

Pharmaceutical  
Multiphase Reactors  
CHE.782

Design of Multiphase  
Flow Processes  
669.266

## 1 Overview of „ParScale“ library

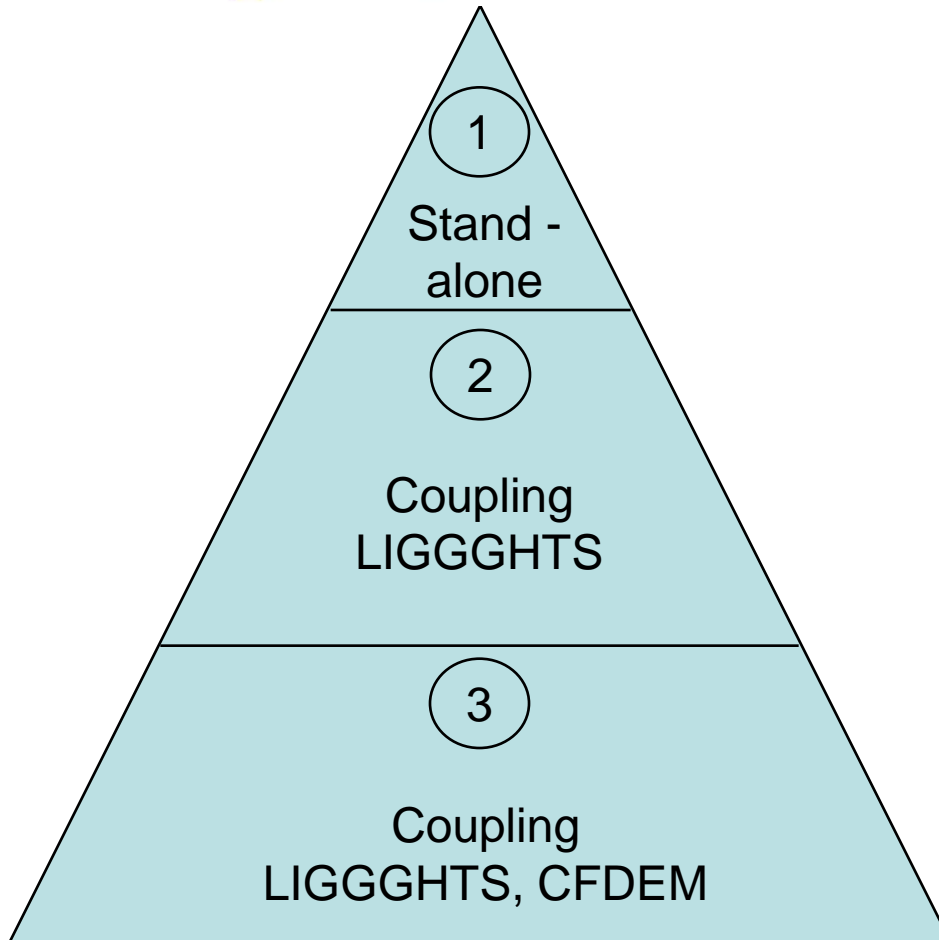
Ass.Prof. Dr. Stefan Radl,  
M. Sc. Thomas Forgber  
Email: [radl@tugraz.at](mailto:radl@tugraz.at)  
Institute of Process and  
Particle Engineering  
Inffeldgasse 13/III  
TU Graz

A part of this teaching material has been  
prepared for NanoSim (<http://sintef.no/NanoSim/>)



NanoSim

NanoSim - A Multi-scale Simulation-Based Design Platform



1

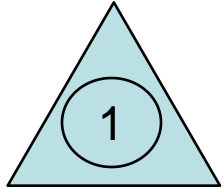
- ParScale for intra particle transport processes
- **Open-source**, stand-alone
- 1-D discretisation, fixed number of grid points
- Reaction, phase change, chemistry, grain scale models

2

- Coupling **ParScale-LIGGGHTS**
- Discrete Element Method (DEM) with resolved intra particle property profiles

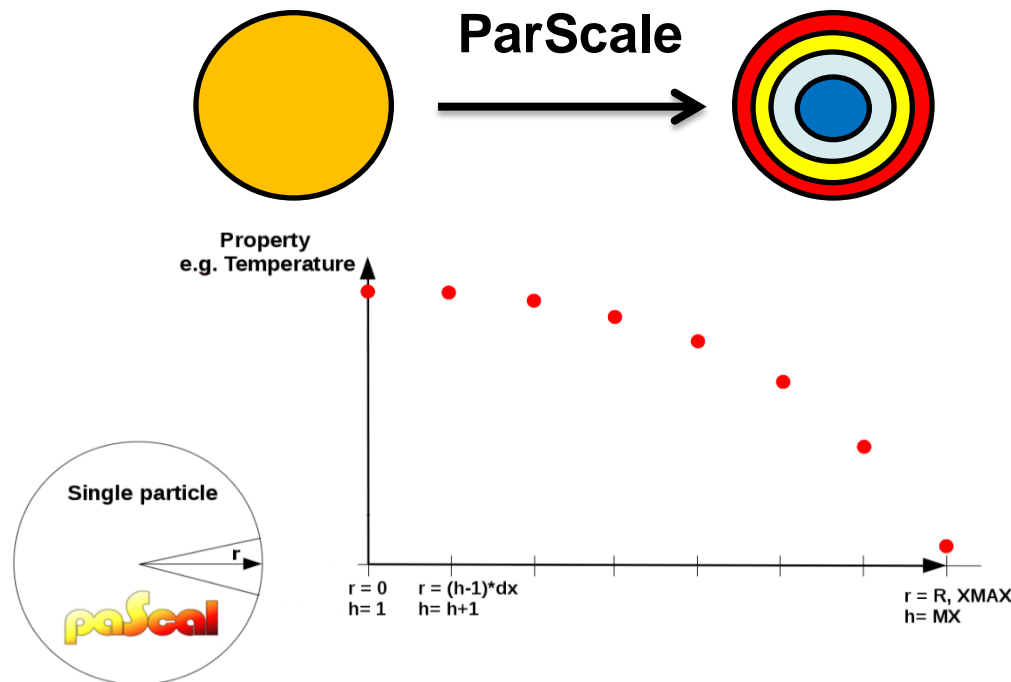
3

- Coupling **ParScale- LIGGGHTS- CFDEMcoupling**
- CFD approach for flow around particles, DEM, intra-particle profiles, fully coupled

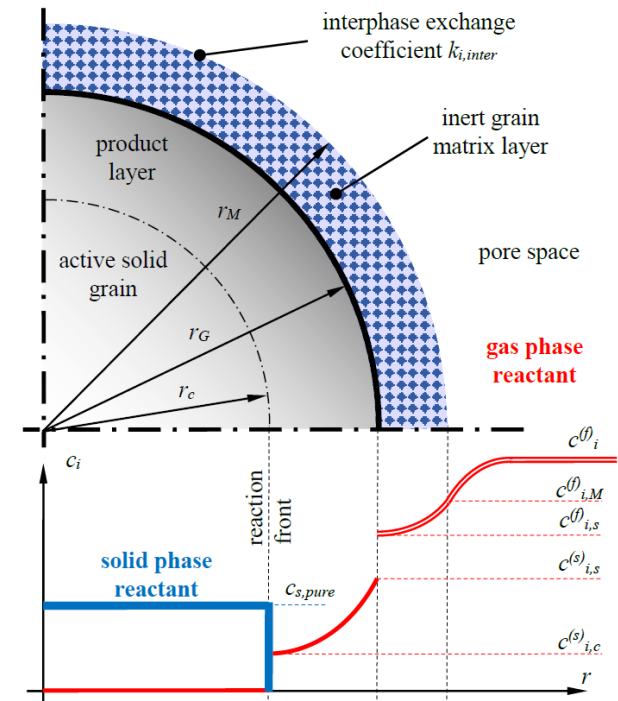


- Open-source library for intra-particle transport processes
- Variety of **chemical models**, relevant physical phenomena, grain effects, **shrinking core model**
- **Three phase particles** including phase change models
- Discretization in **spherical coordinates** or simplified models

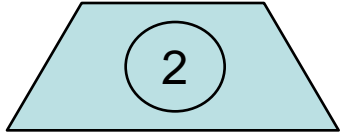
**GOAL: Spatial profile of target property in transient simulation**



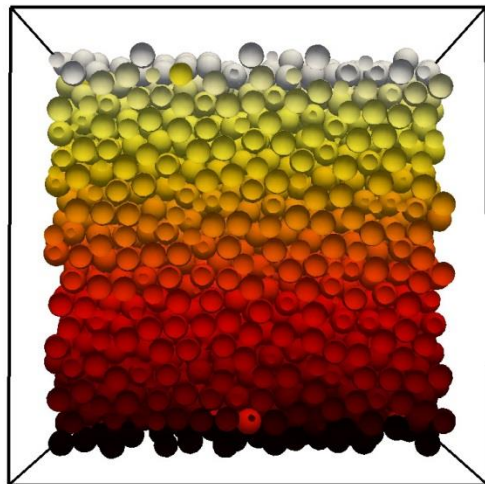
Temperature distribution in a sphere



Concentration profile in a reacting particle.



- Coupling to LIGGGHTS
- Usage of all LIGGGHTS features (contact models, heat transfer,...) with coupling to ParScale



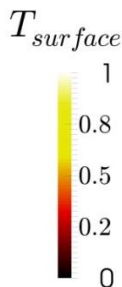
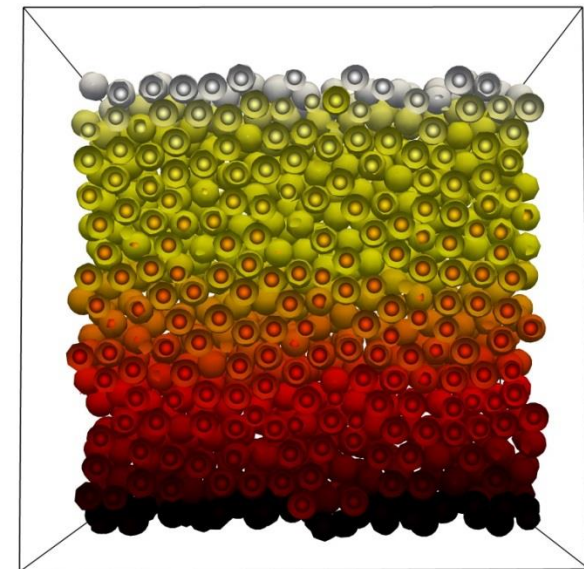
**LIGGGHTS**  
DEM physics

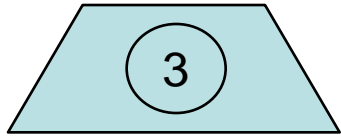


+

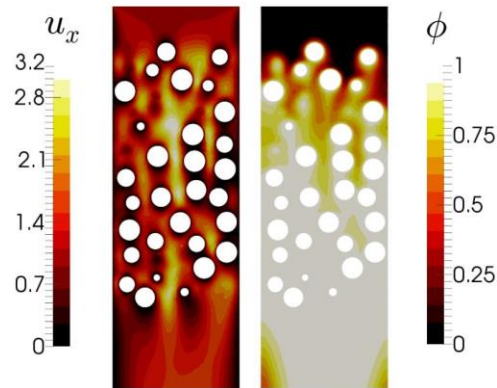
**parScale**

**ParScale**  
for intra-particle  
transport  
processes





- Coupling to LIGGGHTS, CFDEM
- Usage of all coupling features



DNS of fixed particle bed (F. Municchi, TU Graz)

## CFD-DEM

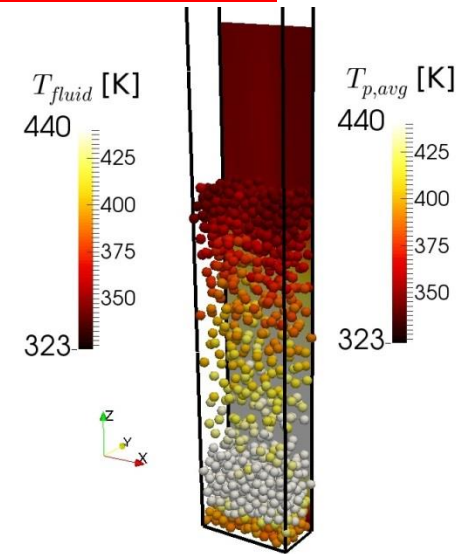
simulation  
to picture  
flow  
physics



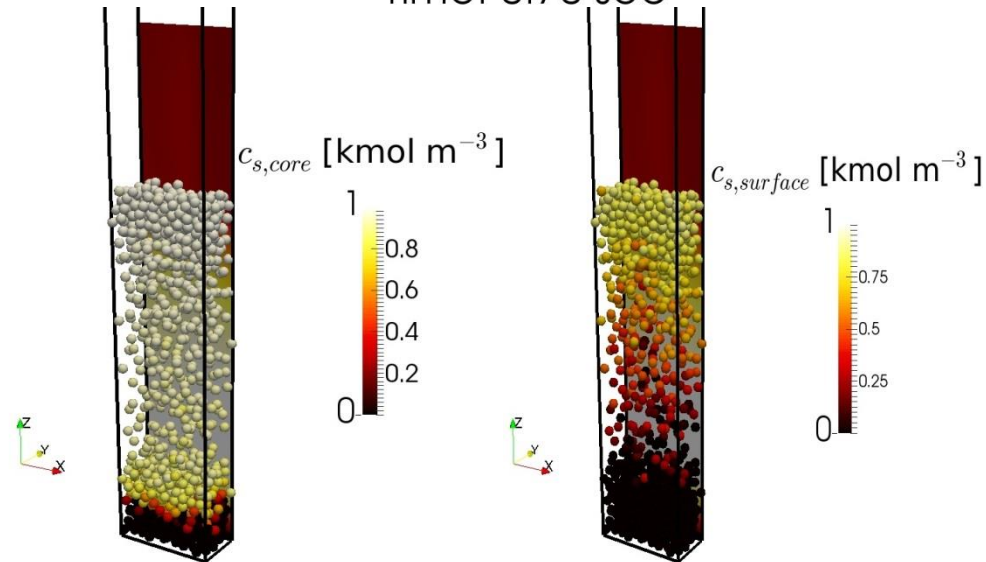
## ParScale

for intra-particle  
transport  
processes

+



Time: 0.70 sec



- For a full feature list and the most recent updates

<https://github.com/CFDEMproject/ParScale-PUBLIC/blob/master/RELEASENOTES.md>



- For help and discussions see forum at [www.cfdem.com](http://www.cfdem.com)

A Compilation of Particle Scale Models.

ParScale is part of the [NanoSim Project](#)

## Graz University of Technology and DCS Computing GmbH releases ParScale 1.1.1 beta

24th of August 2015

### Features

Version 1.1.1-beta is a major upgrade of the ParScale library with extended features to study intra-particle transport phenomena including phase change phenomena (e.g., evaporation of water inside the pores of the particles). Specifically, the following features are new, or have been significantly improved in the latest version of ParScale:

- restructuring of code and documentation that was required for extended ParScale to handle multiple phases
- handling of up to three phases (i.e., solid, liquid, gas), including phase change phenomena. Two phase change models have been added (i.e., "evaporation", as well as "equilibrium sharp"). The volumetric phase change rate can be accounted for in the species transport equations.
- model equations can be used to not only compute concentration profiles, but also update the local phase fraction (e.g., to study the evolution of the local liquid saturation in a porous particle)

# Impressum & Disclaimer

---

**©2015 by Stefan Radl, and other members of the „Simulation Science“ Group at the Institute of Process and Particle Engineering, Graz University of Technology.**

All rights reserved. No part of the material protected by this copyright notice may be reproduced or utilized in any form or by any means, electronically or mechanically, including photocopying, recording or by any information storage and retrieval system without written permission from the author.

LIGGGHTS® is a registered trade mark of DCS Computing GmbH, the producer of the LIGGGHTS® software. CFDEM® is a registered trade mark of DCS Computing GmbH, the producer of the CFDEM®coupling software. This offering is not approved or endorsed by DCS Computing GmbH, the producer of the LIGGGHTS® and CFDEM® coupling software and owner of the LIGGGHTS and CFDEM® trade marks.