Large-scale phase-field sintering simulations of solid state sintering of metallic powders

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Goal

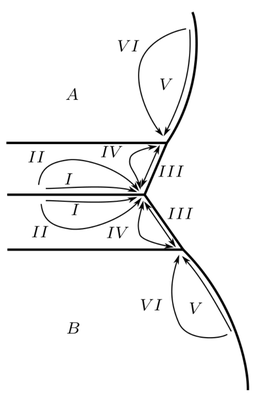
1. Find optimal sintering conditions which deliver parts with the highest densification and the desirable microstructure thus reducing the number of experiments and, therefore, the manufacturing costs.
2. Study how variation of different processing parameters (temperature, time, heating and cooling rates, etc.) influences the obtained densification and microstructure.

Requirements to the modeling tools

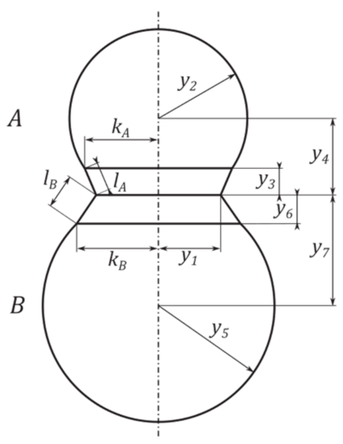
Plausibility	• Both densification and microstructure evolution should be captured
Convenience	• The calibration of the model should be relatively simple and straightforward
Scalability	• The approach should be applicable to packings with large number of particles
Performance	• The simulations should run as fast as possible on either a single PC or a cluster

Computational models

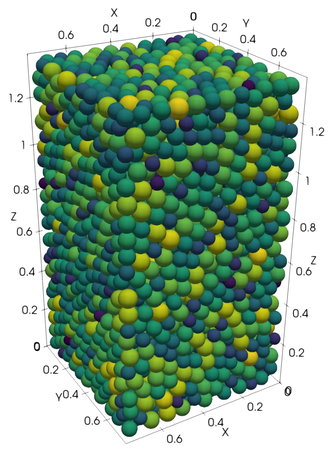
7DoF model | **Discrete element (DEM) model** | **Phase-field (PF) model**



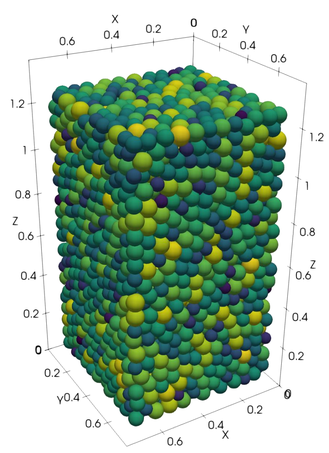
Diffusion paths



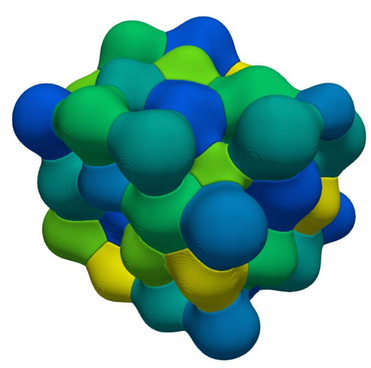
Degrees of freedom



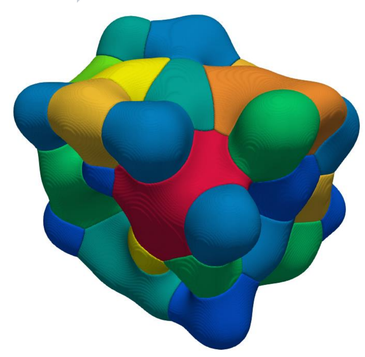
Initial configuration



Final configuration



Early stage sintering



Later stage sintering

Model	Main usage	Plausibility			Convenience	Scalability	Performance
7 DoF	Extract material data from experiments	✔ shrinkage	✔ neck growth	✕ grain growth	Easy to calibrate	2 particles	High
DEM	Early stage sintering	✔ shrinkage	✔ neck growth	✕ grain growth	Easy to calibrate	> 10,000 particles	High
PF	Later stage sintering	✔ shrinkage	✔ neck growth	✔ grain growth	Difficult to calibrate	< 10,000 particles	Low

References:

Thomsen F., et al. (2018): An elementary simulation model for neck growth and shrinkage during solid phase sintering. Materialia 3:338-346. https://doi.org/10.1016/j.mtla.2018.08.031

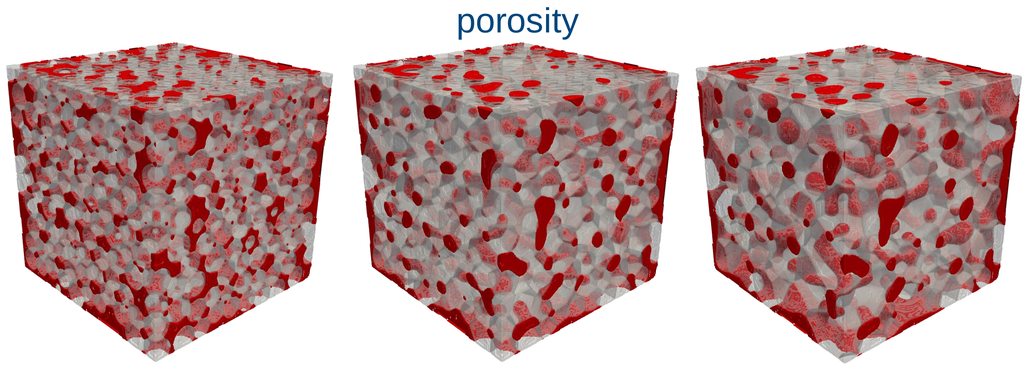
Ivannikov V., et al. (2022): Coupling the discrete element method and solid state diffusion equations for modeling of metallic powders sintering. Computational Particle Mechanics. https://doi.org/10.1007/s40571-022-00486-6

Ivannikov V., et al. (2021): Capturing shrinkage and neck growth with phase field simulations of the solid state sintering. Modelling and Simulation in Materials Science and Engineering 29(7):075008. https://doi.org/10.1088/1361-651X/ac1f87

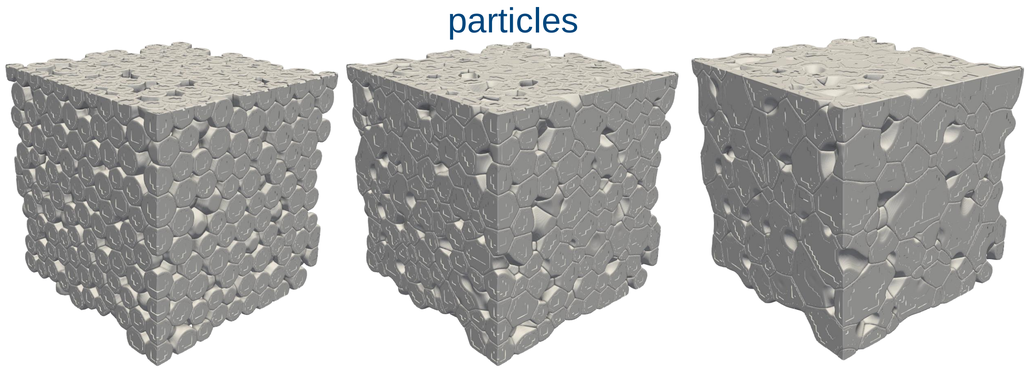
Munch P., et al. (2024): On the construction of an efficient finite-element solver for phase-field simulations of many-particle solid-state-sintering processes. Computational Materials Science 231:112589. https://doi.org/10.1016/j.commatsci.2023.112589

Large-scale phase-field simulations

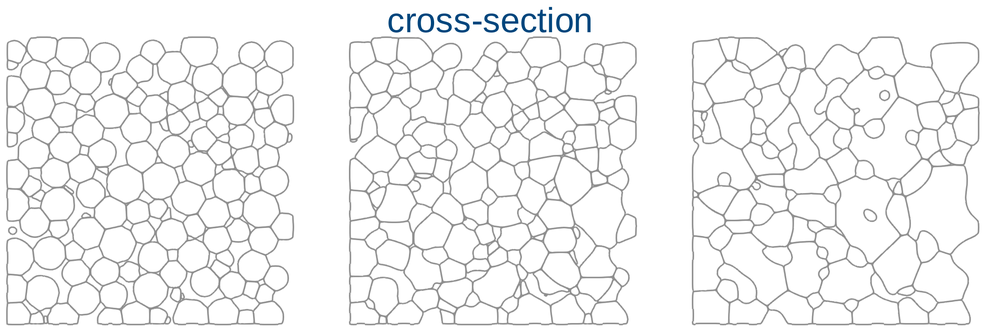
porosity



particles

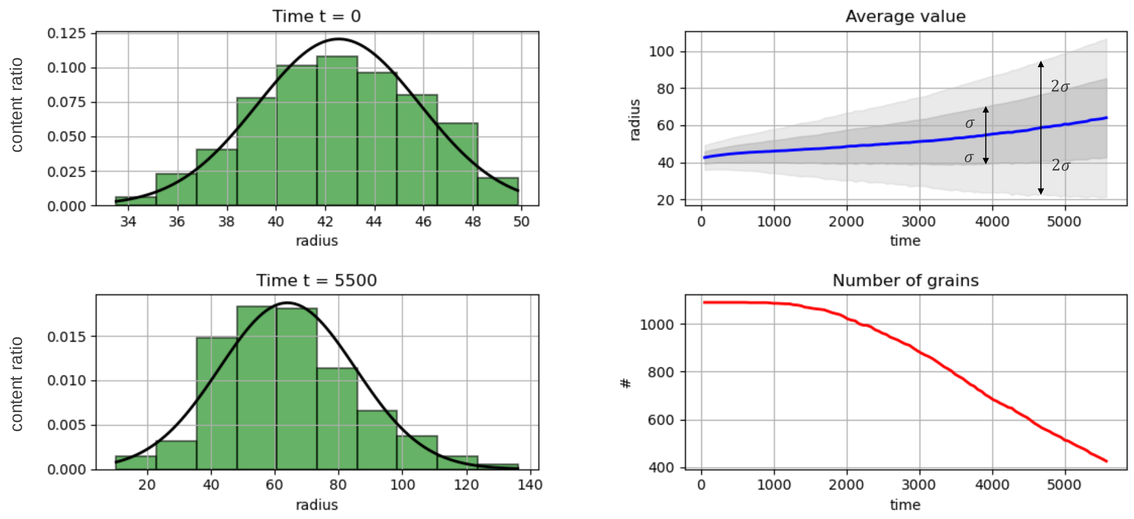


cross-section

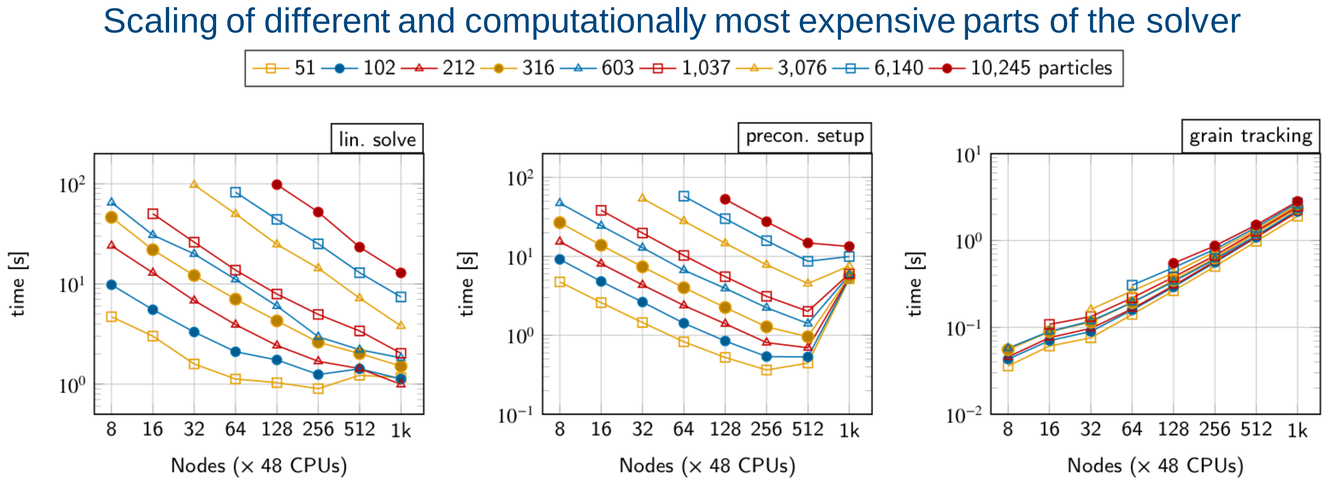


t=0 *t=1000* *t=5500*

Evolution of the grain size distribution during sintering



Scaling of different and computationally most expensive parts of the solver



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