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Mesoscale simulations of particle composites

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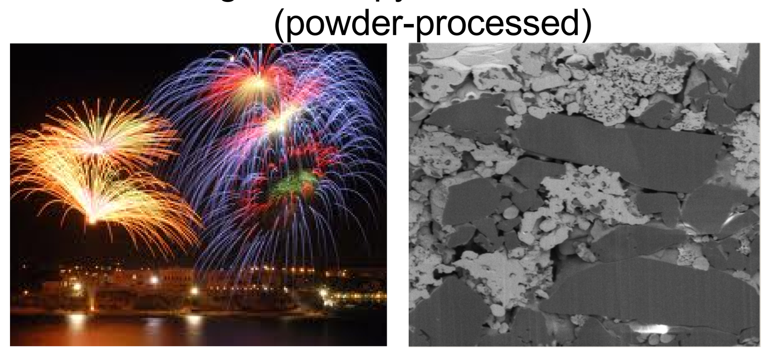
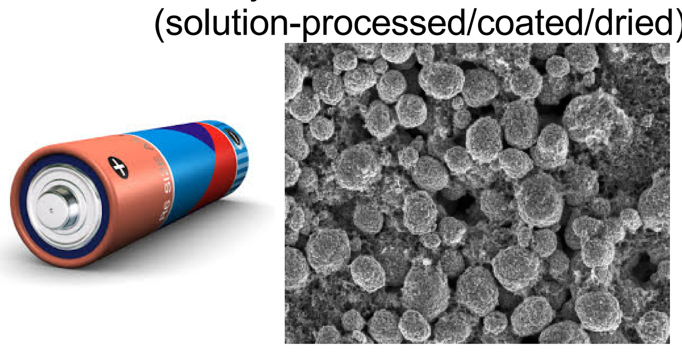
Introduction

Particle suspensions and powders are routinely processed into composite materials in countless manufacturing processes used in energy (e.g. battery electrodes, soil mechanics), defense (e.g. pyrotechnic/energetic materials) and nanotechnology applications. The resulting microstructures are often difficult to predict and control, but can have significant effects on product properties. To this end, we have developed a generic suite of simulation tools for mesoscale simulations relevant to the **processing of particulate suspensions and powders**, as well as the computational **prediction of the resulting composite material properties**.

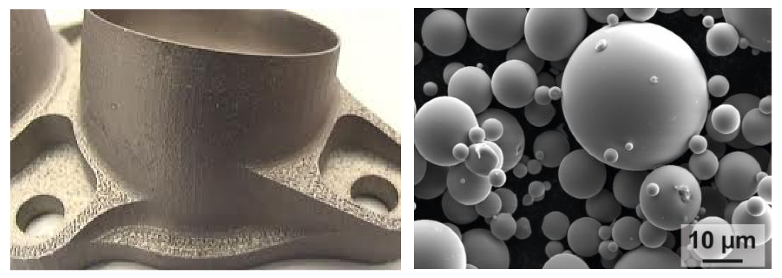
Energetic and pyrotechnic materials (powder-processed)



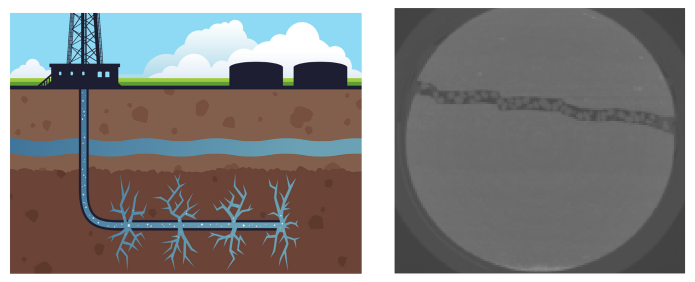
Battery electrode materials (solution-processed/coated/dried)

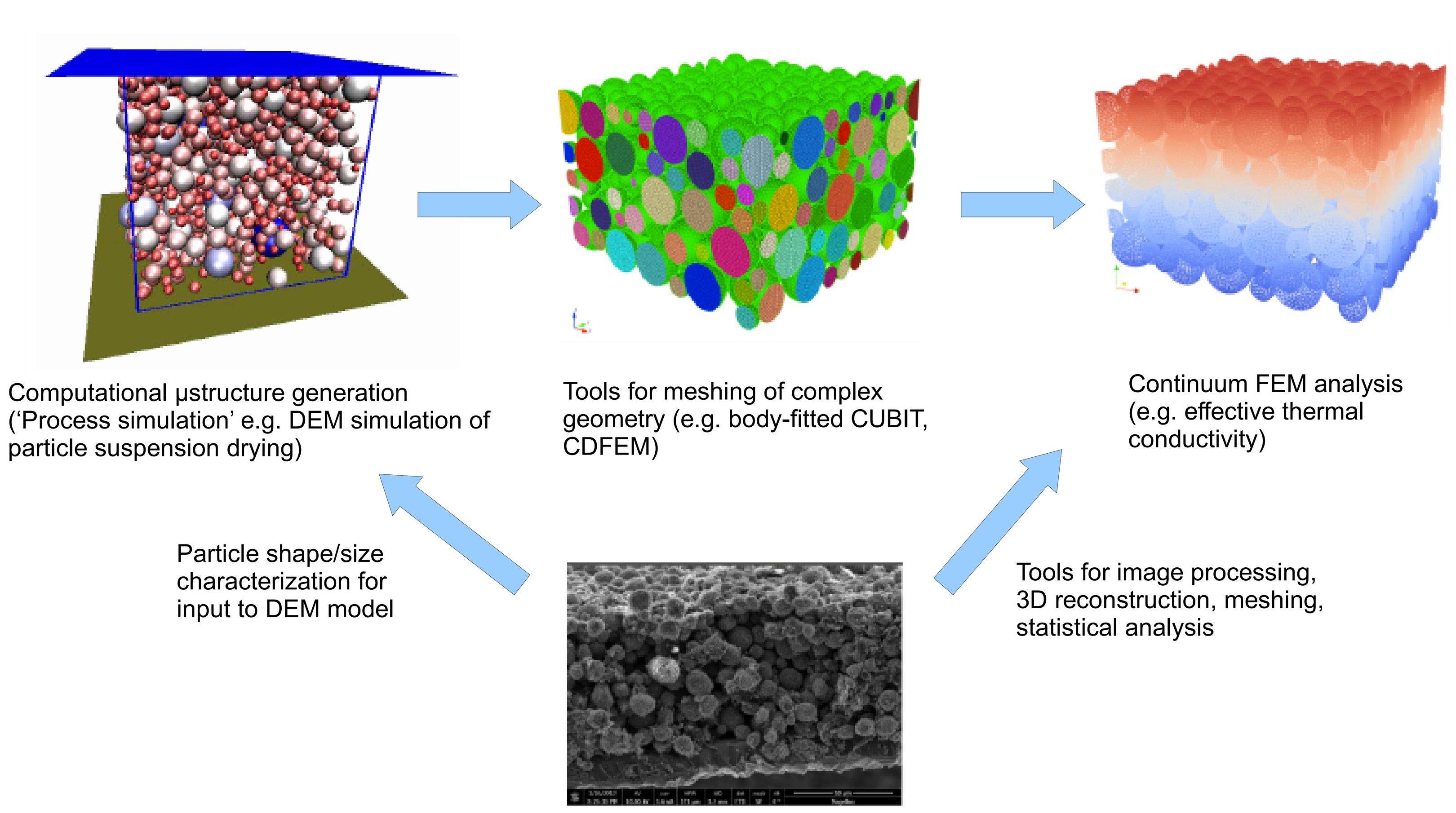


Additive manufacturing/selective laser melting



Geomechanics, e.g. hydraulic fracturing





Computational µstructure generation ('Process simulation' e.g. DEM simulation of particle suspension drying)

Tools for meshing of complex geometry (e.g. body-fitted CUBIT, CDFEM)

Continuum FEM analysis (e.g. effective thermal conductivity)

Particle shape/size characterization for input to DEM model

Tools for image processing, 3D reconstruction, meshing, statistical analysis

Experimental microstructure characterization (e.g. FIB-SEM, µCT)

Acknowledgements and References

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- Leo Silbert (Southern Illinois University)
- Industry partners (former and current CRADA partnerships)

References:

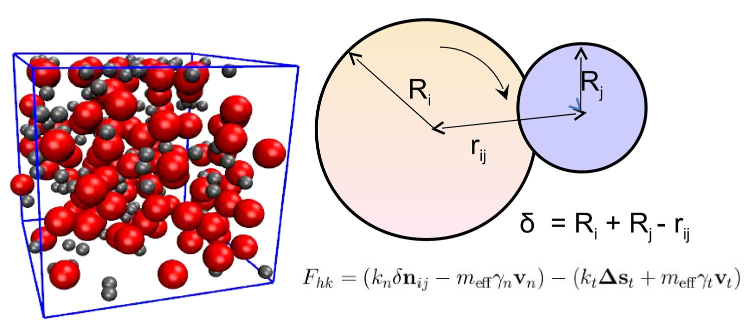
1. Bolintineanu et al, Computational Particle Mechanics, in press (2014)
2. Schunk et al, J Rheol 56:353 (2012)
3. S. Plimpton, J Comp Phys 117:1 (1995) lammps.sandia.gov
4. MA Groeber and MA Jackson, Integrating Materials and Manufacturing Innovation 3:5 (2014) dream3d.bluequartz.net
5. MeshLab, meshlab.sourceforge.net
6. CUBIT, the Sandia National Laboratory automated mesh generation toolkit, cubit.sandia.gov

DEM simulations of microstructure formation (LAMMPS[3])

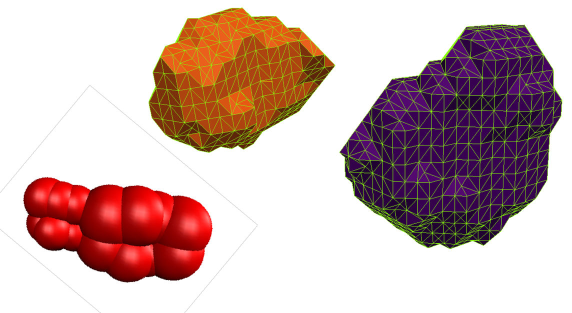
Spherical particles/ simple boundaries

Arbitrary particle shapes/ external geometries

Dry powder



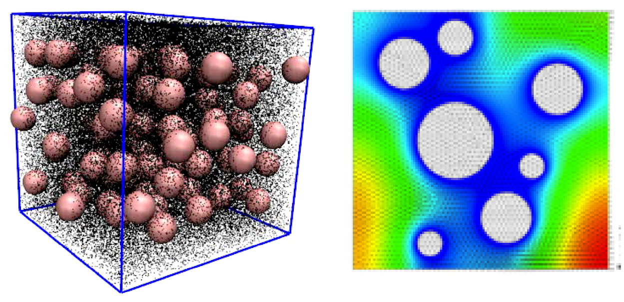
$$F_{hk} = (k_n \delta \mathbf{n}_{ij} - m_{eff}\gamma_n \mathbf{v}_n) - (k_t \Delta \mathbf{s}_t + m_{eff}\gamma_t \mathbf{v}_t)$$

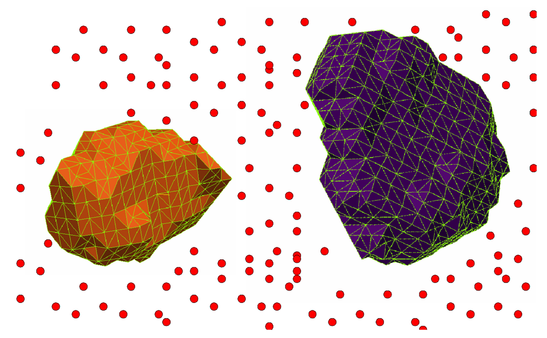


- Well-established granular contact potentials
- Moderate particle polydispersity easily handled
- Complex contact physics (e.g. friction) possible

- Particle shape representation can be challenging. Two current options:
  - Overlapping spheres
  - Tetrahedral mesh (e.g. STL)
- For tet. Mesh, granular contact potentials in development

Solvated particle suspension[1,2]





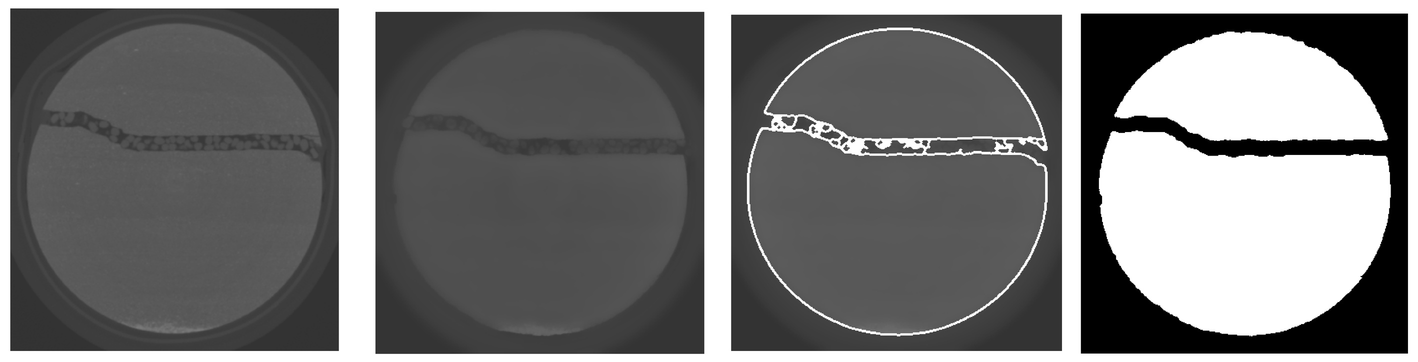
- Hydrodynamic interactions can be dominant:
  - Explicit solvents (e.g. SRD, DPD)
  - Implicit solvents (e.g. SD, FLD)
- For colloidal particles, long-range interactions are significant
- Coupling to continuum codes required for complex solvent rheology

- Hydrodynamic interactions can be modeled only by explicit solvent or coupling to continuum codes
- Colloidal interactions not easily modeled

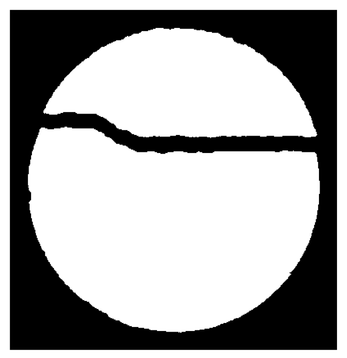
Processing 3D experimental microstructures

Three-dimensional microstructures can be obtained from serial sectioning experiments (e.g. focused ion beam/scanning electron microscopy, or FIB-SEM) or tomography experiments (e.g. X-ray). In some cases, significant challenges still exist with regard to resolution and field of view. We are working to develop highly customizable tools to analyze, segment and import 3D experimental data into in-house finite element codes, both as continuum fields and as solid models. These will be used both for verification of microstructures generated from FIB-SEM data, as well as direct inputs to property prediction simulations.

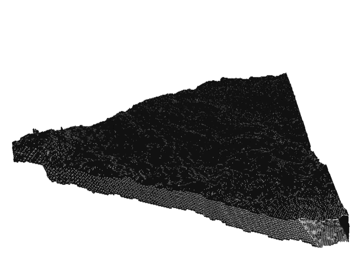
Image processing to segment a tomography scan of a cracked shale sample containing proppant particles. All analysis was carried out within the open source computer vision (OpenCV) and NumPy/SciPy libraries.



Once segmented, regions of interest in the image stack can be converted to surface meshes (e.g. STL files). However, these are unwieldy due to the large number of surface elements (one per pixel/voxel), and additional processing is required to coarsen the surface mesh. Finally, the surface mesh is used to define a solid body geometry (ACIS) which can be meshed to produce a FEM volume mesh. In the example shown here, the crack volume in the shale sample is of interest for fluid flow simulations:

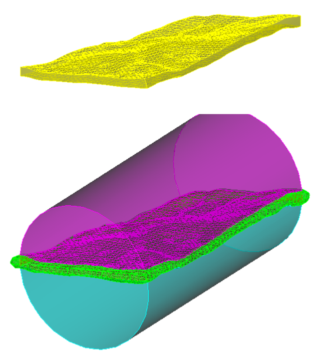


Dream3D[4] (Multi-material marching cubes algorithm)



Mesh coarsening via MeshLab[5] (Poisson surface reconstruction)

Volume meshing (Cubit[6])

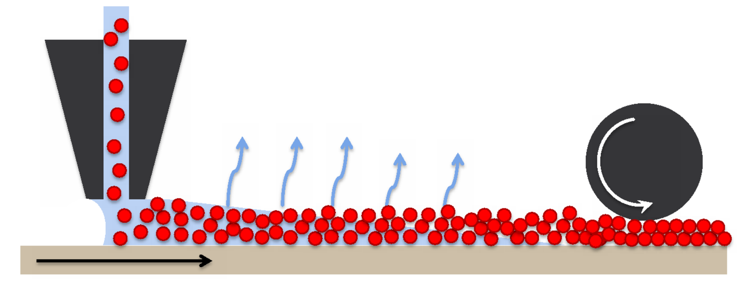


Example 1: Battery electordes (DEM-based microstructure)

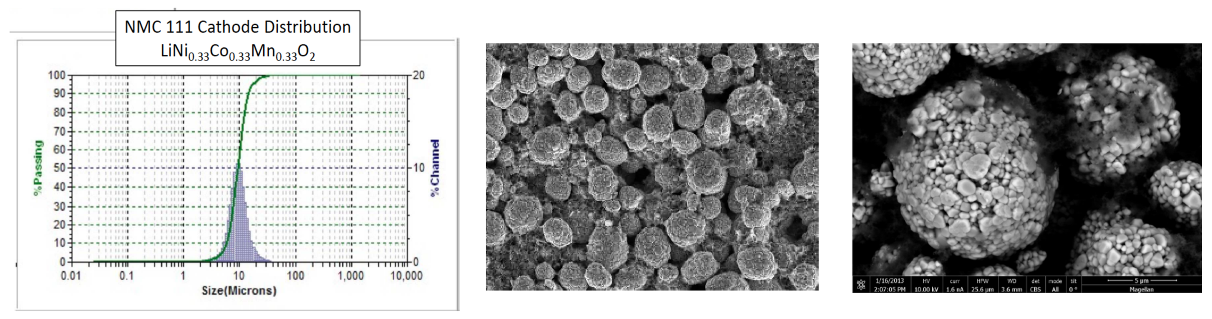
Thin film coating of suspension of $LiNi_xCo_yMn_zO_2$ particles in NMP solvent

Given particle size distribution, process parameters:

- Wet film thickness = ~200µm, dry to obtain a thickness of ~60 µm
- Calendaer to obtain final structure, ~50µm

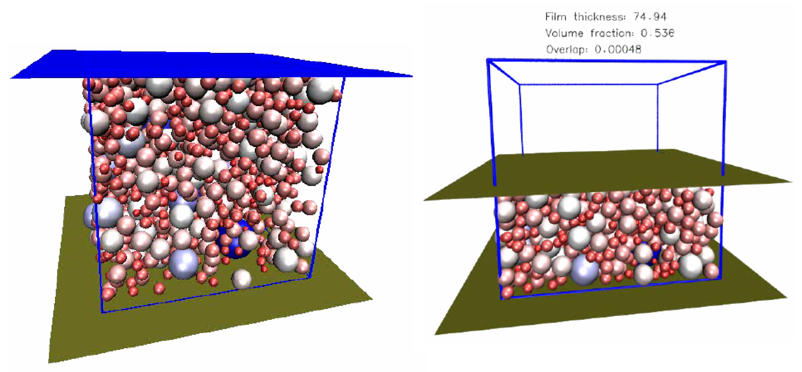


Particle size distribution and SEM images of final(dry) microstructure



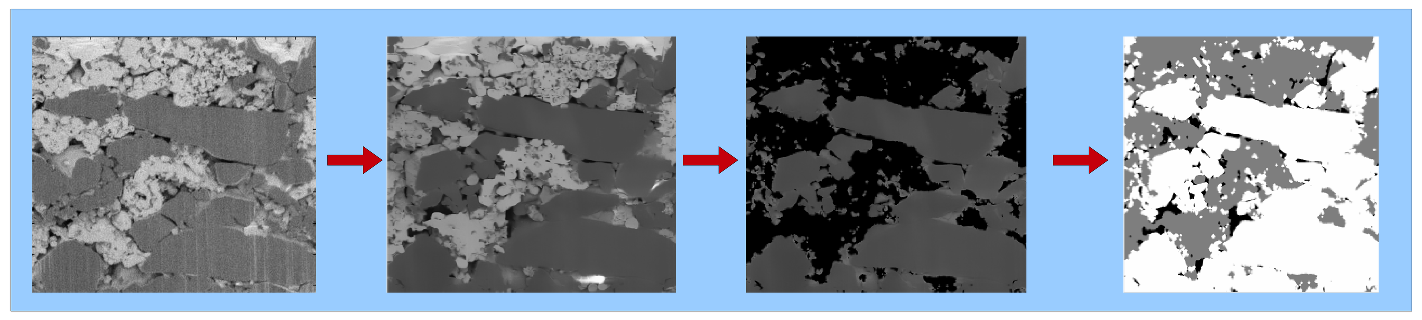
DEM simulations

- Spherical particles with moderate polydispersity
- Implicit solvent (FLD), drying simulated by wall motion
- Granular contact for calendering step
- Several thousand particles, several seconds of real time on desktop compute (actual drying process takes on the order of minutes)

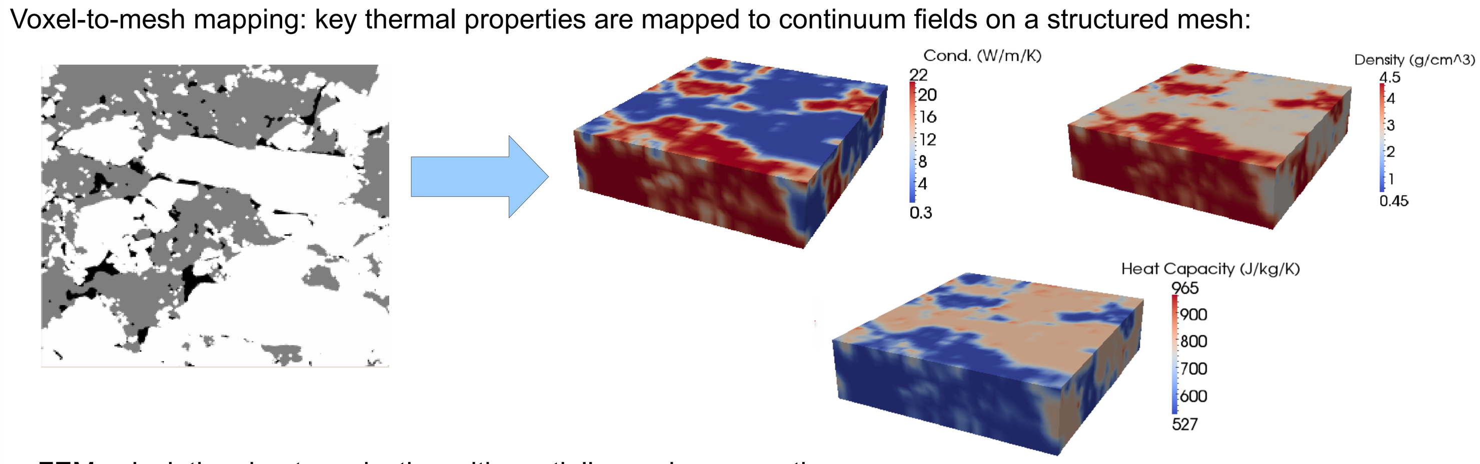


Example 2: Pyrotechnic material (experimental µstructure)

Image processing to segment FIB/SEM stack of Ti/KClO4 pyrotechnic material:



Voxel-to-mesh mapping: key thermal properties are mapped to continuum fields on a structured mesh:

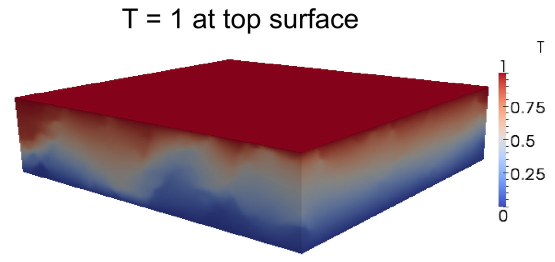


FEM calculation: heat conduction with spatially-varying properties

Transient: $\nabla \cdot (k(\mathbf{x})\nabla T) = \rho(\mathbf{x}) c_p(\mathbf{x}) \frac{\partial T}{\partial t}$

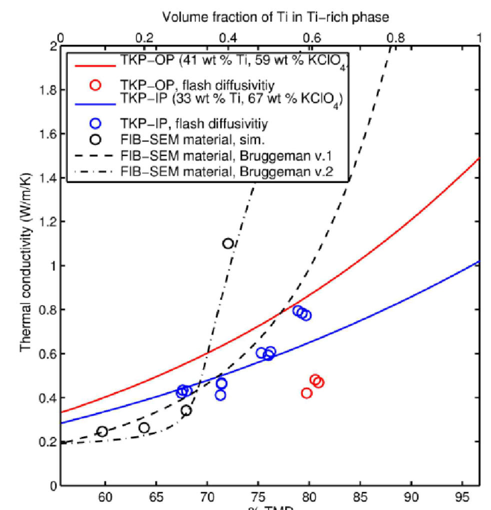
Steady: $\nabla \cdot (k(\mathbf{x})\nabla T) = 0$

T = 1 at top surface



T = 0 at bottom surface

Compute effective conductivity as: $k_{eff} = \frac{-\Delta z \int_A (k(\mathbf{x})\nabla T)_{z=z_0}\, dx\, dy}{\Delta T \int_A dx\, dy}$



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