SAND2011-1697C

COMPUTATIONAL MODELING OF FIELD-ASSISTED SINTERING

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TMS2011

February 27-March 3, 2011 – San Diego, California

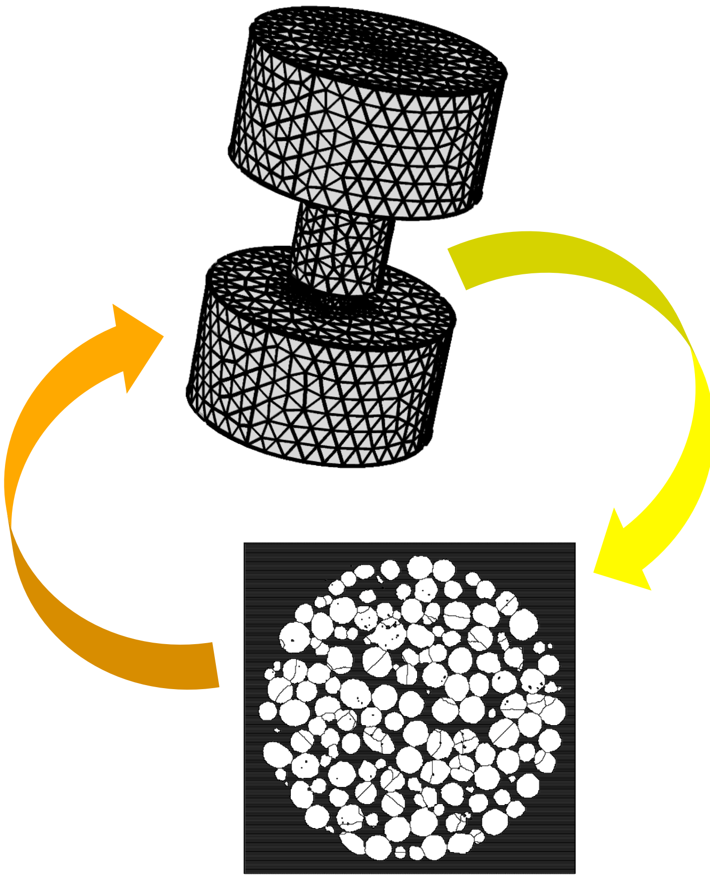
Outline

- Field Assisted Sintering
- Finite Element Analysis (Macroscopic scale)
  - Electrical – Thermal Components
  - Sintering Constitutive Equation
  - Coupling of Components
- Kinetic Monte Carlo Simulation (Mesoscopic scale)
  - Mechanisms of Mass Transport
  - Microstructure Evolution
- Results
- Conclusions

Field Assisted Sintering Technique (FAST)

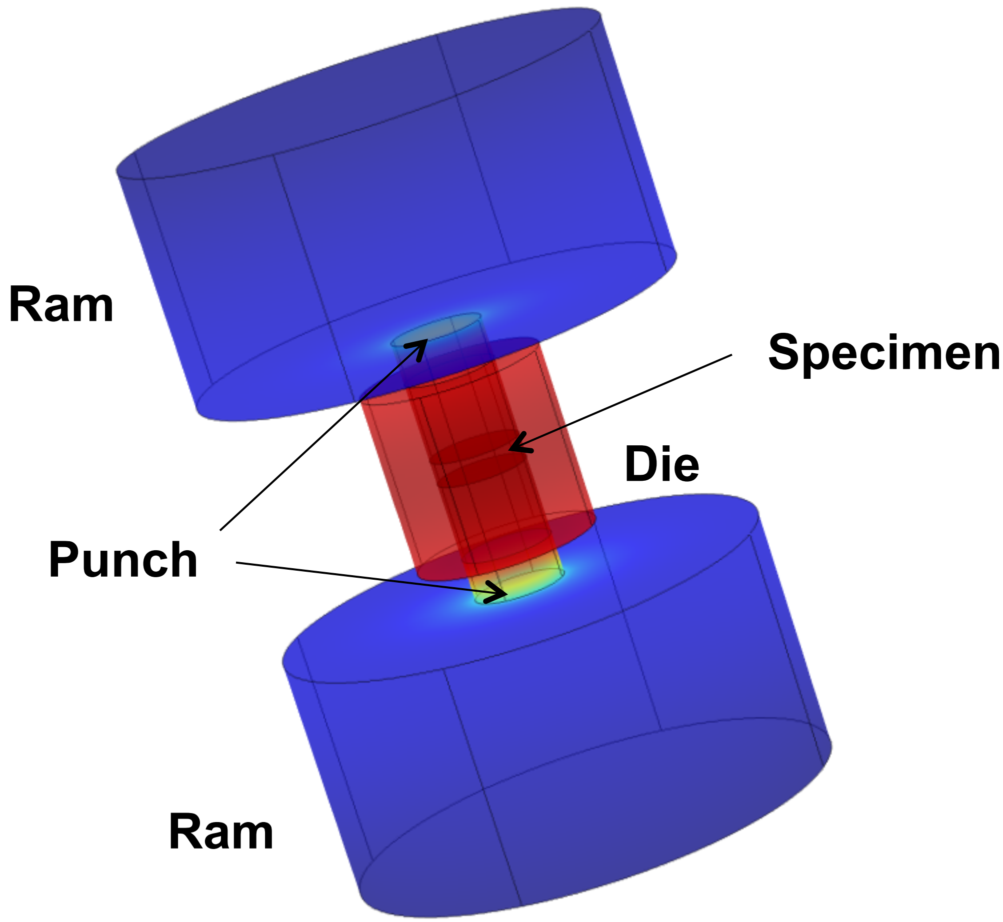
- Non-conventional powder consolidation (FAST, ECAS, SPS)
- Application of an electrical discharge which induces rapid heating (Joule heating)
- Sintering is enhanced: higher densities in shorter times

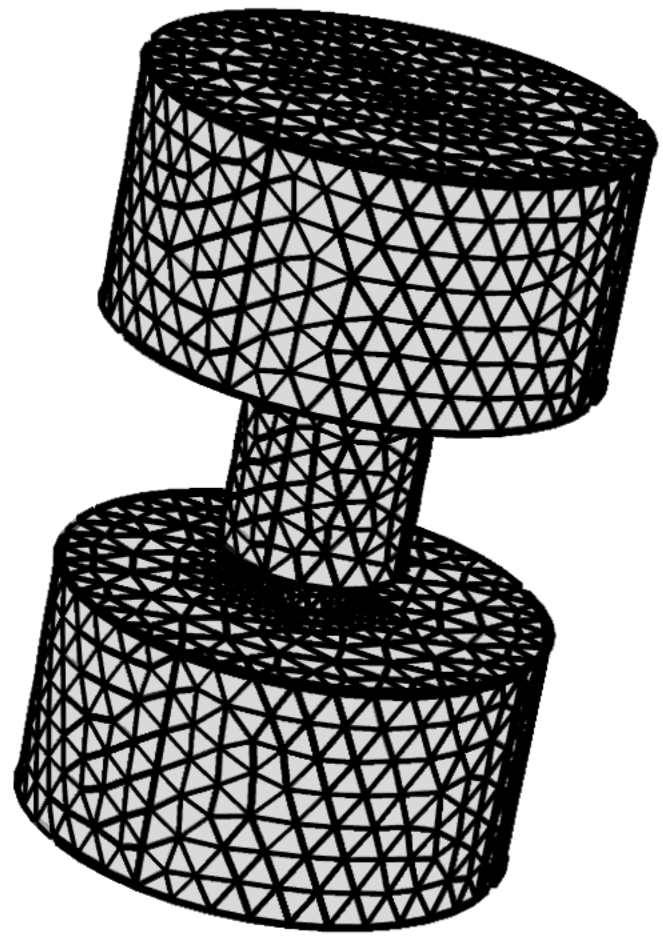
FAST - Computational Modeling



- Gain insight into FAST
- Couple multi-physics phenomena
- Simulate densification using local conditions
- Correlate / incorporate microstructure information

Finite Element Analysis (FEA) - COMSOL





FEA - Coupled Components I

$$-\nabla \cdot (\sigma_{el} \nabla V) = 0$$

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k_T \nabla T) = \sigma_{el} \left| \nabla V \right|^2$$

Variables: ***T*, *V*, *t***

Parameters: ***ρ*, C_p, k_T, σ_{el}**

- **Thermal and electrical conduction problems coupled: material parameters depend on T**

FEA – Densification Description

$$\sigma_{ij} = \frac{\sigma(W)}{W}\left[\varphi\,\dot{\varepsilon}_{ij} + \left(\psi - \frac{1}{3}\varphi\right)\dot{e}\,\delta_{ij}\right] + P_L\,\delta_{ij}$$

Functions of Porosity

Macro-scale State

Applied stress	σ_{ij}
Equivalent Strain Rate	W
Strain rate	$\dot{\varepsilon}_{ij}$
Shrinkage rate	$\dot{e}$

Functions of Porosity

Sintering stress	$P_L = P_{L0}(1-\theta)^2$
Bulk viscosity mod.	$\psi = \frac{2}{3}\frac{(1-\theta)^3}{\theta}$
Shear viscosity mod.	$\varphi = (1-\theta)^2$

E. A. Olevsky. “*Theory of sintering: from discrete to continuum*”. Materials Science and Engineering, R23 (1998), pp. 41-100.

FEA - Coupled Components II

Electrical Conduction

$$-\nabla \cdot (\sigma_{el} \nabla V) = 0$$

Heat Transfer by Conduction

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k_T \nabla T) = \sigma_{el} \left|\nabla V\right|^2$$

Sintering Constitutive Equation

$$\sigma_{ij} = \frac{\sigma(W)}{W}\left[\varphi \dot{\varepsilon}_{ij} + \left(\psi - \frac{1}{3}\varphi\right)\dot{e}\,\delta_{ij}\right] + P_L \delta_{ij}$$

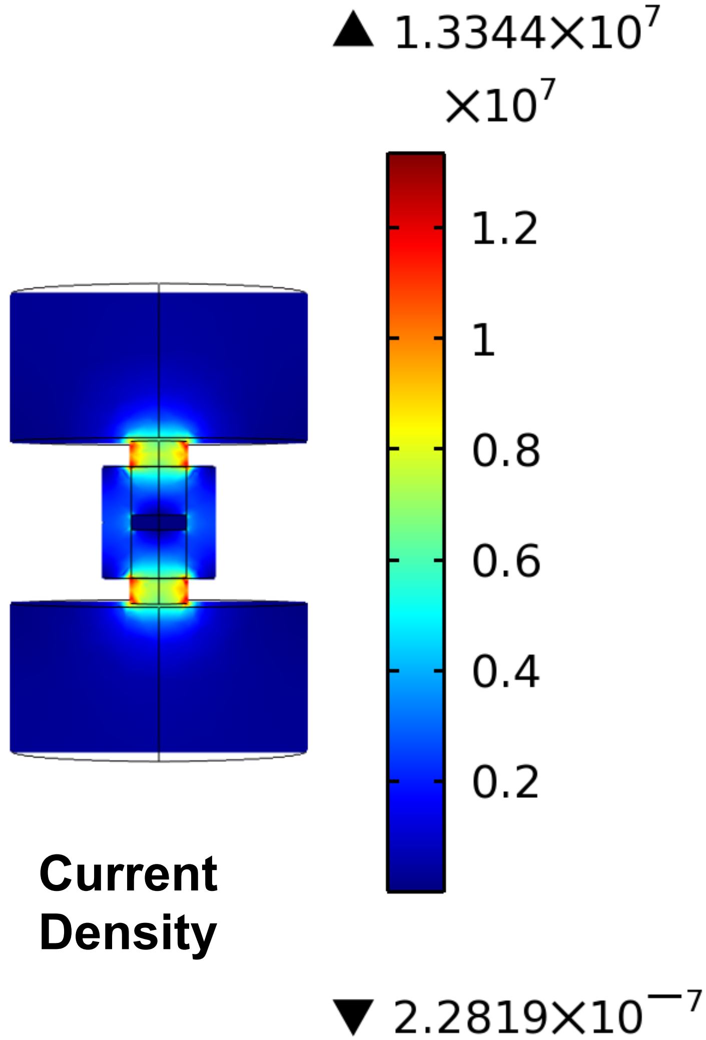
Densification

$$\frac{\dot{\theta}}{1-\theta} = \dot{e}$$

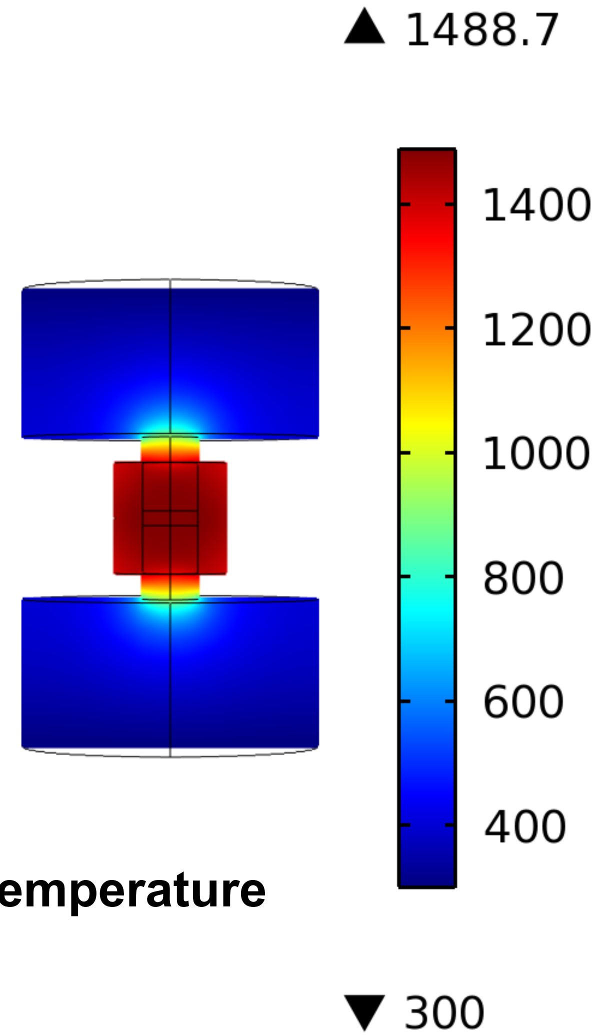
$$\sigma(W) = A W^m$$

$$A = \tilde{A} T^m \exp\left(\frac{m\,\Delta H_{SD}}{RT}\right)$$

Results – FEA – FAST

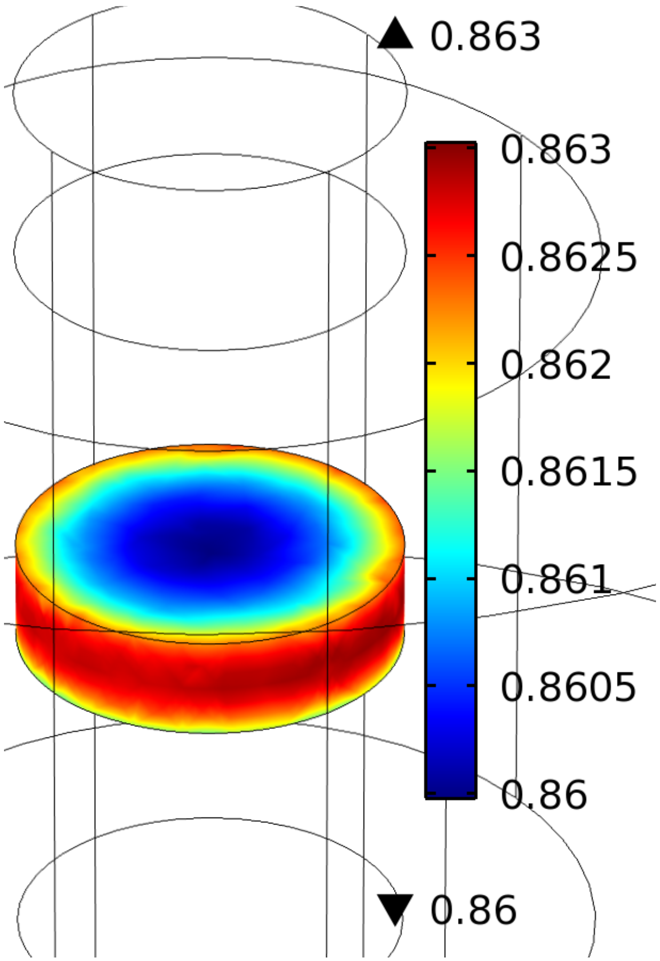


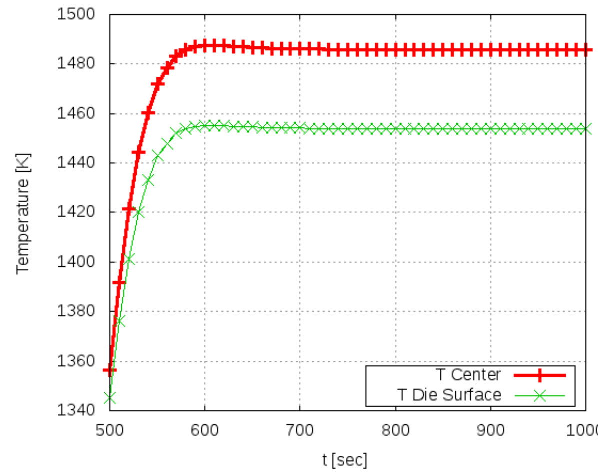
Current Density

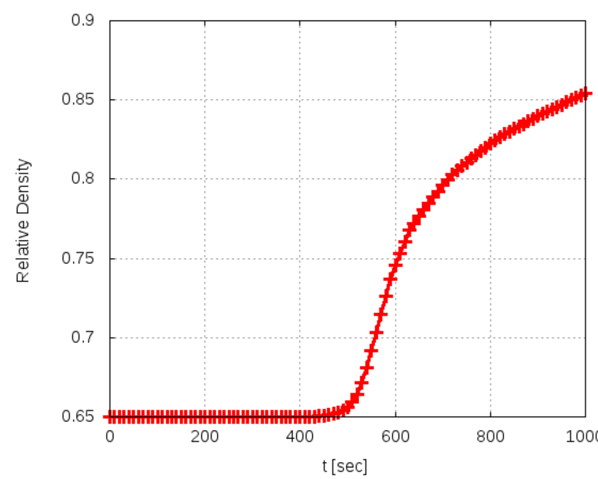


Temperature

Results – FEA – FAST





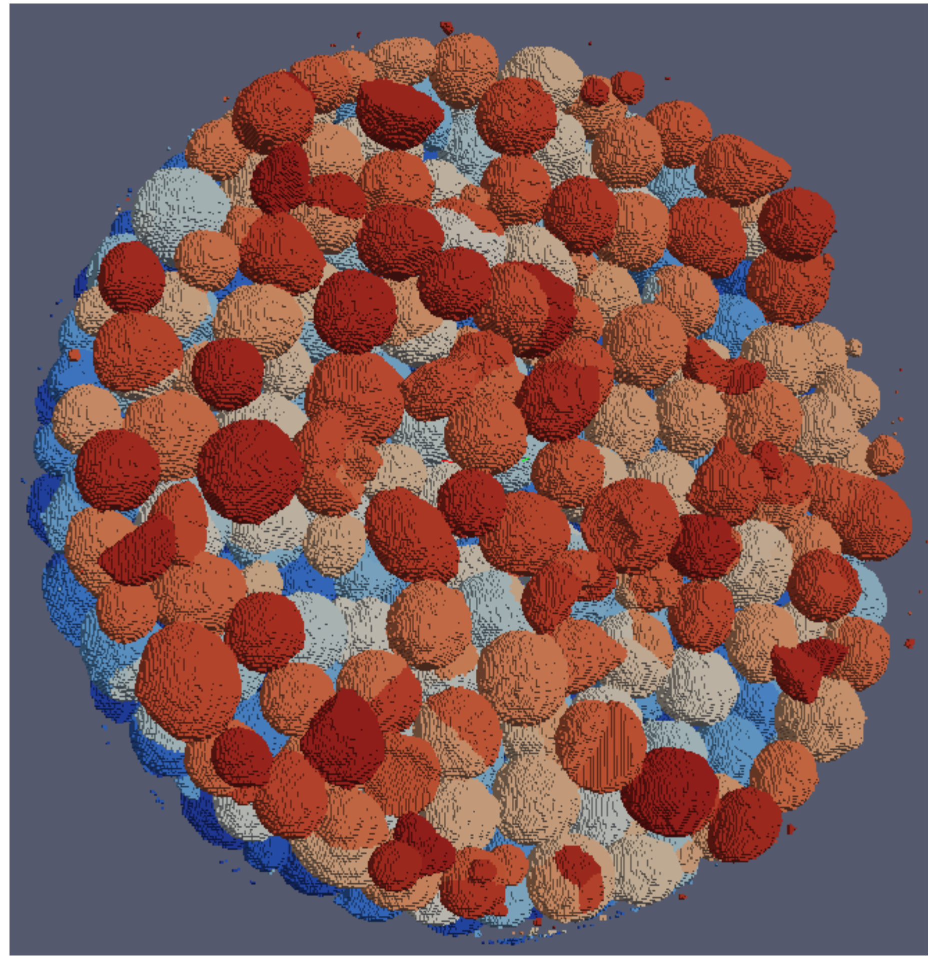


FEA Simulation – Challenges

- Material parameters are difficult to obtain
- Constitutive parameters are approximate (analysis of simplified microstructures)
- More realistic scenario is to consider the pore-grain structural evolution
- Need to investigate inter-particle neck for better understanding of FAST
- Conventional model: no field effects considered

Kinetic Monte Carlo Simulation (kMC)

- **Monte Carlo simulation: useful for systems whose complexity renders them intractable by other formal means**
- **kMC + Sintering: simple model providing insight about the mechanisms of mass transport**
- **kMC + Sintering + Parallel implementation: ability to include larger number of particles (SPPARKS)**



kMC Model - Description

1. Simulation space: 3D cubic lattice
2. Events: Mechanisms of mass transport
3. Evolution: Metropolis Algorithm

$$P = \begin{cases} \exp\left(\dfrac{-\Delta \mathrm{E}}{\mathrm{k_B} T}\right) & for \quad \Delta \mathrm{E} > 0 \\ 1 & for \quad \Delta \mathrm{E} \leq 0 \end{cases}$$

4. Energy Function: interfacial free-energy

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{26}(1-\delta(q_i, q_j))$$

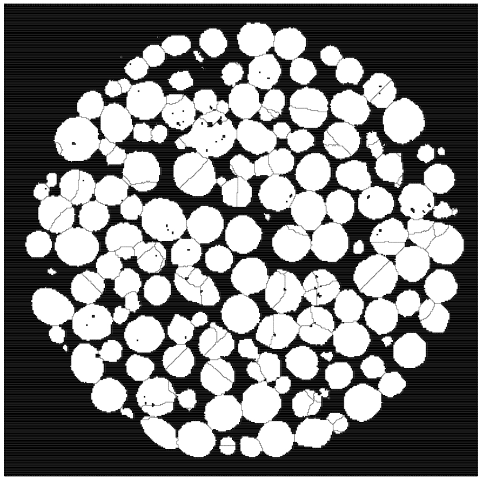
kMC Model – Mass Transport Mechanisms

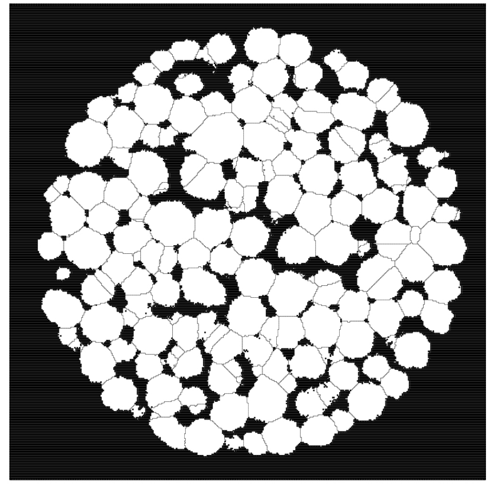
- Grain Growth
  - Short-range diffusion of atoms
  - Pinning caused by evolving porosity
- Pore Migration
  - Surface diffusion leading to pore shape evolution and coarsening
- Vacancy Formation and Annihilation
  - Grain boundary diffusion of vacancies
  - Vacancy annihilation leading to densification

M. Braginsky, V. Tikare and E. Olevsky. "*Numerical simulation of solid state sintering*". International Journal of Solid and Structures, 42 (2005), pp. 621-636.

kMC – Microstructure Evolution

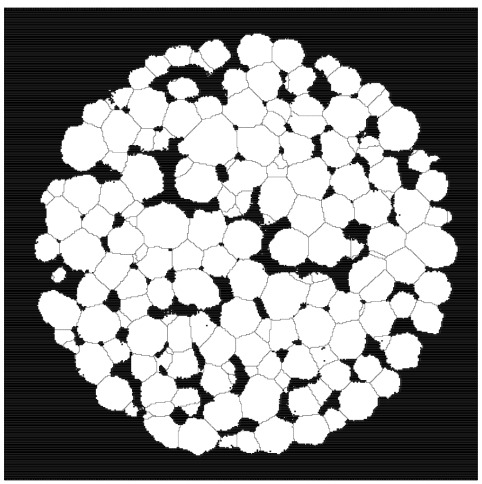
0 MCS
69 %

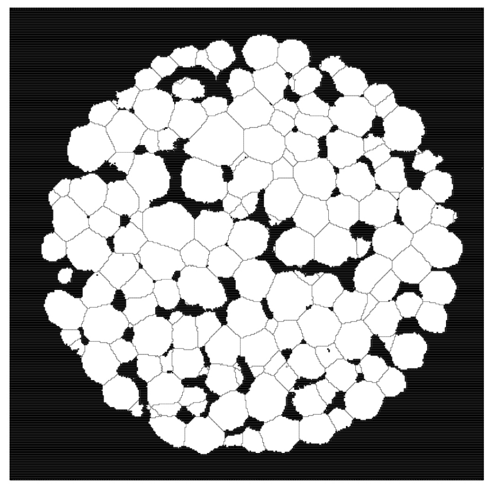




1200 MCS
78 %

2400 MCS
81 %



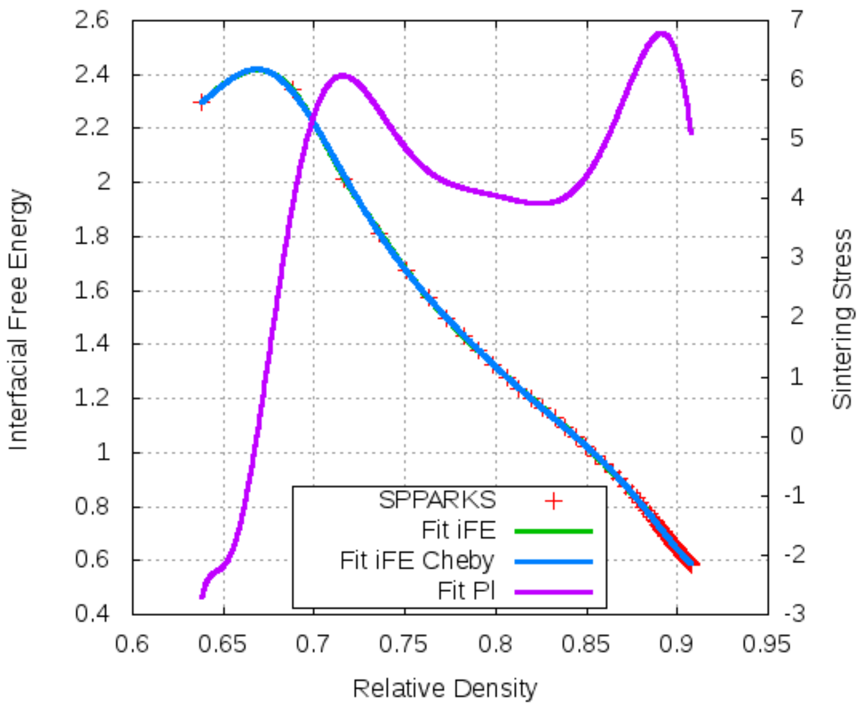


3600 MCS
83 %

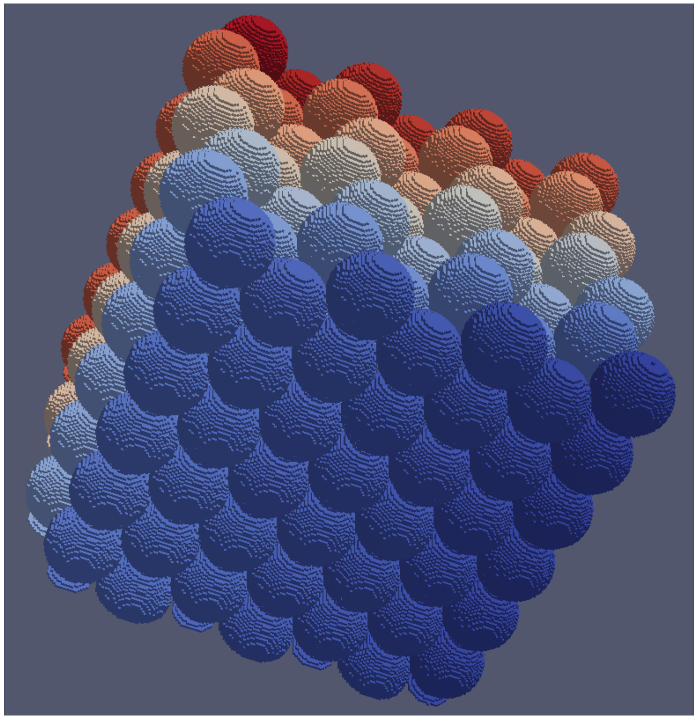
kMC – P_L Sintering Stress Estimation

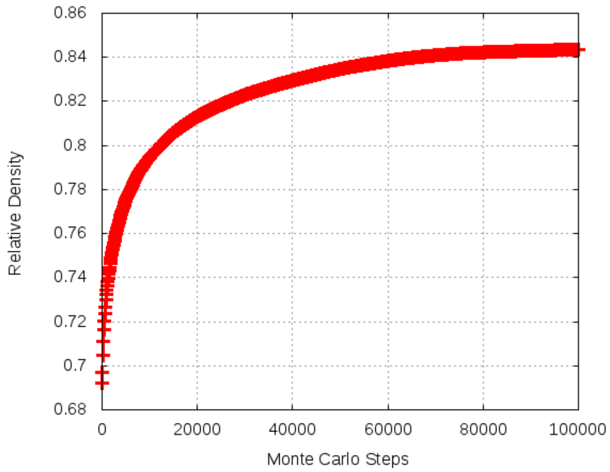
$$P_L = \left.\frac{\partial F}{\partial v}\right|_T$$

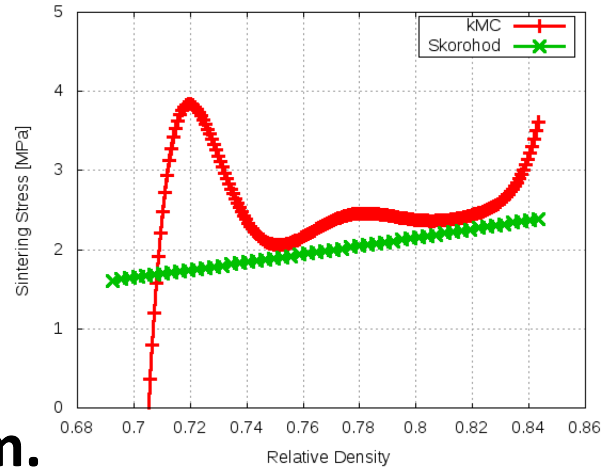
1. Calculate interfacial free energy *F*
2. Compute a Chebyshev polynomial fit of interfacial free energy based on spline
3. Differentiate the Chebyshev polynomial with respect to specific volume *v*



Results – Close Packing

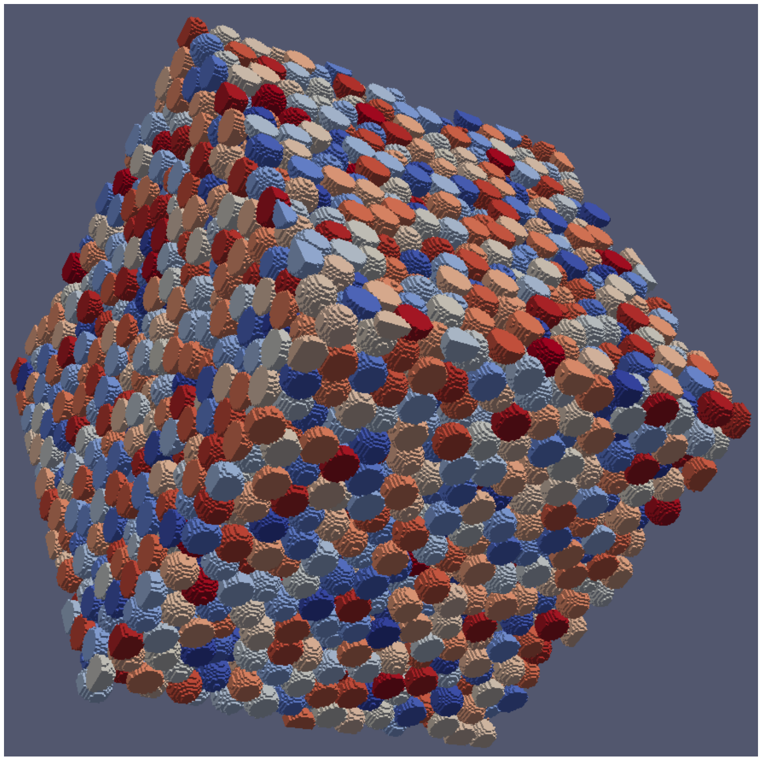


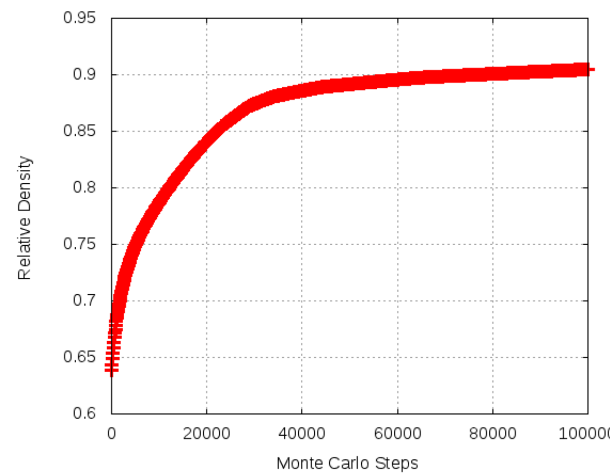


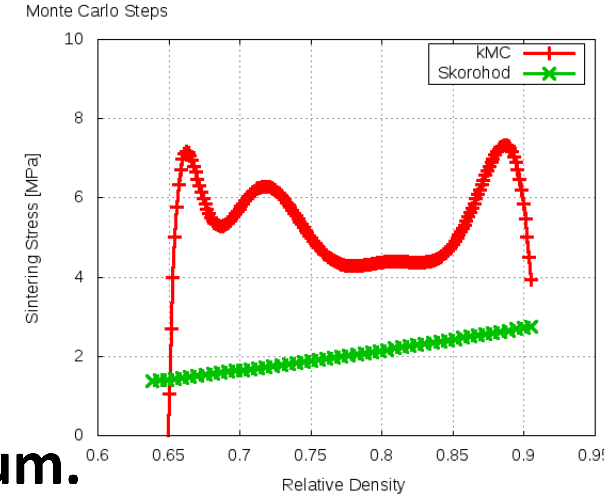


Close packing 340 particles, r_0= 2.5 um.

Results – Random Packing

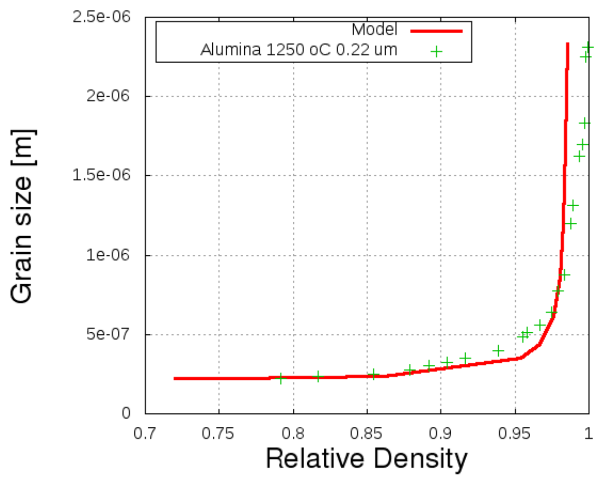






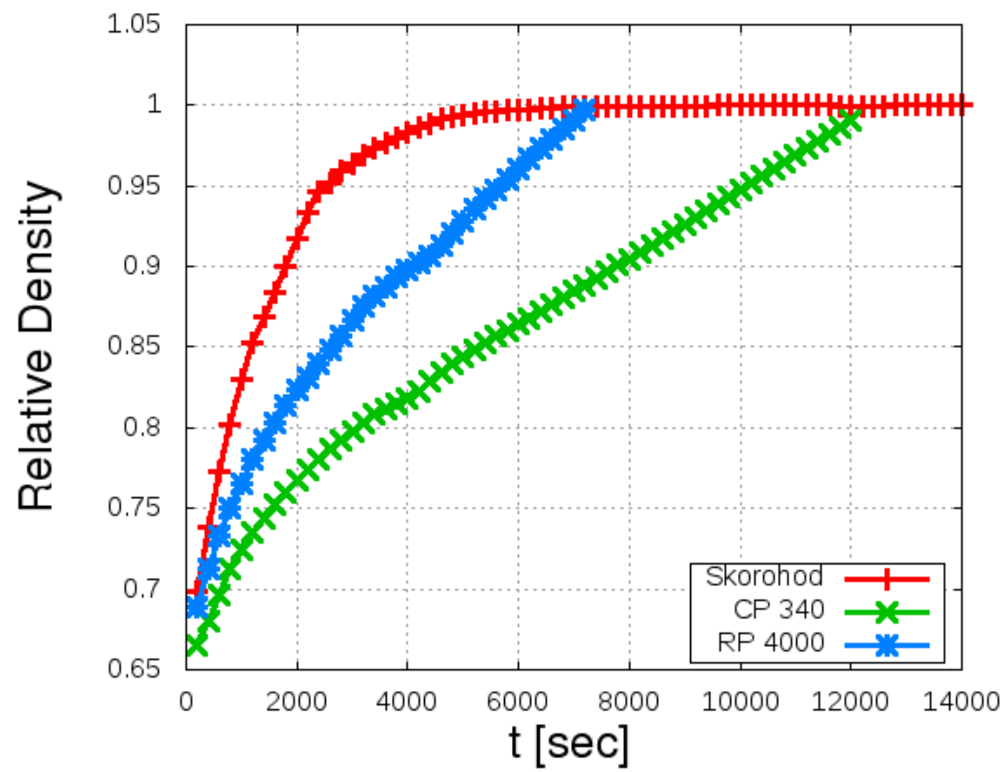
Random packing 4000 particles, r_0= 1 um.

Results – FEA + kMC – Free Sintering



$$\sigma(W) = AW$$

$$A = \tilde{A}T\exp\left(\frac{\Delta H_{SD}}{RT}\right)$$



Free sintering: (left) Parameter match, (right) Densification

Conclusions

- A FEA code coupling electrical, thermal and displacement fields has been implemented
- The continuum theory of sintering is incorporated enabling the evolution of the densification based on local conditions, thus a true spatial density distribution could be obtained
- Microstructures provide qualitative and quantitative exploration of sintering evolution
- Few a-priori assumptions regarding the geometry of the system are required
- Other meso-scale effects could be incorporated

Acknowledgements

NSF

ARDEC

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P T Lab

Powder Technology Laboratory