CFD-DEM Modeling at High Temperatures

Effects of Gas Density Change and Radiation

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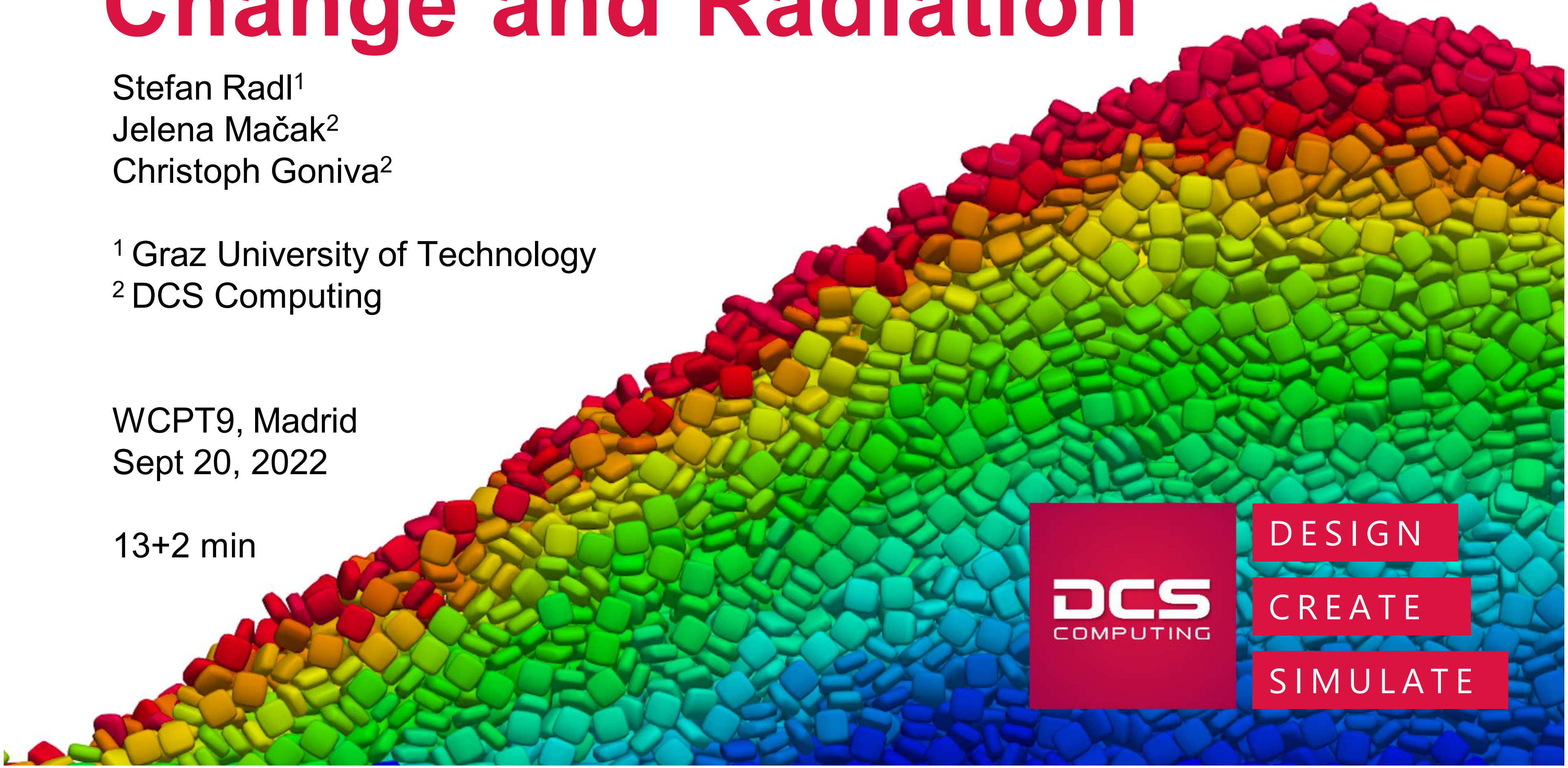
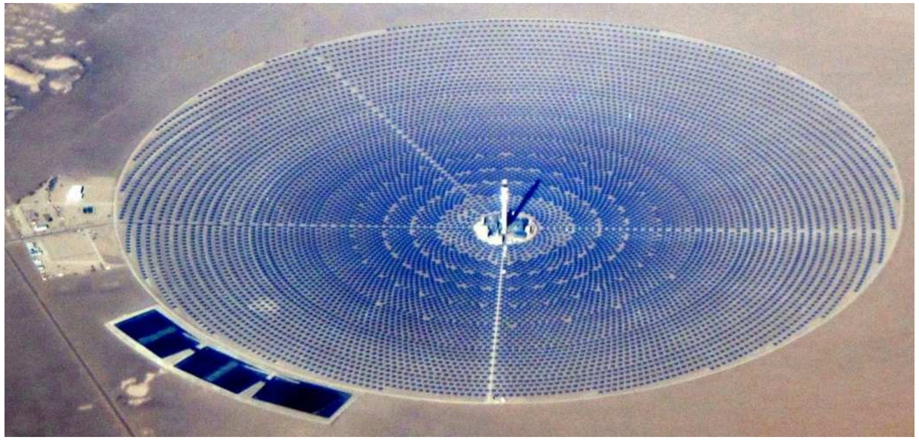
13+2 min



Motivation

- **energy** plays a central role in our society

- natural gas, **solar, battery**[1] and nuclear energy sources with the following characteristics
  - particles (or solid walls)
  - fluid = gas (**ideal gas law**)
  - temperatures above 1000 [°C]
  - **radiative transport**



https://en.wikipedia.org/wiki/Crescent_Dunes_Solar_Energy_Project

Golubkov et al., RSC Adv., 2018, 8, 40172

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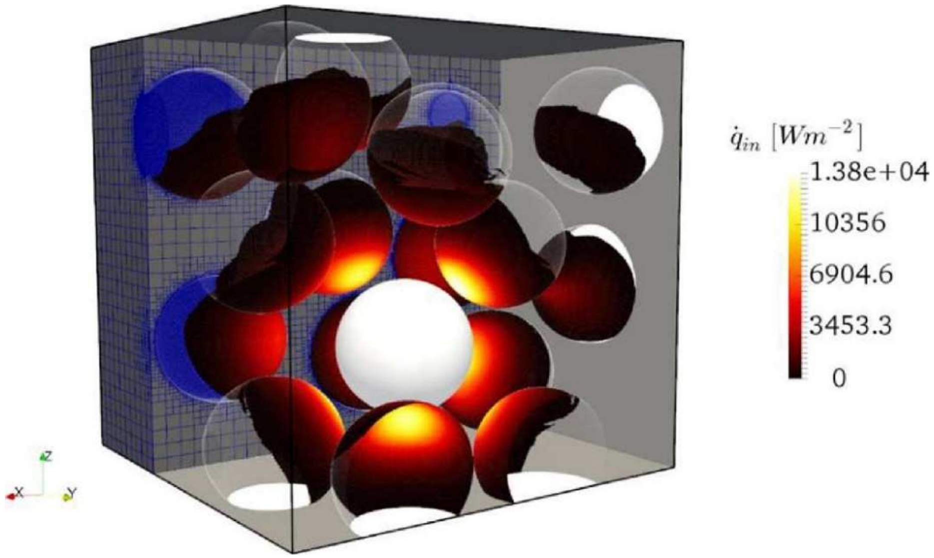
[1] during venting/thermal runaway

Motivation

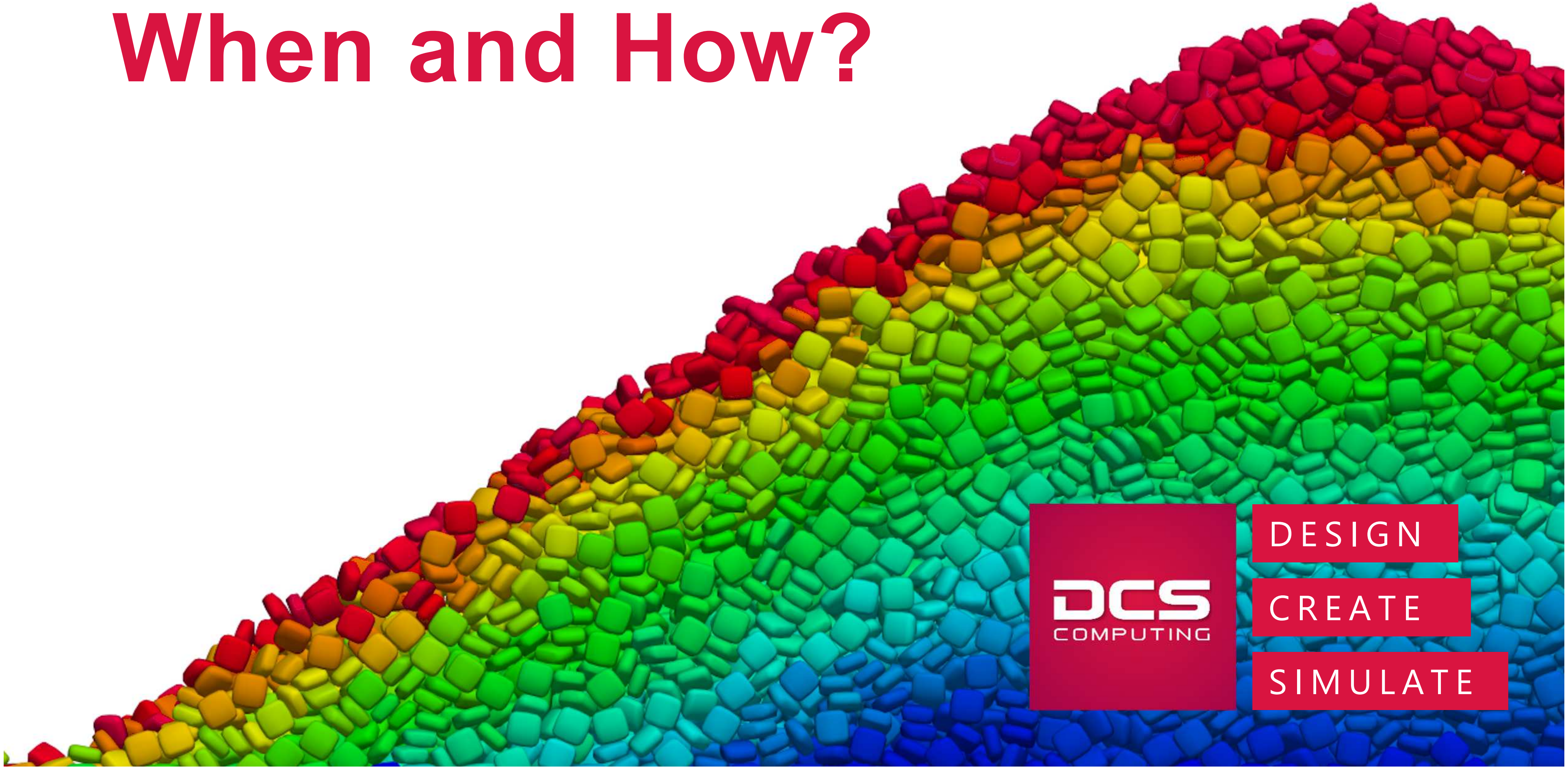
- „additional“ **computational cost** for radiation modeling, need for specialized compressible solver (more complex)
- **chemical reactions** may occur on surfaces at elevated temperature
- improvements in **predictive power** can be substantial (+/- 50 [K], +/-100% reaction rate!)



Forgber and Radl (Pow. Technol. 2018, 323, 24-44; doi:10.1016/j.powtec.2017.09.014)

PART 1

Compressibility: When and How?



DCS COMPUTING

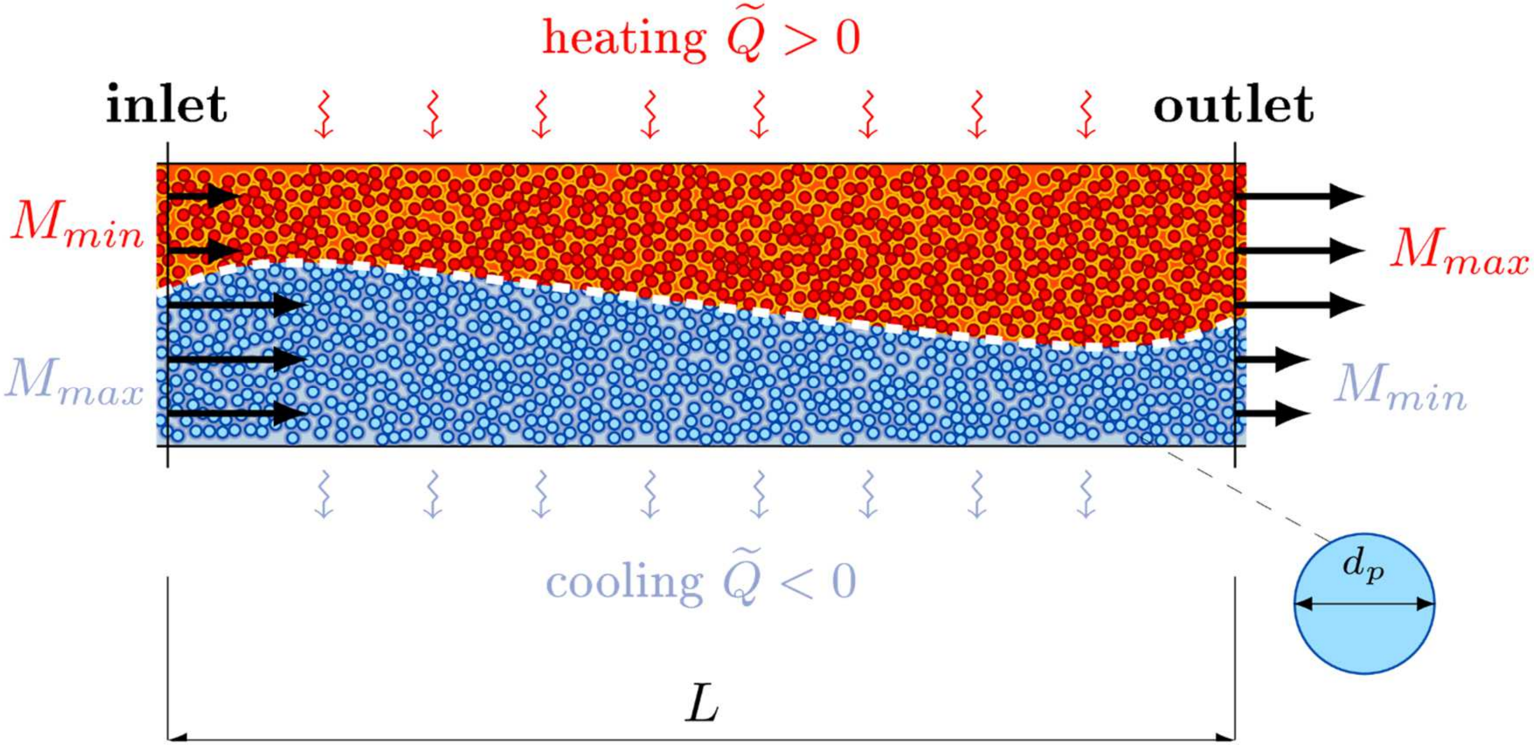
DESIGN

CREATE

SIMULATE

Heat transfer only

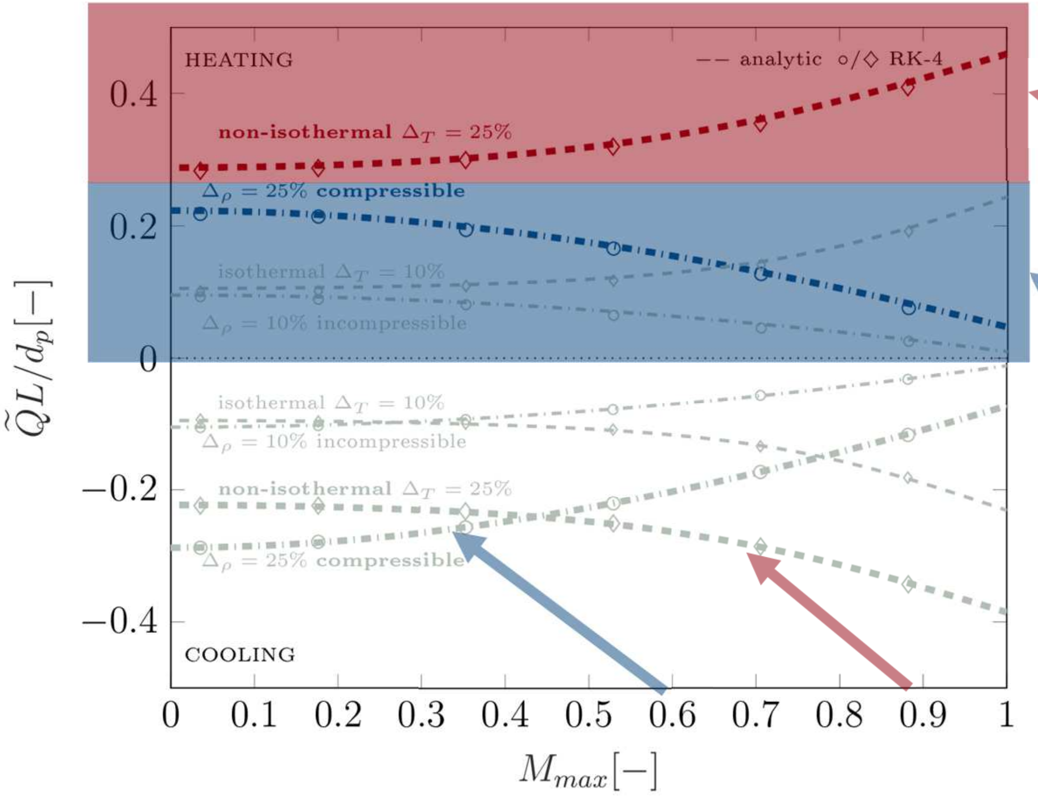
Mačak et al. (Pow. Technol. 2021, 394, 44-61; doi:10.1016/j.powtec.2021.08.017)



$$M^2 = \frac{u^2}{\kappa\, R\, T}$$

$$\tilde{Q} = \frac{6\,\phi_p}{Pr}\frac{Nu(Re,Pr)}{Re}\left(\frac{T_p}{T_{fluid}} - 1\right)$$

Heat transfer only



non-isothermal flow

$$\tilde{Q}\,\frac{L}{d_p} \geq 0.3$$

compressible flow

$$\tilde{Q}\,\frac{L}{d_p} \geq 0.2$$

- **non-isothermal heated flow** is always “compressible”
- bounding curves are **not symmetric**! Be careful if cooled or heated…

Conclusion Part 1

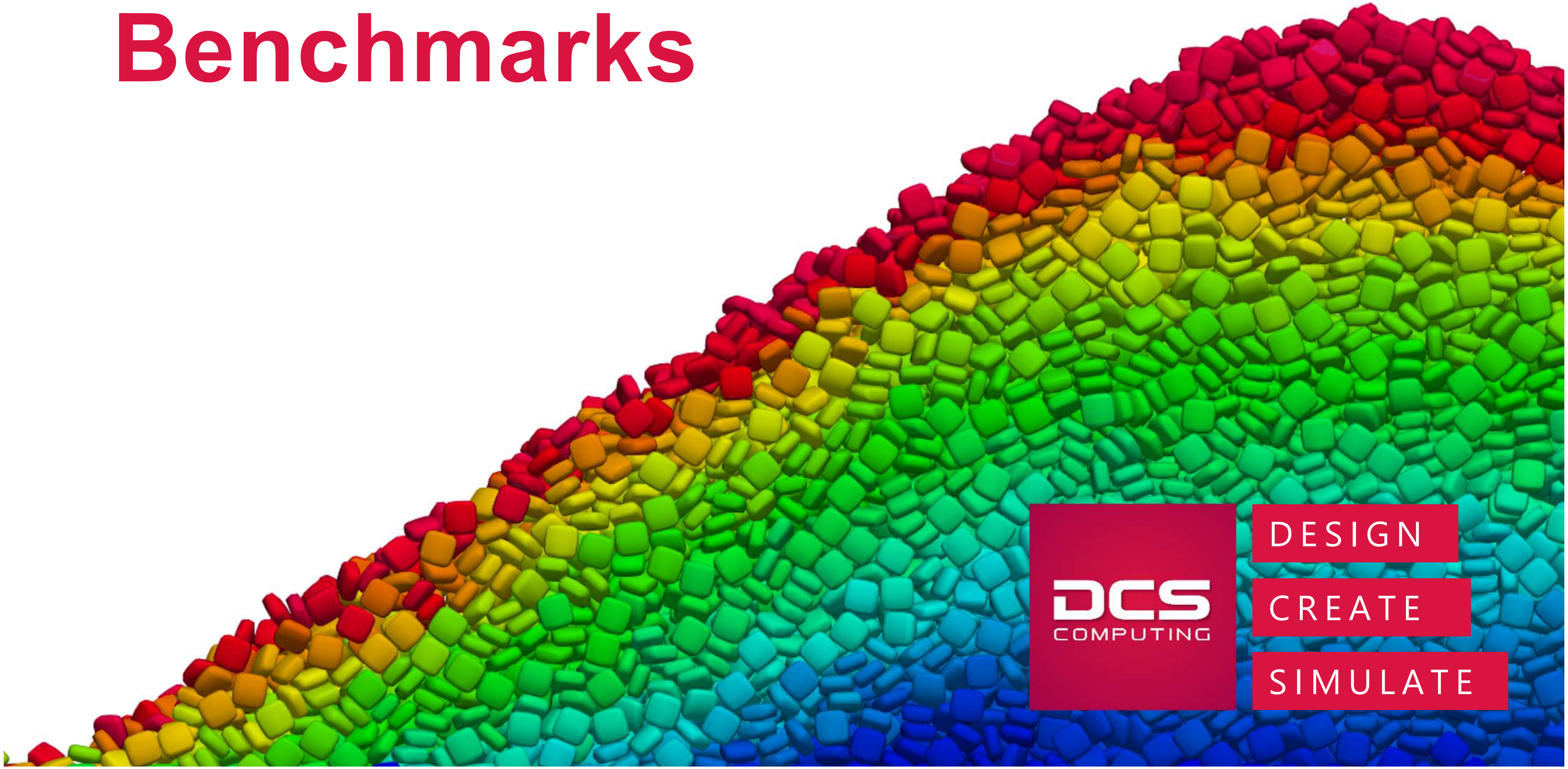
Dimensional analysis and laws of gas dynamics enable us to build a “**compressible or not” regime map** for gas-particle flows

Large particles appear more challenging with respect to **cluster-scale compressibility effects in FBs** than smaller ones. Reason: **length scale** of clusters increases strongly with particle size

Classical **CFD-DEM solvers** with variable density (**cfdemSolverRhoPimple**; will be soon available via https://github.com/CFDEMproject) show excellent agreement with (semi-)analytic solutions up to ***Ma*** **= 0.1 (<5% deviation)**. Need to push this limit…

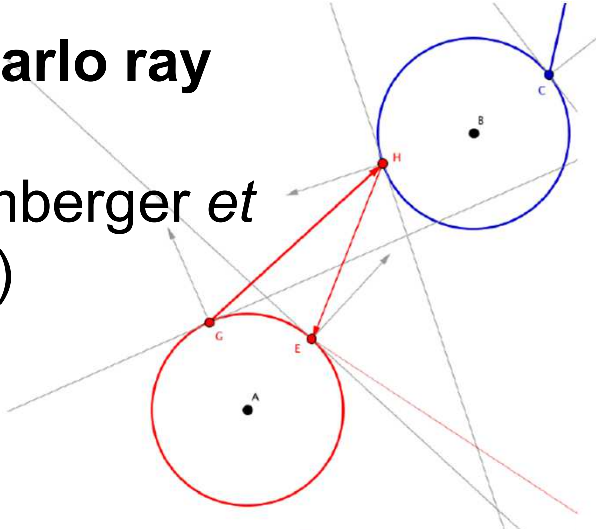
PART 2

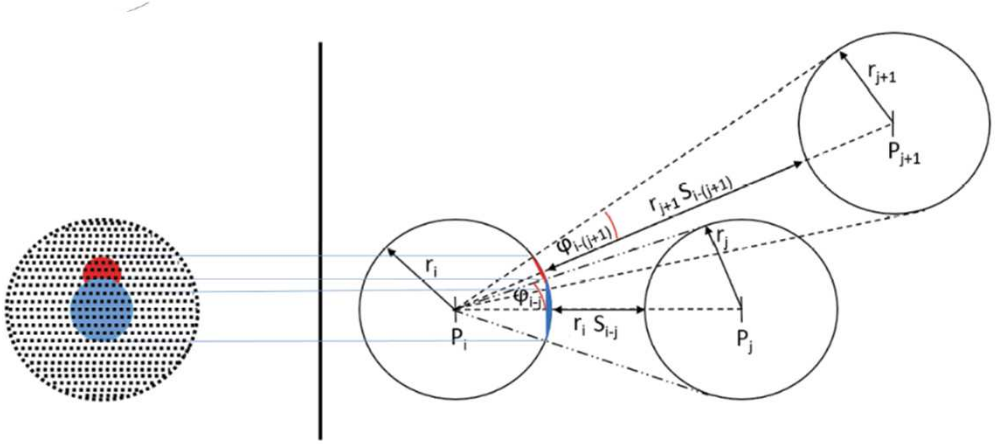
Radiation: P1 and Benchmarks

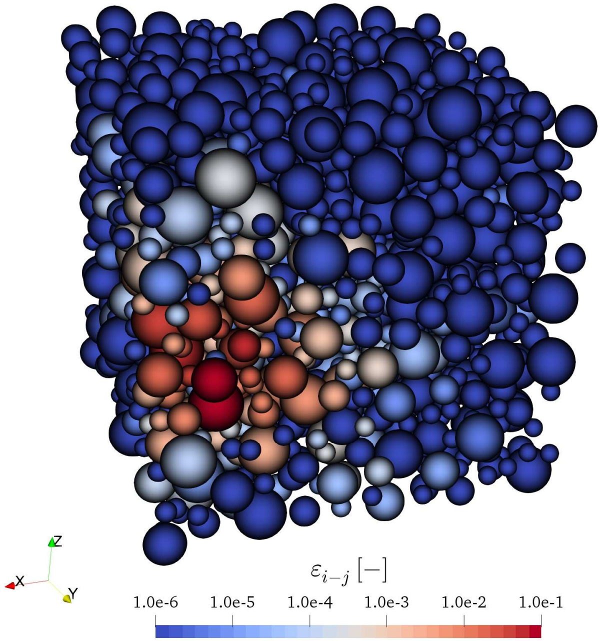


Particle-Based Radiation Modeling

Monte-Carlo ray tracing
(e.g., Amberger *et al*.,(2013)





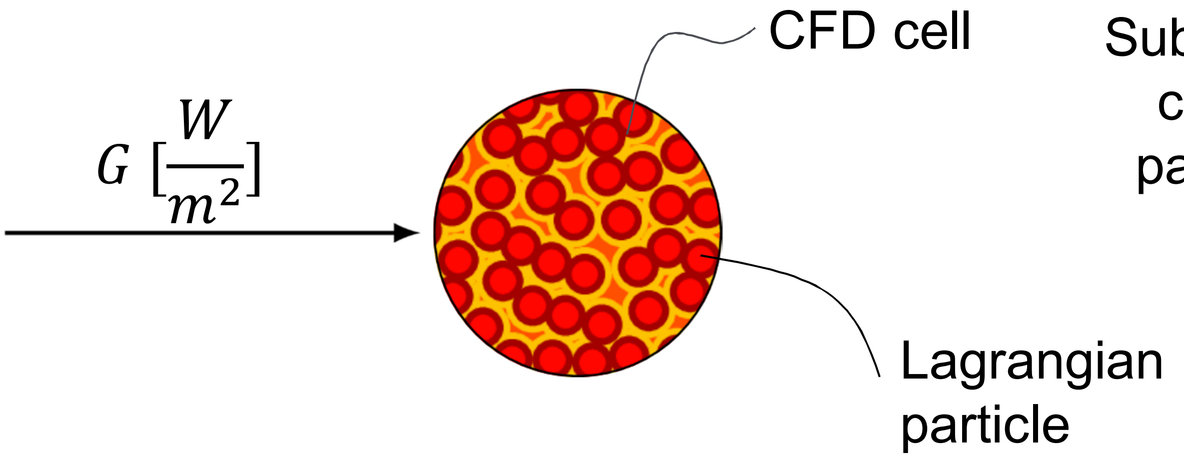


View factor-based
Forgber *et al*., 2018;
Tausendschoen *et al.*,
2021…2023

!!Computationally Expensive!!

P1 **continuum** approximation

…is a PDE for G: **the incident radiation ("what heats particles")**



Sub "p" quantities calculated from particle props. & positions

$$\nabla^2\left(\frac{1}{3(\kappa_f+\kappa_p)+\sigma_f+\sigma_p(3-A_1)}\,G\right)$$

$$=(\kappa_f+\kappa_p)G\ -4e_f\sigma T^4-E_p$$

total diffusivity Γ of radiation [m]

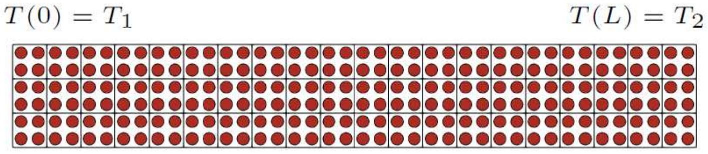
total absorption [W/m³]

fluid's emission [W/m³]

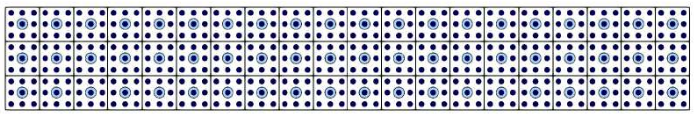
particles' emission [W/m³]

P1 benchmark I: packed bed

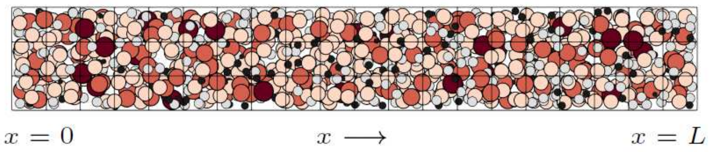
…**bed-average heat flux** calculated from G is well predicted…



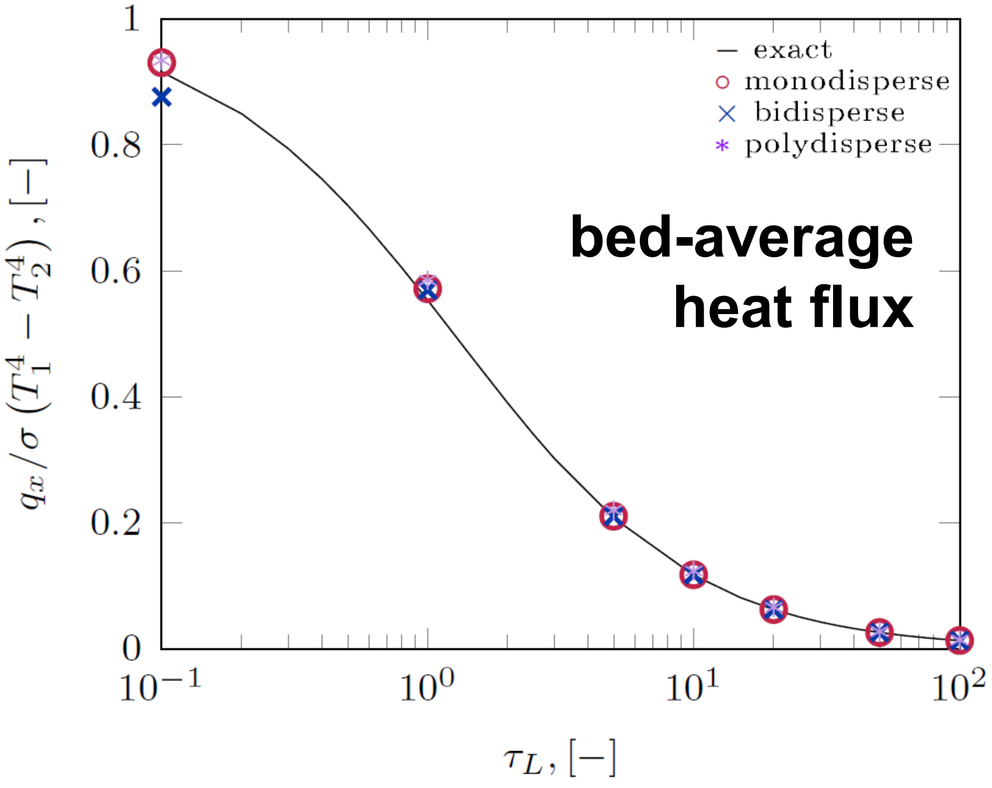
(a) monodispersion



(b) bidispersion



(c) polydispersion



bed-average heat flux

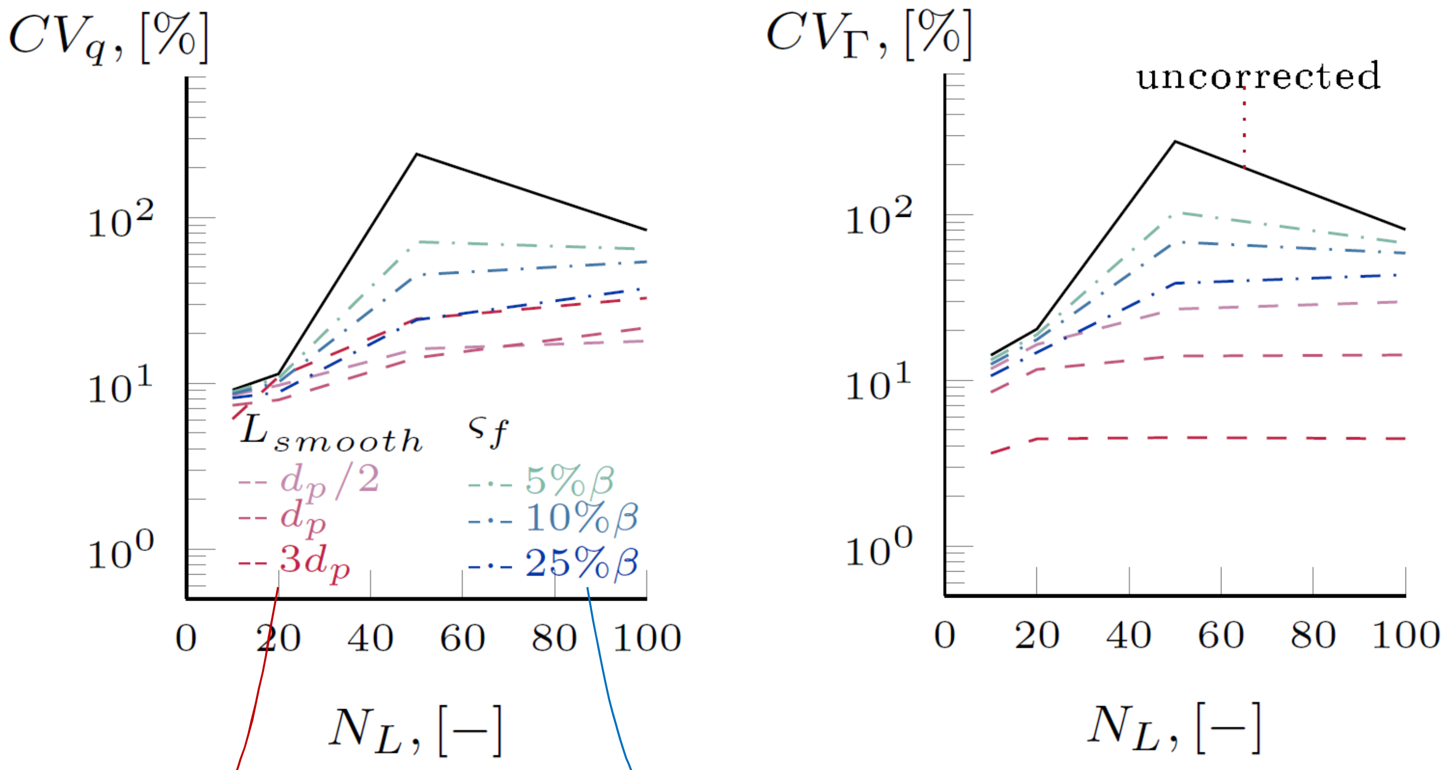
(optical thickness, opacity)

…and coarse grained variants, at steady state or transient (data not shown)

Mačak et al. (under preparation).

P1 benchmark I: packed bed

…however. the devil is in the detail: variation **within bed**

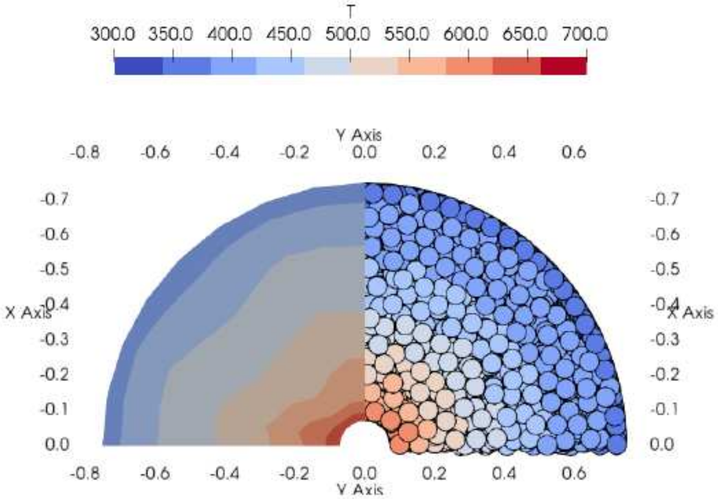


…Γ (diffusion) smoothing …or pseudo-scattering

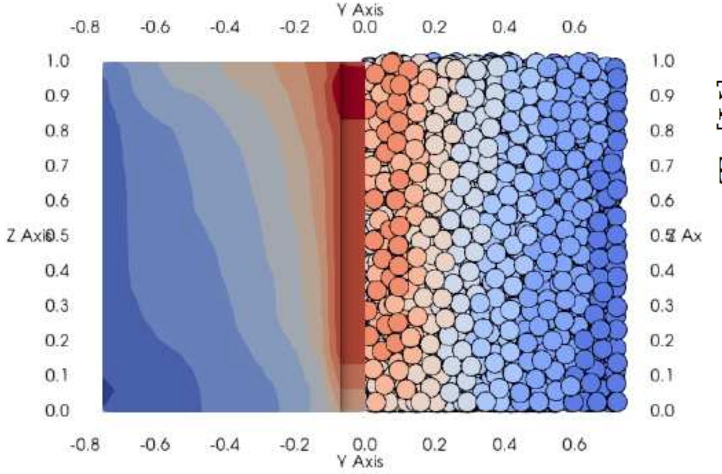
Mačak et al. (under preparation).

P1 benchmark II: cylindrical bed + N_2 flow

- height: 1 [m], diameter: 1.5 [m]
- **„full“ CFD-DEM solver** with variable density + radiation
- **calibration** of P-P conduction parameters (DEM side)

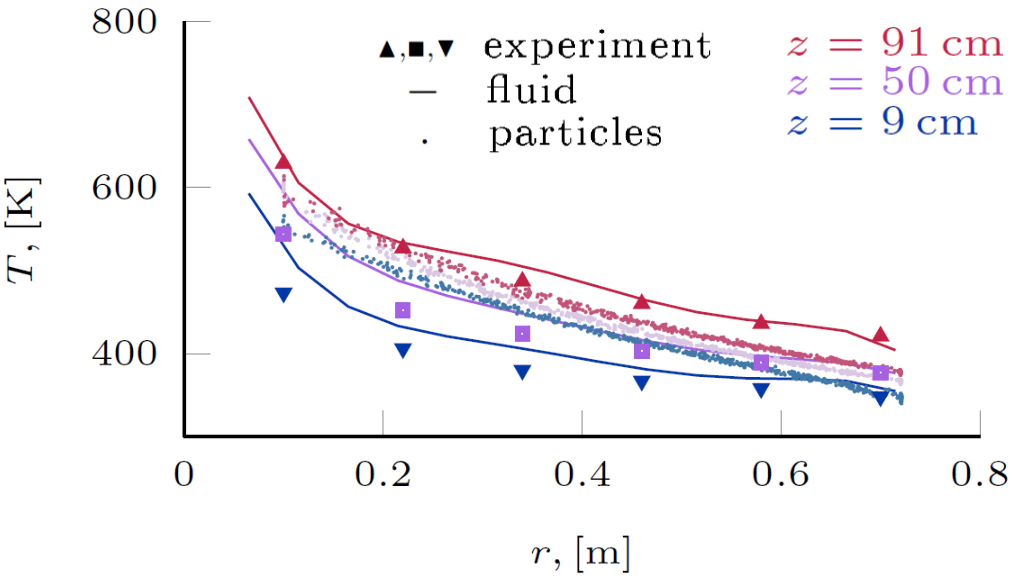


(a) 5 kW: top



(c) 5 kW: vertical cross-section

5 kW: full heat transfer, calibrated



Mačak et al. (under preparation).

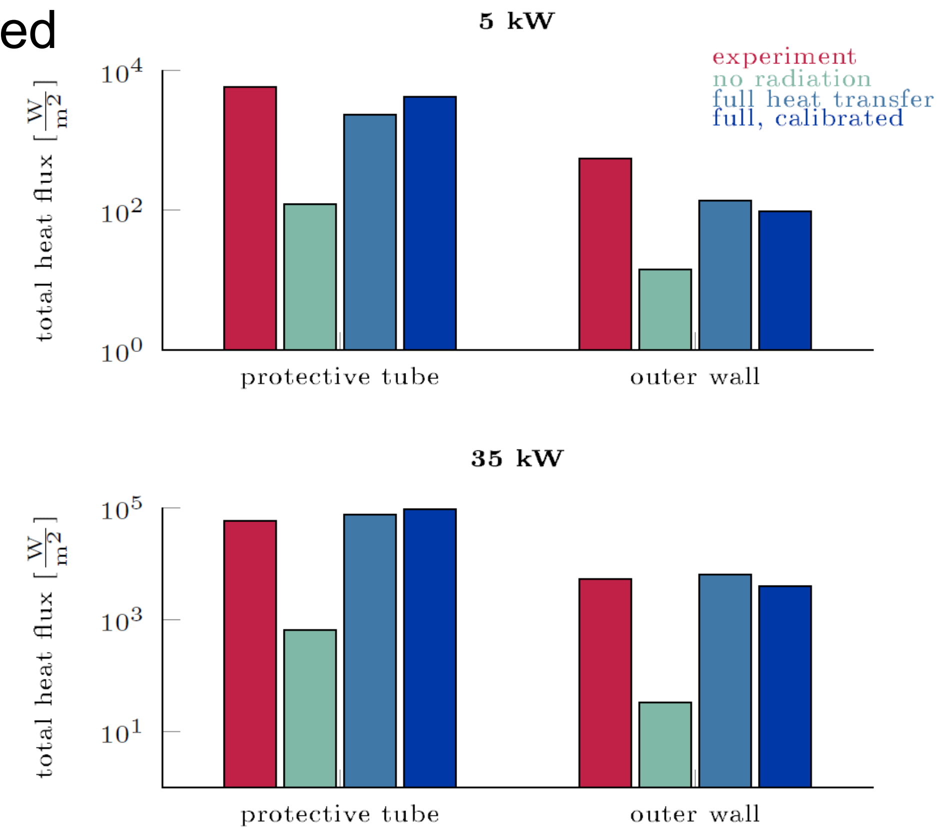
Conclusion Part 2

The P1 model **does an acceptable job** in “granular only” applications, if

- **appropriate (coarse) mesh**, or
- **Γ-smoothing**, or
- **pseudo-scattering** is employed

For gas-particle suspensions: calibration necessary to mimick conduction correctly (roughness, fluid at contact points)

(Buoyancy-driven) **fluid flow is still a challenge,** same as **intra-particle temperature distribution**



Mačak et al. (under preparation).

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MATHEGRAM

Thank you!

Questions?

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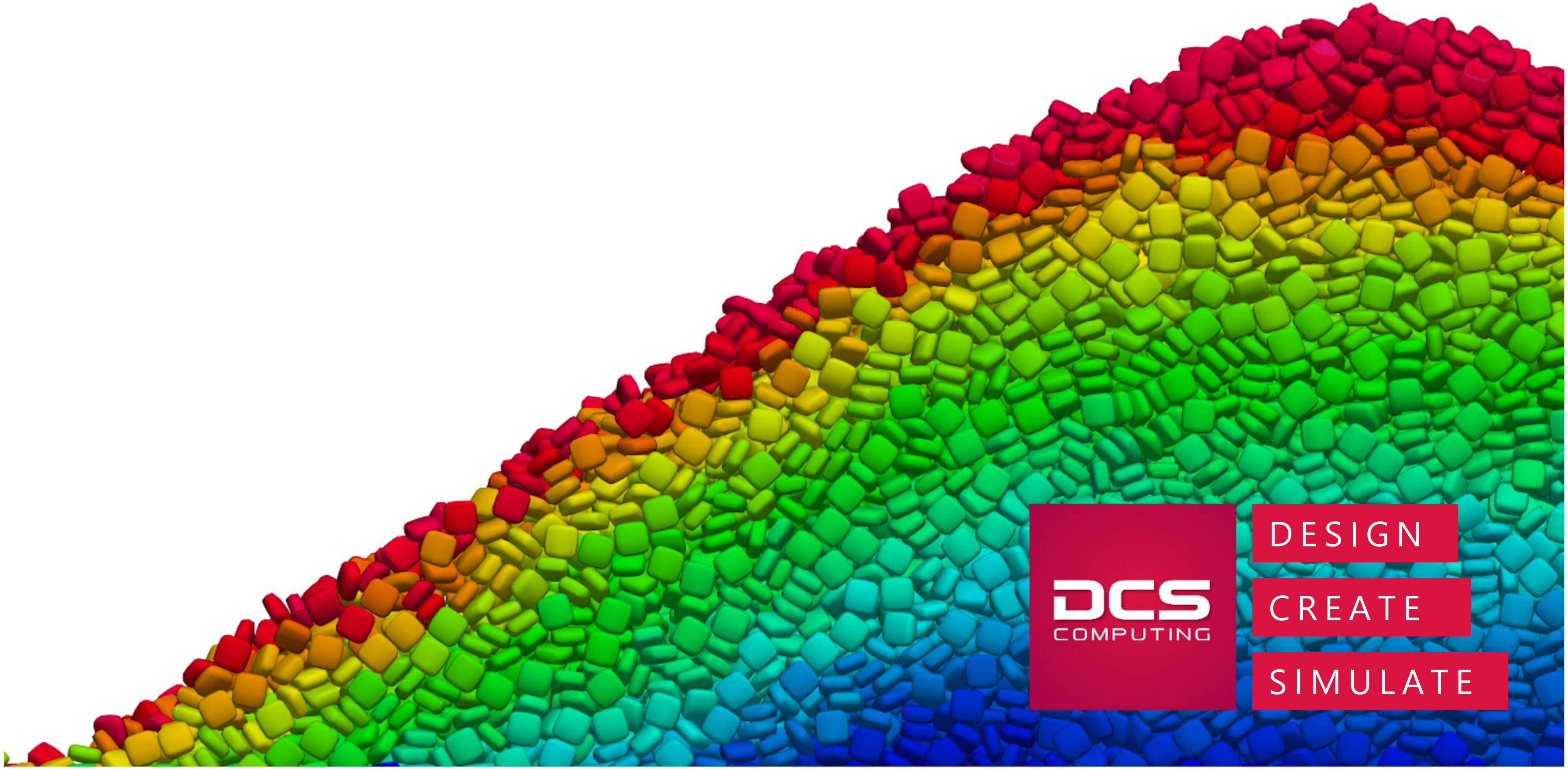
DCS COMPUTING

DESIGN
CREATE
SIMULATE

More Showcases



DCS COMPUTING

DESIGN

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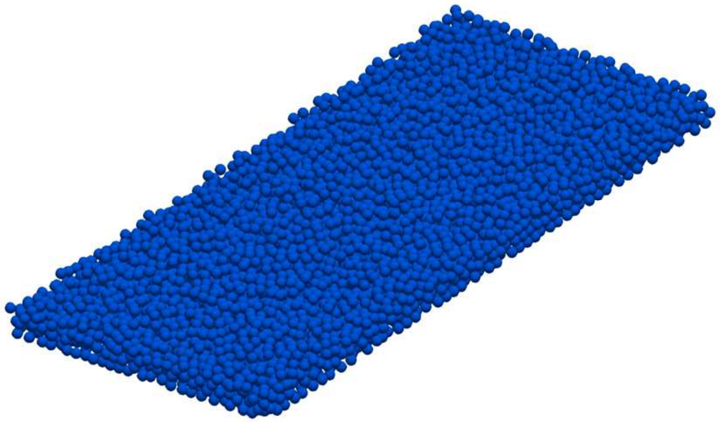
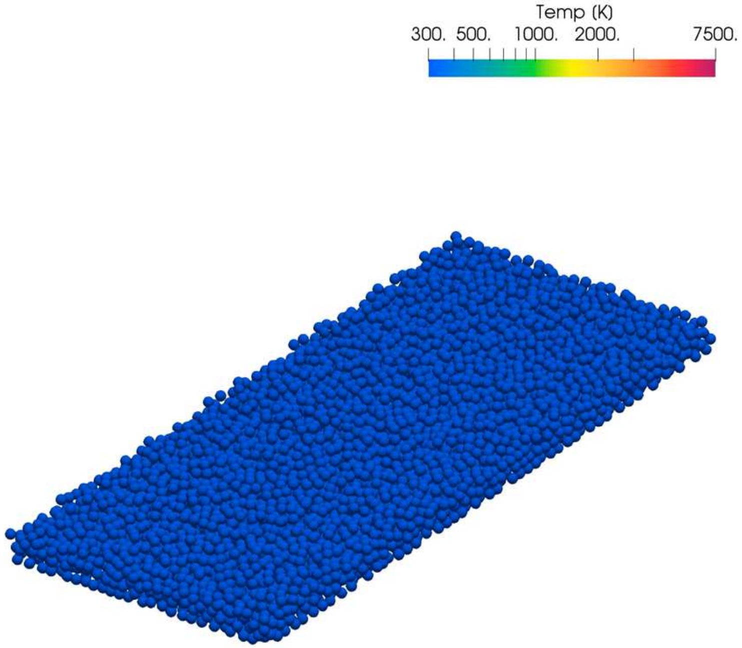
SIMULATE

Application: Laser heat source



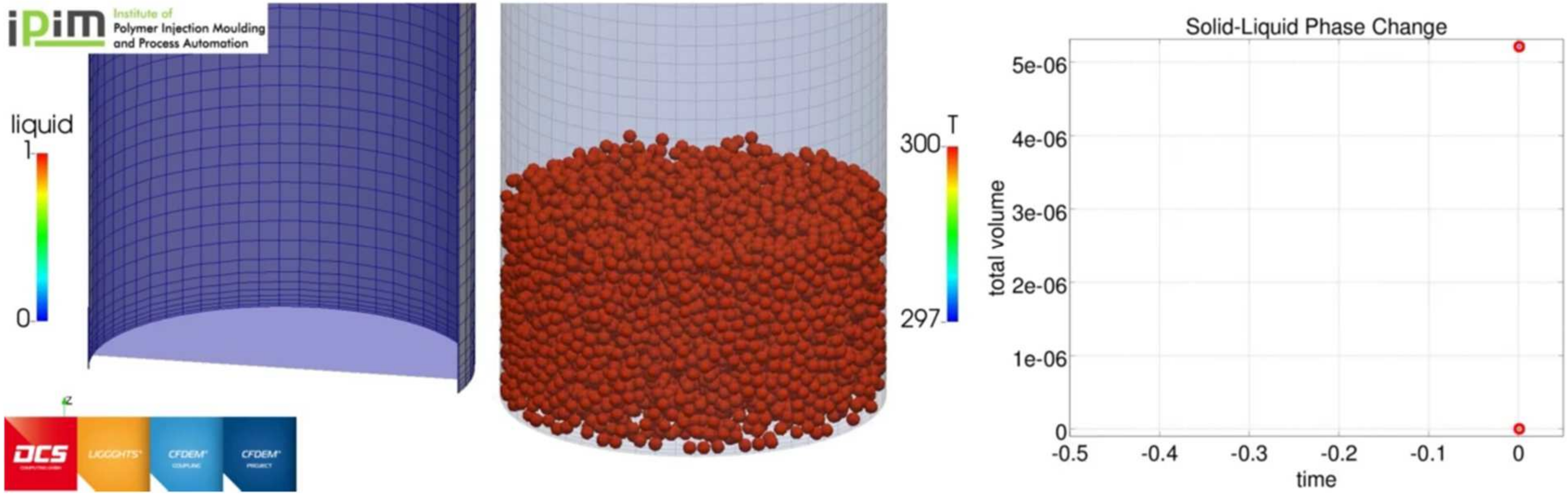
radiation



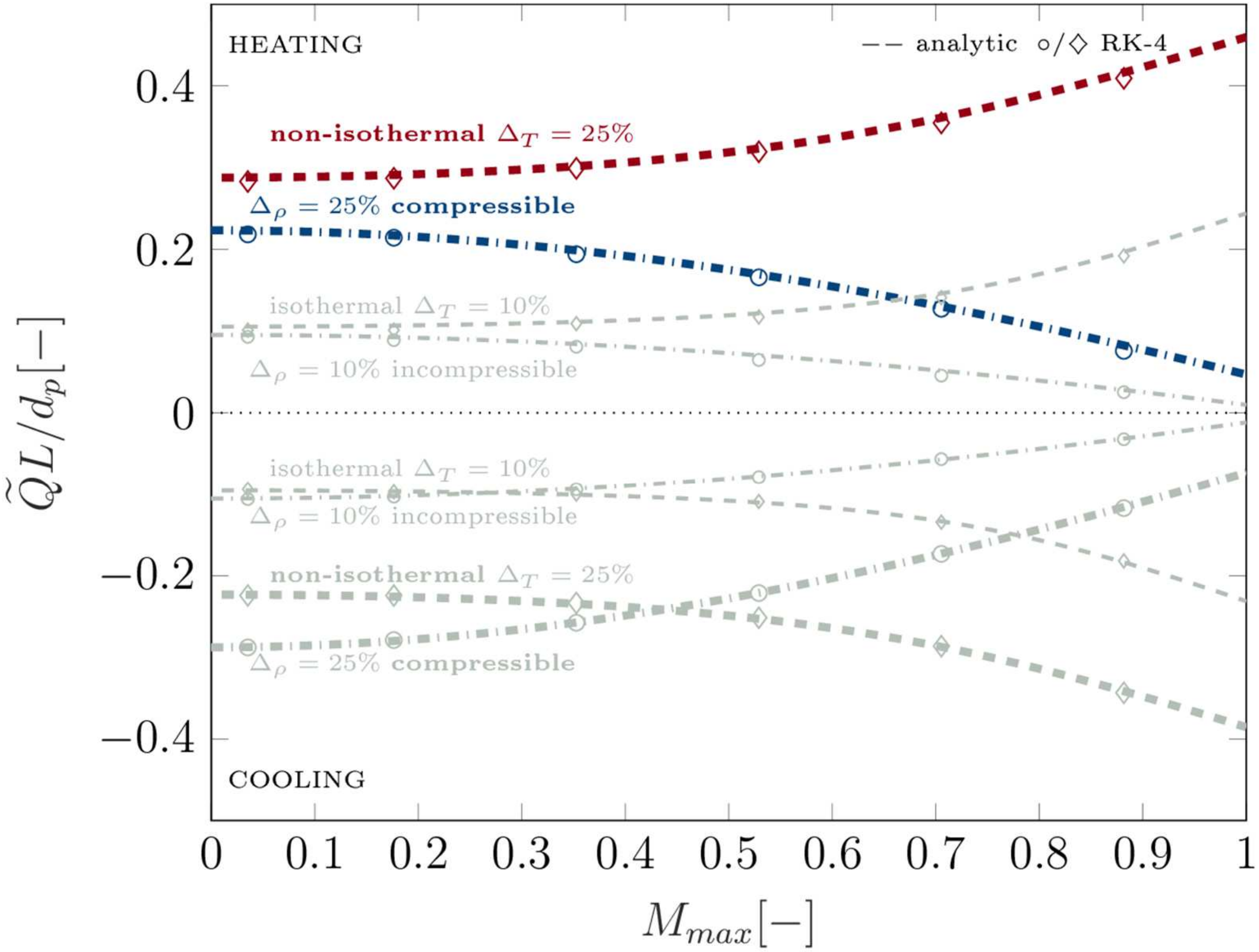
radiation +conduction

Application: towards selective laser melting

- phase change
- convective heat transfer with ambient gas
- substrate influence
- effect of temperature gradient on solid and fluid properties . . .



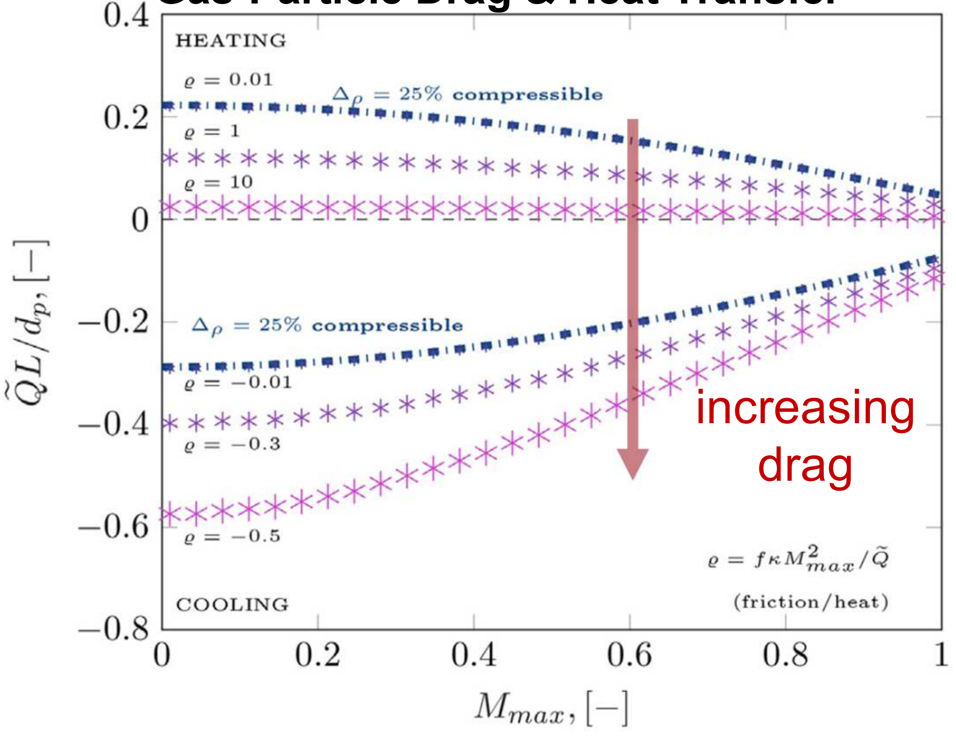
Heat transfer only



- dimensionless bed length is a **key player**
- a simple **map** to make a decision on closures and flow solver

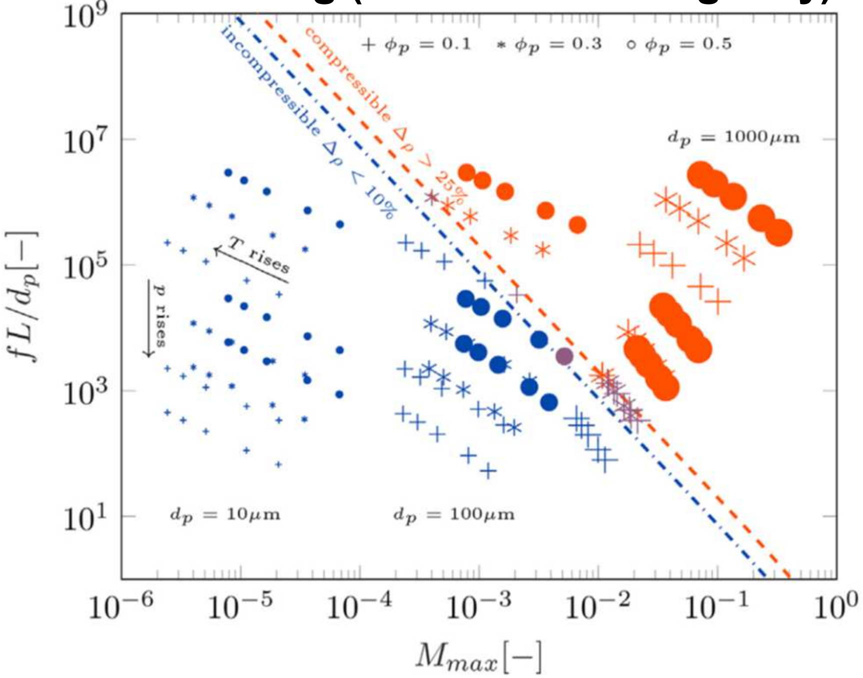
Phenomena Combos & Fluidized Bed App

Gas-Particle Drag & Heat Transfer



combinations of phenomena possible: semi-analytical solution

Clustering (Gas-Particle Drag only)



Application FB: **Low pressure** and **large particles** yield „more cluster-scale compressible“ problems