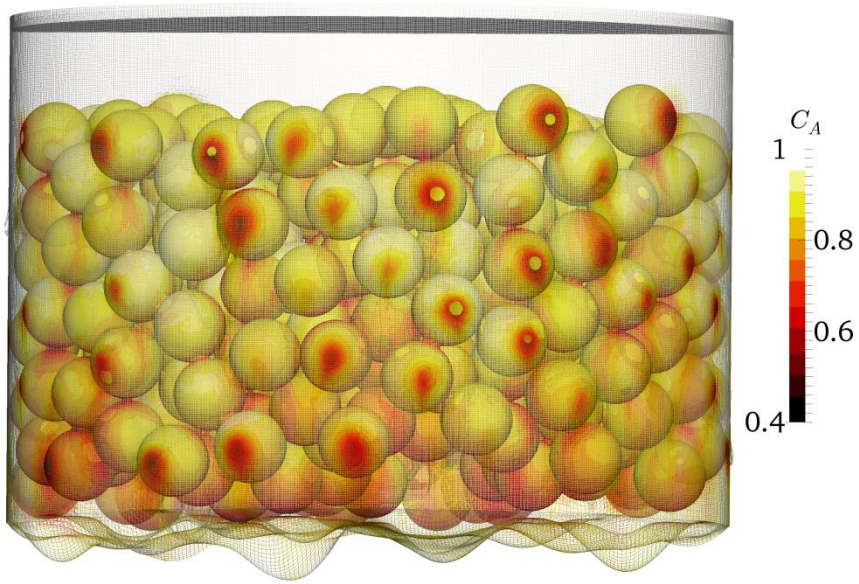


Instantaneous concentration fields in the wake of a single particle (Re = 500).

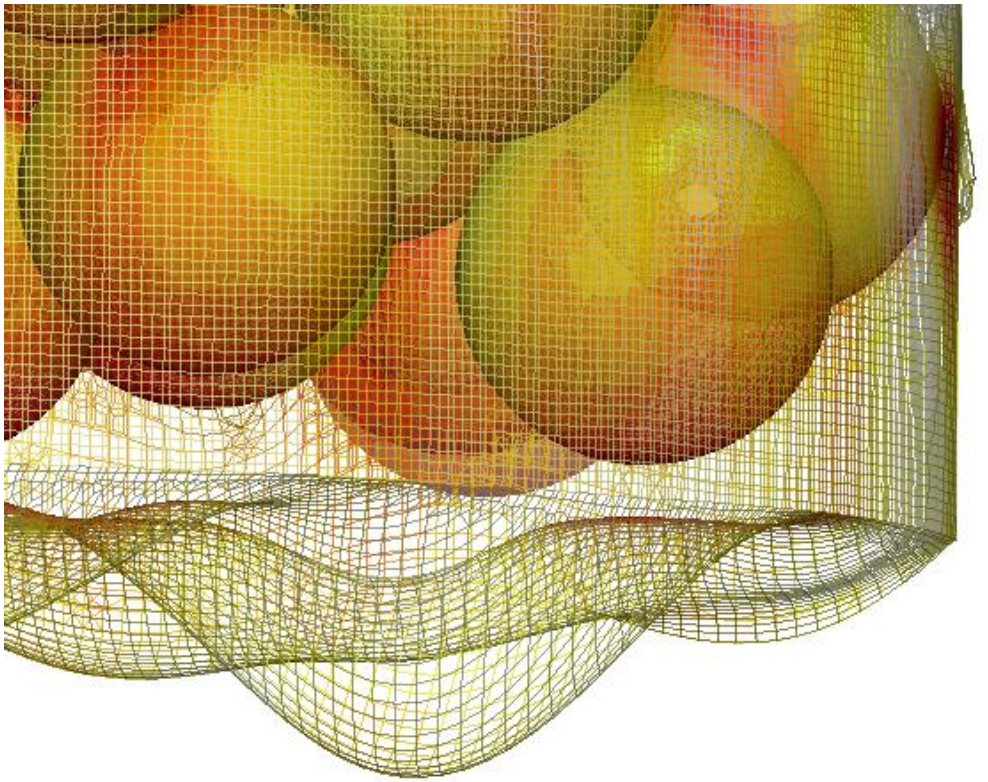
Why Modeling Reactive Flows?

2 - Scientific Curiosity

- Modeling on **multiple levels** (co-current or sequential) and **exploitation of "big data"** is key.



Concentration field in liquid catalytic reactor
(Re ~ 1, Sc ~ 500,
Master Thesis Rafael Pichler, 2015).



Which Modeling Tools Exist?

1 - Multipurpose Continuum Solvers

- Matlab /octave / Julia
- OpenFOAM®
- CFDEM®
- ANSYS Fluent
- AVL Fire®

2 - Multipurpose Lagrangian Solvers

- Yade / WooDEM
- LAMMPS / LIGGGHTS®
- SimPARTIX®
- EDEM
- Itasca PFC

Open-source

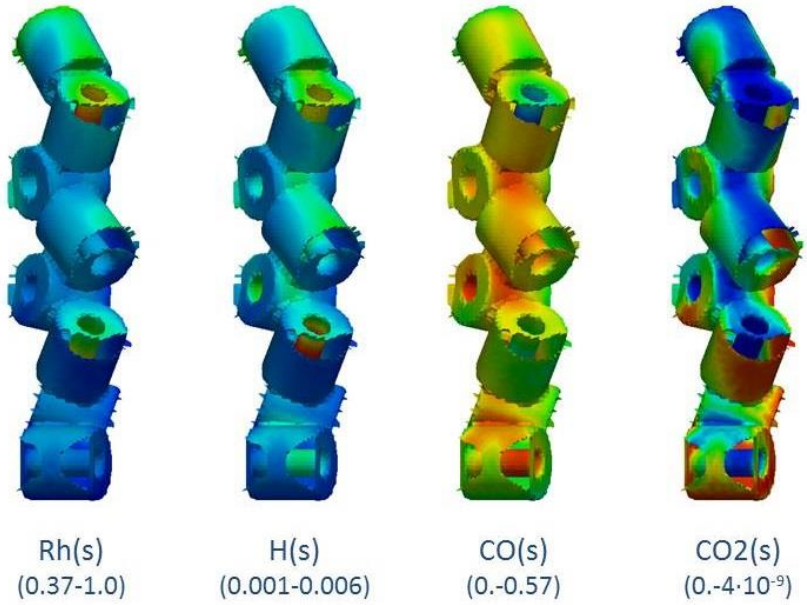
Open Issues

1. **Sub-Particle** scale modeling (first step: OpenFOAM®'s „pyrolysisModel")
2. Advanced **data analysis** tools in parallel (first step: swak4Foam)
3. Efficient **parallelization** for Euler-Lagrange co-simulations
4. Advanced **coupling models** (i.e., for the fluid-particle interaction force)

Which Modeling Tools Exist?

3 - Kinetics & Transport Tools

- CANTERA
- OpenFOAM® / CatalyticFoam
- DETCHEM / DC4OpenFOAM
- CHEMKIN



Adsorbed species mass fraction distribution on the surface of non-porous particles
http://www.catalyticfoam.polimi.it

Open Issues

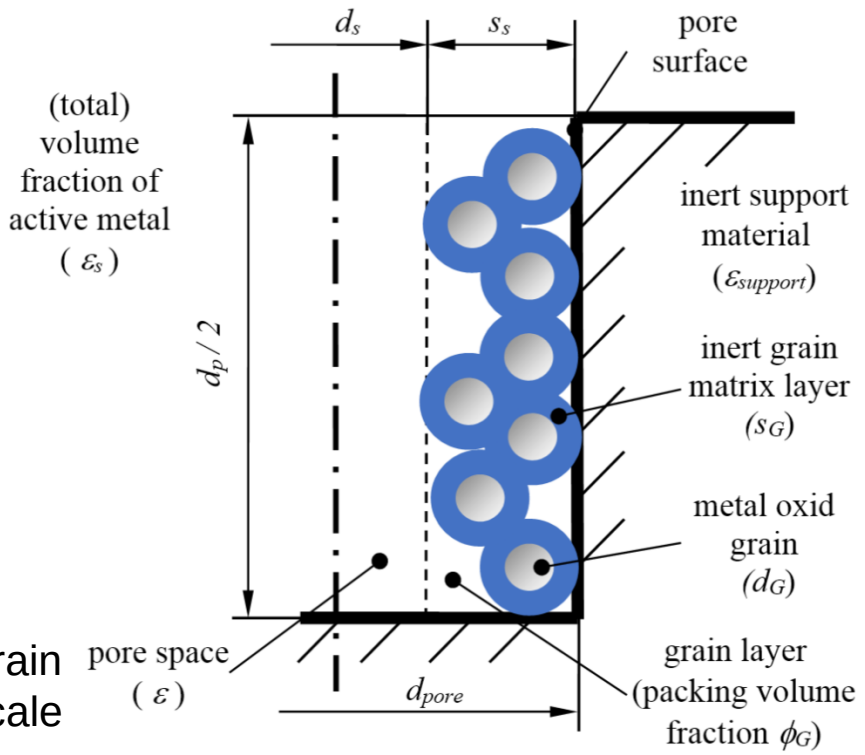
1. **Coupling** to high-performace CFD solvers missing
2. Limited to 1D transport in a **single particle**
3. Particles cannot **move**
4. Transport in **porous particles** missing

Open-source

What is ParScale?

A Compilation of Particle Scale Models

- Model transport and reactions in **porous particles** with **“grains”**
- Designed for **stiff systems** (CVODE as integrator)
- ParScale can manage **large particle clouds** with O(10^6) particles in parallel via LIGGGHTS®-based data containers

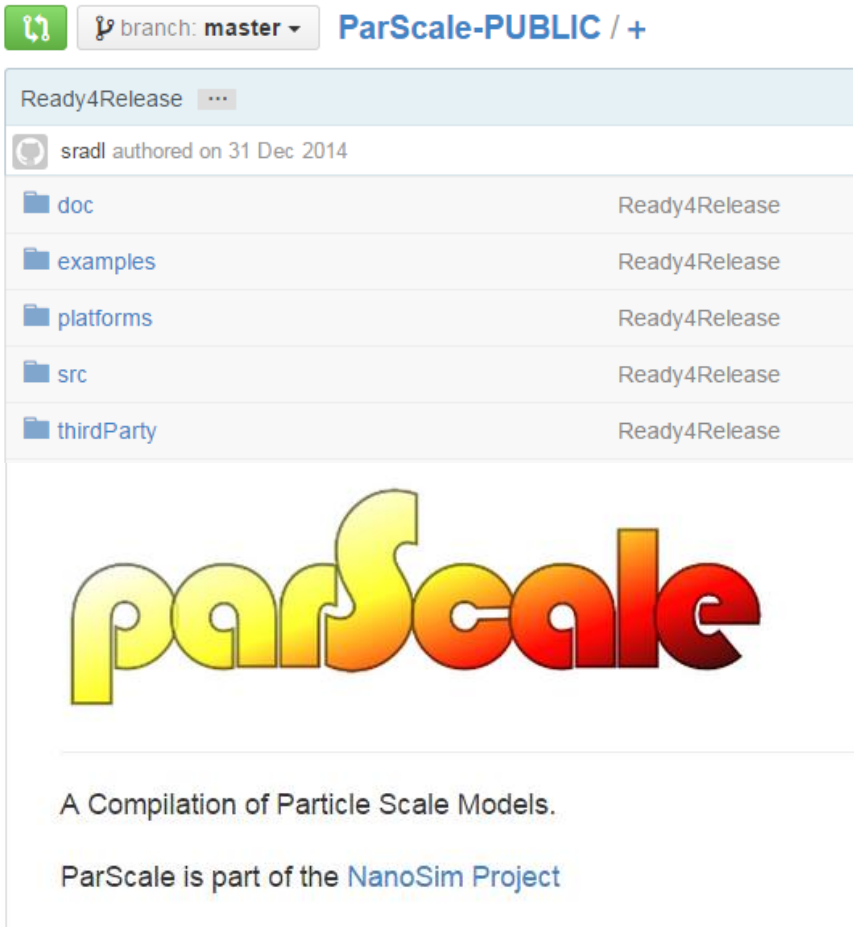


Typical pore and grain model available in ParScale

What is ParScale?

A Compilation of Particle Scale Models

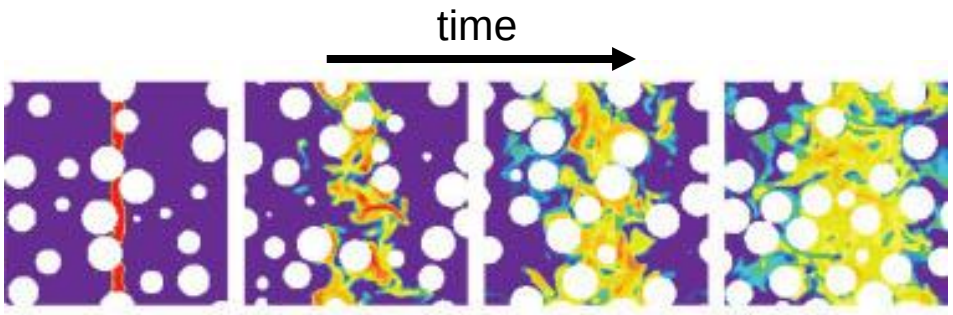
- Designed to run in **standalone mode**, or to be linked with **LIGGGHTS®**
- **Flexible** (Matlab-like input script; arbitrary number of species, CHEMKIN file format interface)
- Licensed under **LGPL**
- https://github.com/CFDEMproject/ParScale-PUBLIC



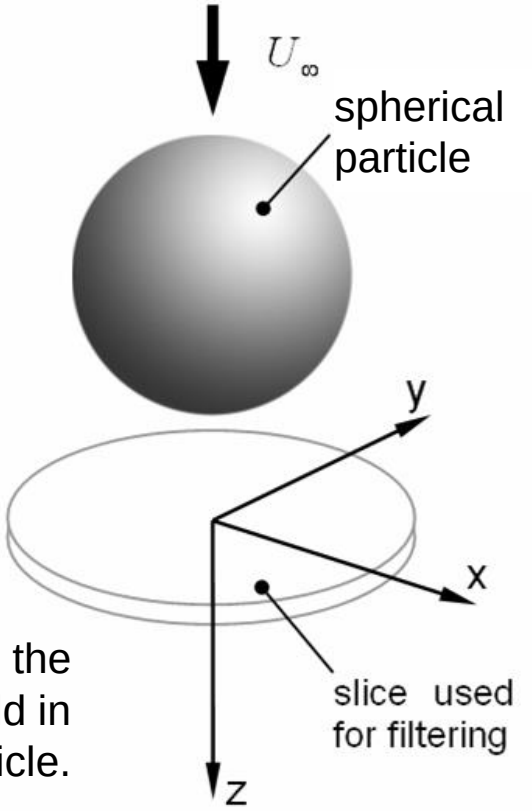
What is Filtering?

A Spatial Data Analysis Strategy

- **Filtering = Spatial averaging** of **microscopic quantities**, e.g., forces, concentration & temperature fields, reaction rates to obtain **effective quantities.**
- Example: Measure **Dispersion Coefficients**



Dispersion of a concentration pulse (Derksen, 2008).



Sketch of the setup used for the filtering of the concentration field in the wake of a particle.

What is Filtering?

The Filtering Toolbox CPPPO

- Spatial averaging **across multiple processors**
- Designed as **library** to be linked to **OpenFOAM®**
- **CSV interface** (e.g., ANSYS Fluent output)
- **Flexible** (Matlab-like input script; filtering, sampling and binning operations configured at runtime)
- Licensed under **LGPL**

branch: C3PO_dev ▾ CFDEMcoupling-RADL / src / c3po / +

This branch is 31 commits ahead, 13 commits behind master

Major Update of sampling ···

sradl1981 authored 13 hours ago

..

applications	Merge master in C3PO_dev
core	Major Update of sampling
doc	Major Update of sampling
etc	Removed bugs
examples	Major Update of sampling
interface_CSV	Removed bugs
interface_OF	Update

CPPPO

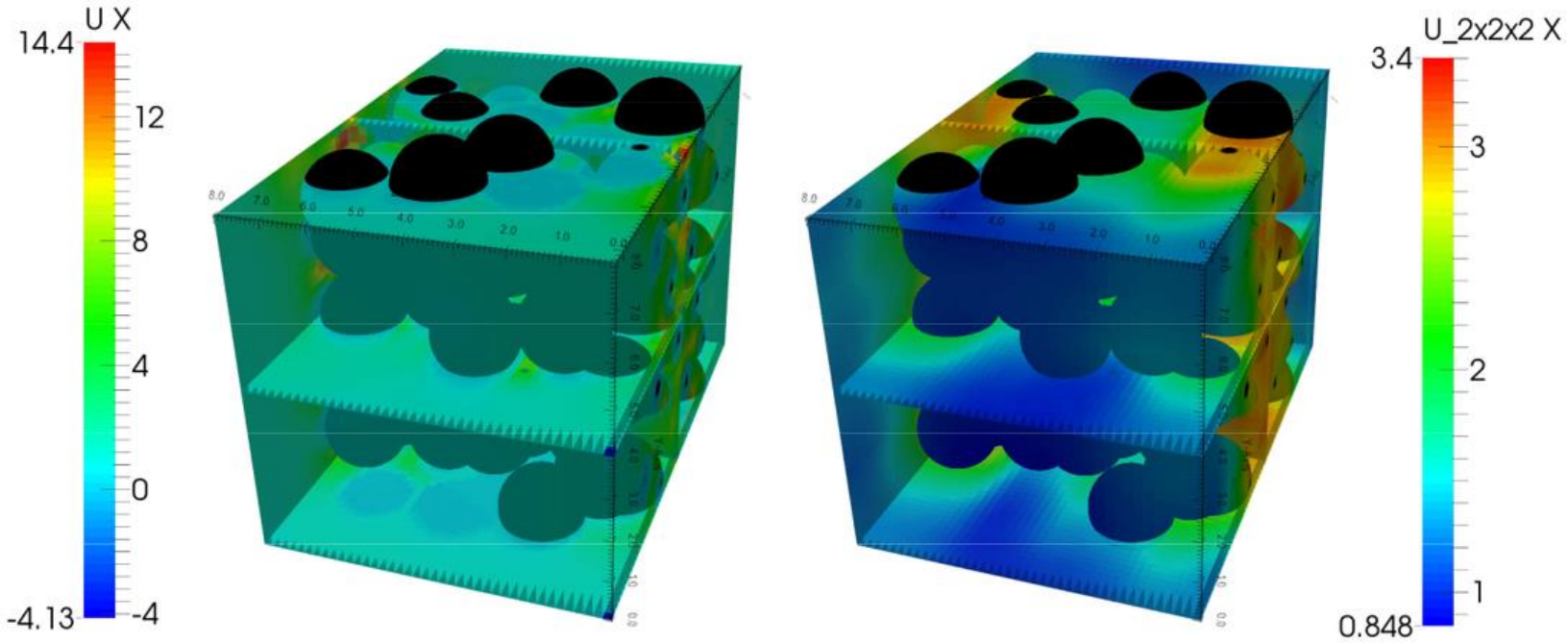
A Compilation of Fluid-Particle Post Processing routines.

CPPPO is part of the NanoSim Project

What is Filtering?

Spatial Data Analysis – An Example

- **Direct numerical simulation** of flow around a random particle ensemble
- On-the-fly top-hat filtering during a CFDEM® run using CPPPO



Conclusion

IPPT uses CFDEM® as the main Euler-Lagrange(-Euler) simulation engine

- Based on **OpenFOAM®**
- Parallel efficient **up to ~ 128 cores**
- Improved models & algorithms (e.g., coupling, forces, sprays, etc.)
- Open-Source (**NOT** all is public!)

ParScale is an open-source particle-scale simulation tool

- **Continuum and shrinking-core** type of models
- **Grain models** (e.g., model oxide layer formation)

CPPPO is a data analysis tool for "heavy jobs"

- **Spatial averaging** in parallel
- Sampling & binning of raw data for on-the-fly data compression

Outlook

Announcement

OpenFOAM® User Meeting (PFAU X)

The Institute for Process and Particle Technology is pleased to host the “PFAU X” (*Palaver OpenFOAM Users Austria - the Austrian User Group*).

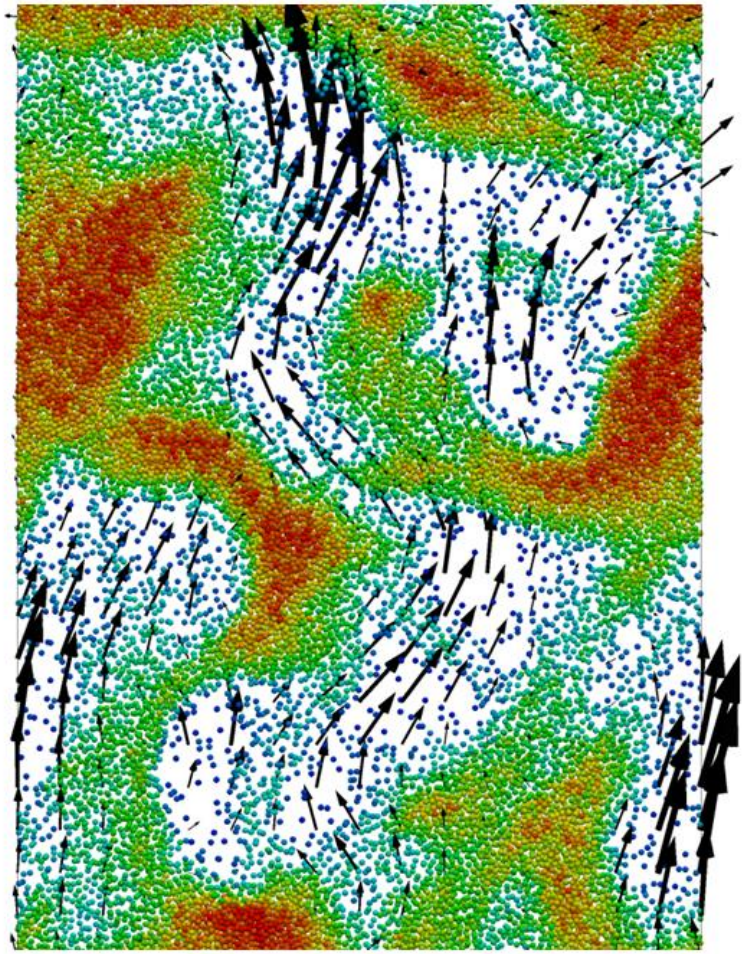
The meeting will take place on

Wednesday, July 8, 2015
10.00 a.m. - 4.00 p.m.

in

Lecture Room “HS i8”
Inffeldgasse 13, TU Graz

PFAU meetings are informal, and provide a channel for open discussions on finished, ongoing or future projects related to the development and usage of OpenFOAM®.



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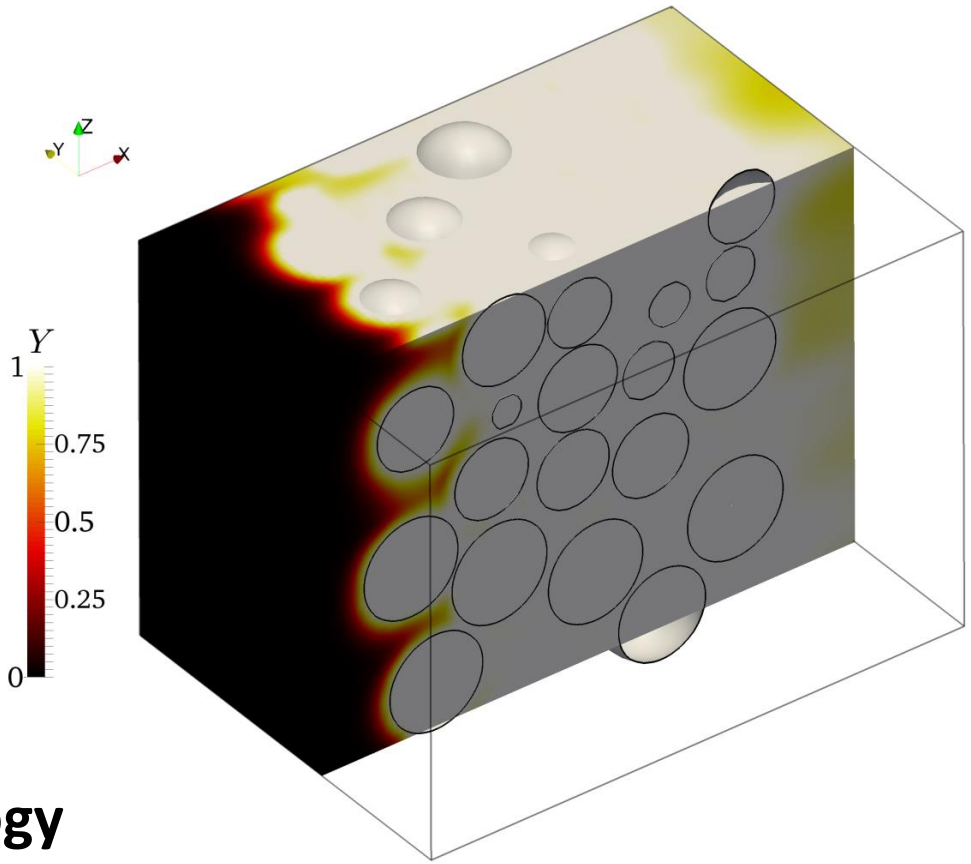

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