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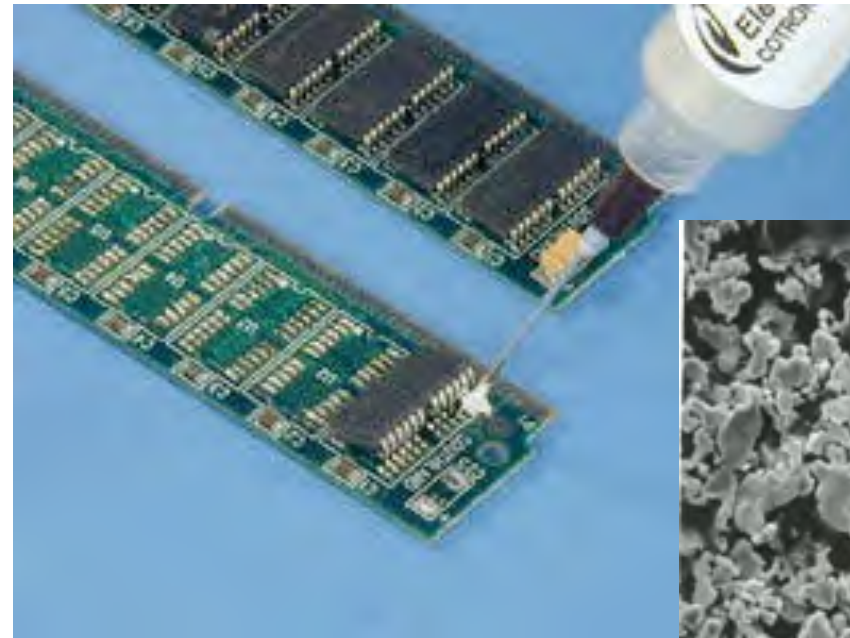
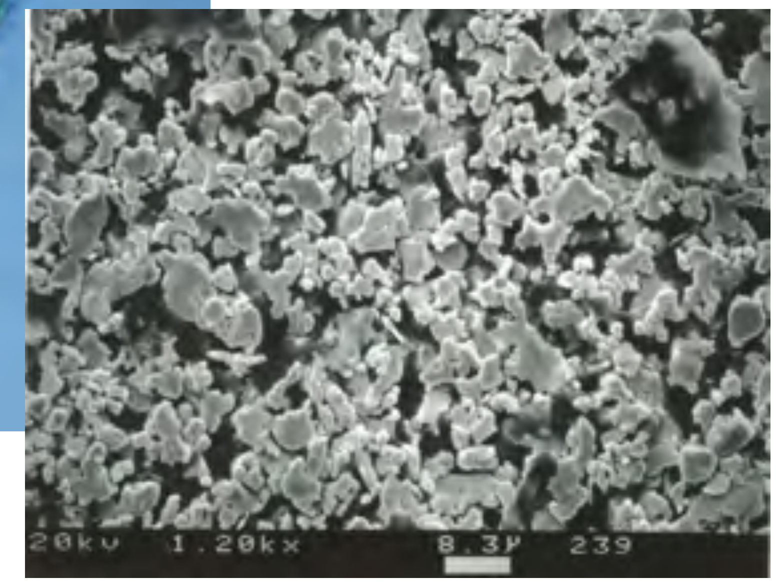
High-performance Image-based Modeling of Failure in Heterogeneous Materials with Application to Thin Layers

Karel Matouš

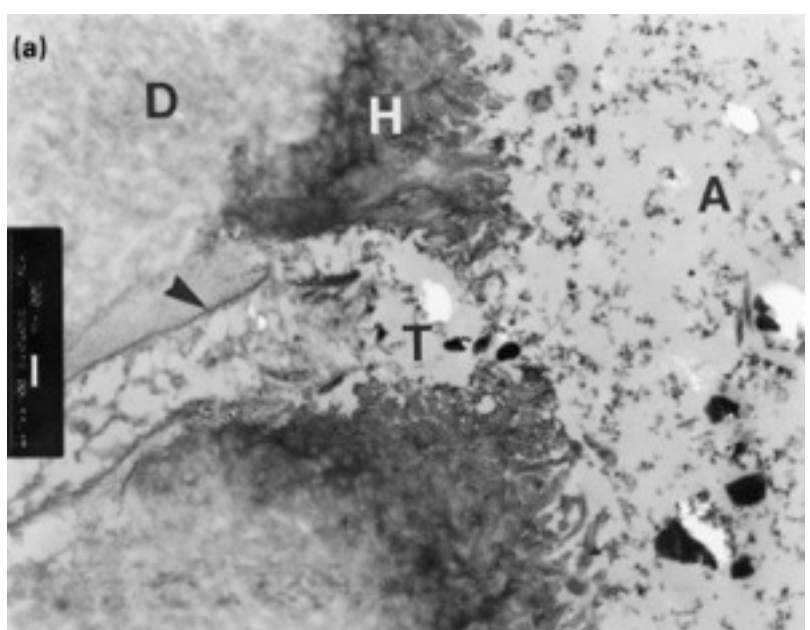
M. Mosby and A. Gillman

Motivation



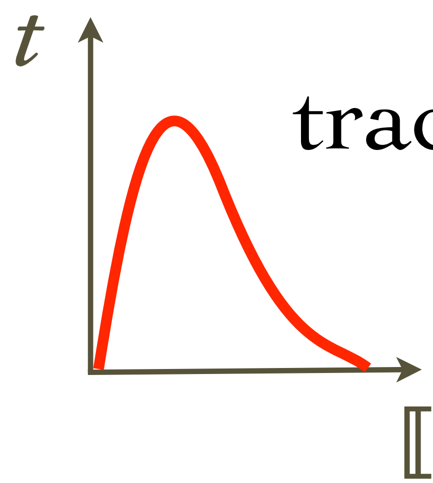


S. Xu, D. Dillard and J. Dillard

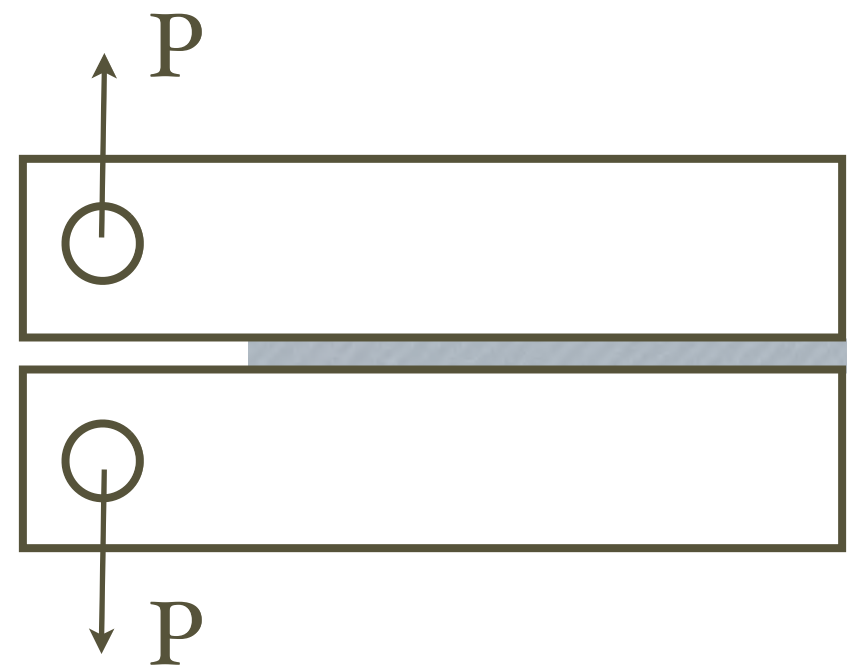


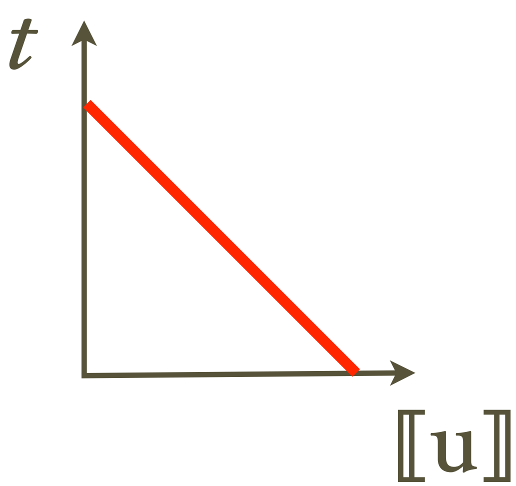
Motivation

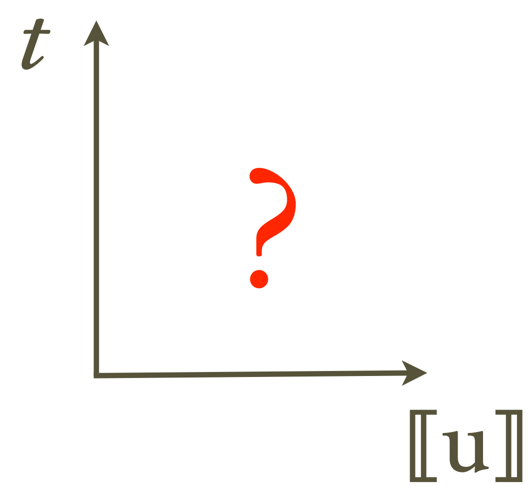
- Cohesive modeling

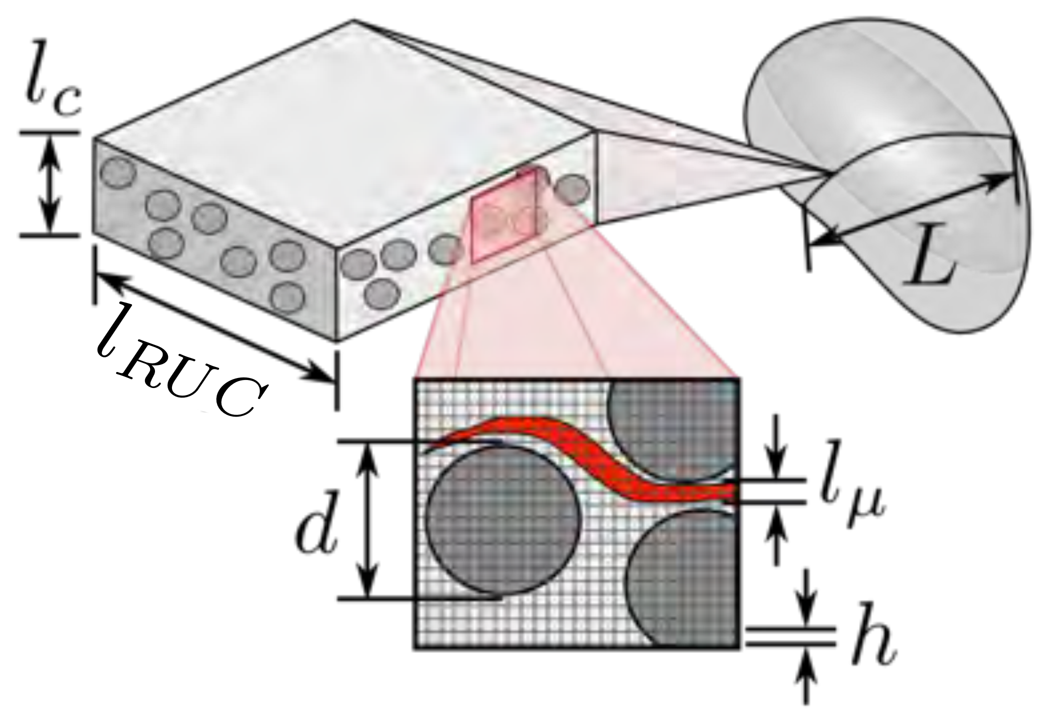


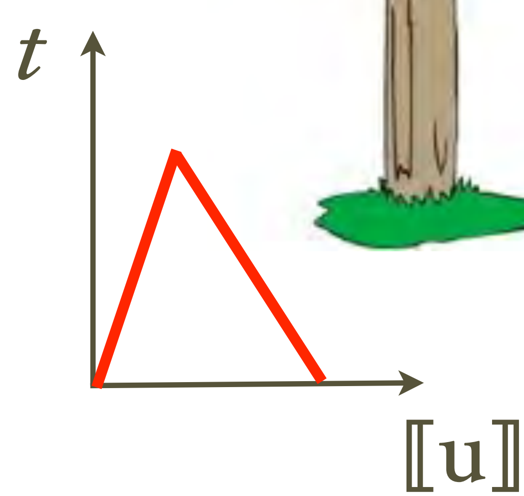
traction-separation law











$$L \gg l_c > d > l_\mu > h$$

- Cohesive law based on lower scale physics

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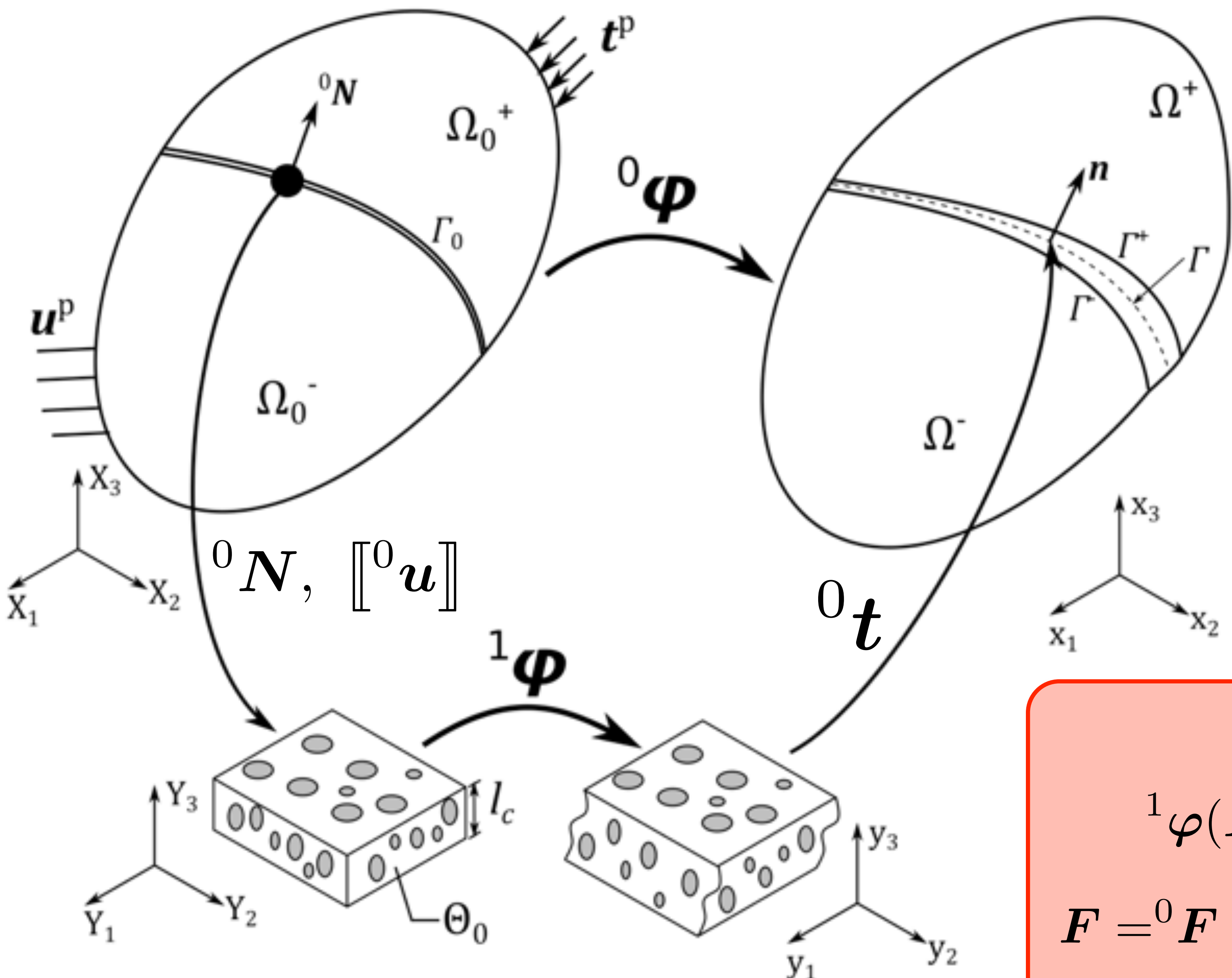
Multiscale Cohesive Model

- Critical assumption: $l_c \ll \mathcal{O}(L)$



Matouš et al., 2008

Mosby and Matouš, 2014

Adherends

$$^0\varphi(X) = X + {}^0u(X) \quad \in \Omega_0^\pm$$

$$^0F = 1 + \nabla_X {}^0u(X) \quad \in \Omega_0^\pm$$

Macro Interface: Average Deformation Gradient

$$[\![{}^0\varphi(X)]\!] = {}^0\varphi^+ - {}^0\varphi^- = [\![{}^0u(X)]\!] \quad \text{on } \Gamma_0$$

$$^0F = 1 + \frac{1}{l_c}[\![{}^0u(X)]\!] \otimes {}^0N \quad \text{on } \Gamma_0$$

Micro Interface

$$^1\varphi(X, Y) = {}^0F(X)Y + {}^1u(Y) \quad \in \Theta_0$$

$$F = {}^0F + \nabla_Y {}^1u(Y) = 1 + \frac{1}{l_c}[\![{}^0u(X)]\!] \otimes {}^0N + \nabla_Y {}^1u(Y) \quad \in \Theta_0$$

Strong and Weak Forms

Macroscale Strong Form

$$\nabla_{\boldsymbol{X}} \cdot {}^0\boldsymbol{P} + \boldsymbol{f} = \boldsymbol{0} \quad \in \ \Omega_0^{\pm}$$

$${}^0\boldsymbol{P} = \frac{\partial^0 W}{\partial^0 \boldsymbol{F}} \quad \in \ \Omega_0^{\pm}$$

Boundary Conditions

$${}^0\boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}^p \quad \text{on } \partial\Omega_0^{\mathrm{t}}$$

$${}^0\boldsymbol{u} = {}^0\boldsymbol{u}^p \quad \text{on } \partial\Omega_0^{\mathrm{u}}$$

$$\boldsymbol{t}^+ + \boldsymbol{t}^- = \boldsymbol{0} \quad \text{on } \Gamma_0$$

Macroscale Weak Form

$${}^0\mathcal{R} = \int_{\Omega_0^{\pm}} {}^0\boldsymbol{P} : \nabla_{\boldsymbol{X}}(\delta^0\boldsymbol{u})\,\mathrm{dV} - \int_{\Omega_0^{\pm}} \boldsymbol{f} \cdot \delta^0\boldsymbol{u}\,\mathrm{dV} - \int_{\partial\Omega_0^{\mathrm{t}}} \boldsymbol{t}^{\mathrm{p}} \cdot \delta^0\boldsymbol{u}\,\mathrm{dA} + \int_{\Gamma_0} {}^0\boldsymbol{t} \cdot [\![\delta^0\boldsymbol{u}]\!]\,\mathrm{dA} = 0$$

Microscale Strong Form

$$\nabla_{\boldsymbol{Y}} \cdot {}^1\boldsymbol{P} = \boldsymbol{0} \quad \in \ \Theta_0$$

$${}^1\boldsymbol{P} = \frac{\partial^1 W}{\partial \boldsymbol{F}} \quad \in \ \Theta_0$$

$$\boldsymbol{F} = \boldsymbol{1} + \frac{1}{l_c}[\![{}^0\boldsymbol{u}(\boldsymbol{X})]\!] \otimes {}^0\boldsymbol{N} + \nabla_{\boldsymbol{Y}}\,{}^1\boldsymbol{u}(\boldsymbol{Y})$$

Hill-Mandel Lemma

- Microscale weak form
- Yields closure on ${}^0\boldsymbol{t}$
- Restrictions on BC

Hill-Mandel Lemma

$$\inf_{[\![{}^0\boldsymbol{u}]\!]} {}^0W([\![{}^0\boldsymbol{u}]\!]) = \inf_{{}^0\boldsymbol{F}} \inf_{{}^1\boldsymbol{u}} \frac{l_c}{|\Theta_0|} \int_{\Theta_0} {}^1W\left({}^0\boldsymbol{F}([\![{}^0\boldsymbol{u}]\!]) + \nabla_Y {}^1\boldsymbol{u}\right) \mathrm{dV}$$

$${}^1\boldsymbol{P} = \left.\frac{\partial^1 W}{\partial \boldsymbol{F}}\right|_{\boldsymbol{F}={}^0\boldsymbol{F}+\nabla_{\boldsymbol{Y}} {}^1\boldsymbol{u}}$$

$${}^0\boldsymbol{t} = \frac{\partial^0 W}{\partial [\![{}^0\boldsymbol{u}]\!]}$$

$${}^1\mathcal{R} = \frac{l_c}{|\Theta_0|} \int_{\Theta_0} {}^1\boldsymbol{P} : \nabla_{\boldsymbol{Y}}(\delta^1\boldsymbol{u}) \, \mathrm{dV} = 0$$

$${}^{[\![{}^0\boldsymbol{u}]\!]}\mathcal{R} = \left({}^0\boldsymbol{N} \cdot \frac{1}{|\Theta_0|} \int_{\Theta_0} {}^1\boldsymbol{P} \, \mathrm{dV} - {}^0\boldsymbol{t}\right) \cdot [\![\delta({}^0\boldsymbol{u})]\!] = 0$$

At microscale **equilibrium** $${}^0\boldsymbol{t} = {}^0\boldsymbol{N} \cdot \frac{1}{|\Theta_0|} \int_{\Theta_0} {}^1\boldsymbol{P} \, \mathrm{dV}$$

- No assumption on form of ${}^0\boldsymbol{t}$

Microscale Boundary Condition Admissibility

$$\frac{1}{|\Theta_0|} \int_{\Theta_0} \nabla_{\boldsymbol{Y}} {}^1\boldsymbol{u} \, \mathrm{dV} = \frac{1}{|\Theta_0|} \int_{\partial\Theta_0} {}^1\boldsymbol{u} \cdot \boldsymbol{N}_\Theta \, \mathrm{dA} = \boldsymbol{0}$$

$$\begin{cases} {}^1\boldsymbol{u} = \boldsymbol{0} & \text{on } \partial\Theta \\ {}^1\boldsymbol{u}^+ = {}^1\boldsymbol{u}^- \;||\; \bar{\boldsymbol{t}}^+ = -\bar{\boldsymbol{t}}^- & \text{on } \partial\Theta \\ \bar{\boldsymbol{t}} = \boldsymbol{0} & \text{on } \partial\Theta \end{cases}$$

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Constitutive Response of Adhesive Layer

- Isotropic damage law

$$^1W(\boldsymbol{F},\omega) = (1-\omega)\,^1W(\boldsymbol{F})$$

- Damage surface

$$g(\bar{Y},\chi^{\mathrm{t}}) = G(\bar{Y}) - \chi^{\mathrm{t}} \leq 0$$

$$G(\bar{Y}) = 1 - \exp\left[-\left(\frac{\bar{Y}-Y_{in}}{p_1 Y_{in}}\right)^{p_2}\right], \qquad H = \frac{\partial G(\bar{Y})}{\partial \bar{Y}}$$

- Irreversible dissipative evolution equations

$$\dot{\omega} = \dot{\kappa} H \quad \rightarrow \quad \dot{\omega} = \mu\langle \phi(g) \rangle$$

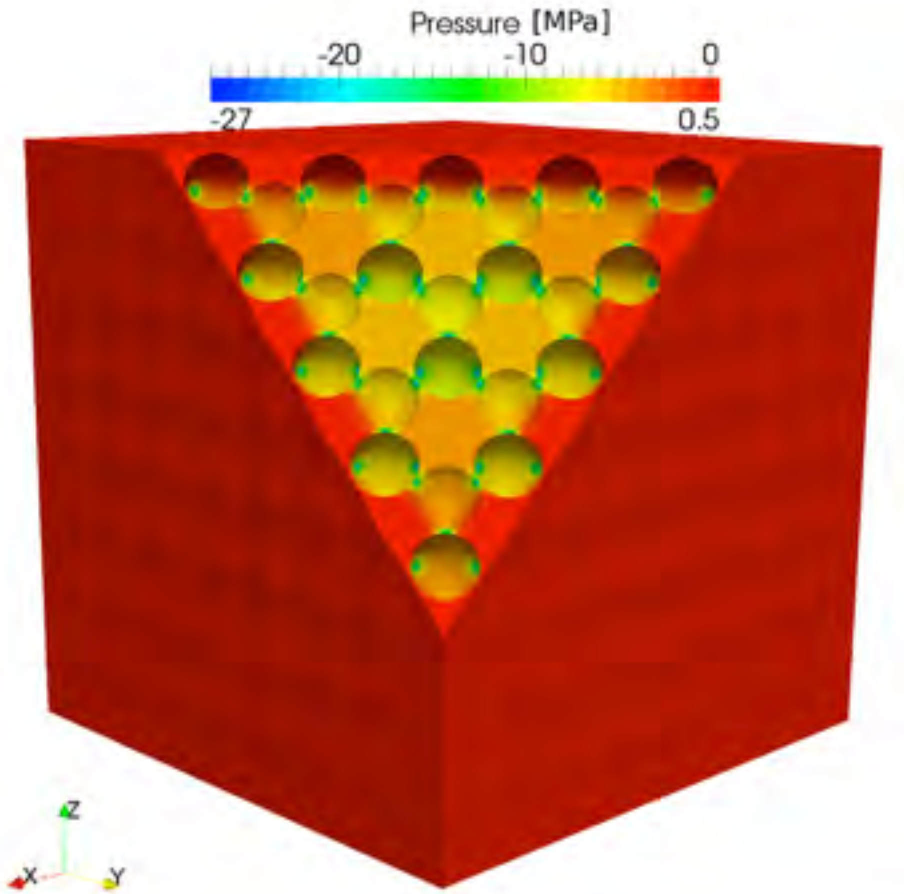
$$\dot{\chi}^{\mathrm{t}} = \dot{\kappa} H \quad \rightarrow \quad \underbrace{\dot{\chi}^{\mathrm{t}} = \mu\langle \phi(g) \rangle}_{\text{viscous regularization}}$$

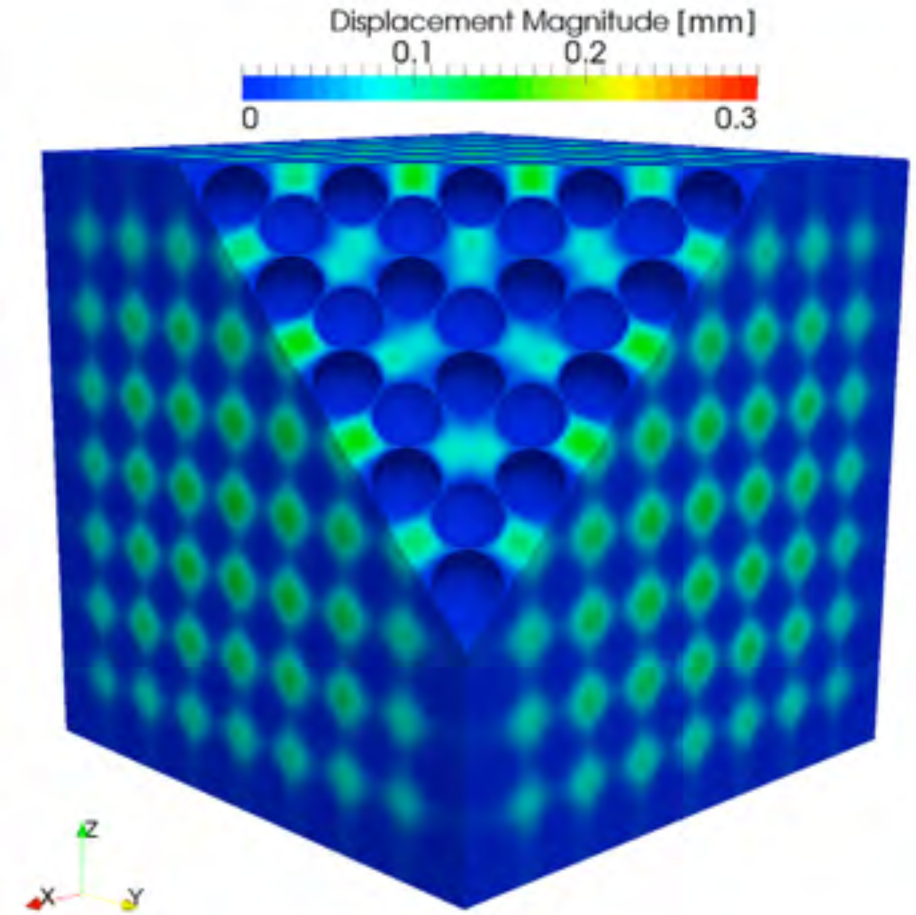
$1/\mu \approx \tau$ [s]

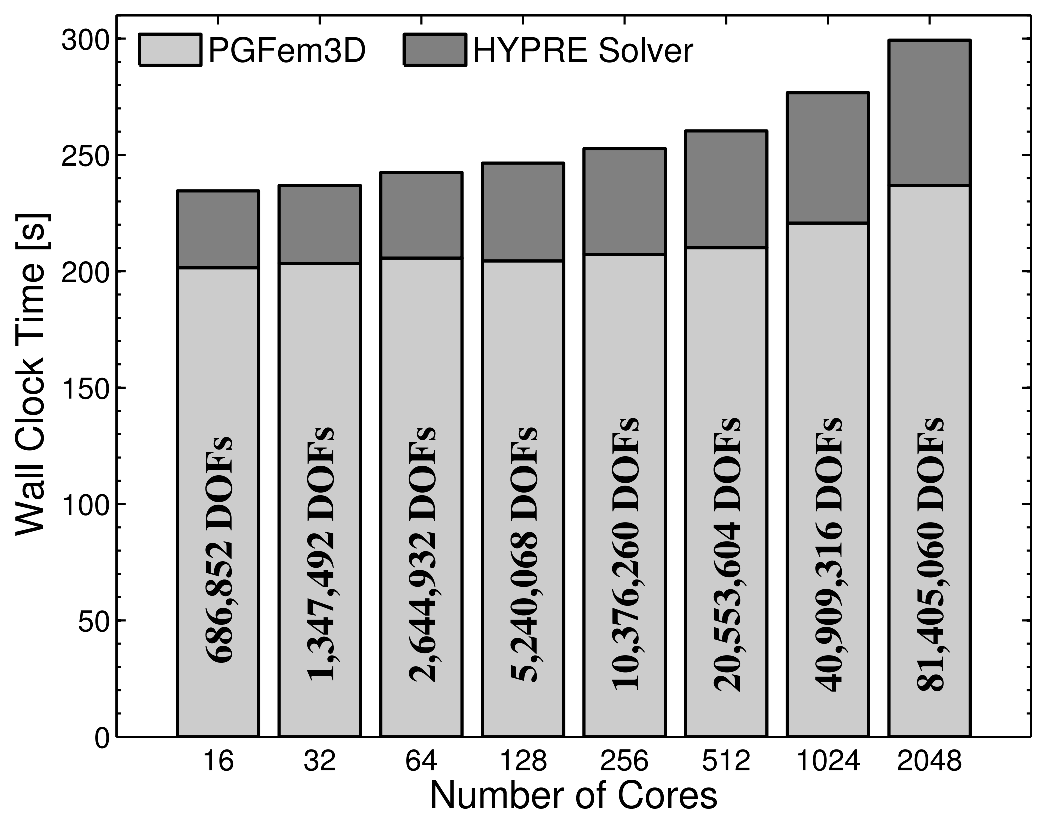
Epoxy τ-$\mathcal{O}(10^{-6}\text{-}10^{-2})$

- Different constitutive laws can be used

High Performance Computing - Weak Scaling







- Highly scalable finite strains *PGFem3D* solver

N_n=23,841,057 N_e= 123,168,768

- four nonlinear steps
- four iterations

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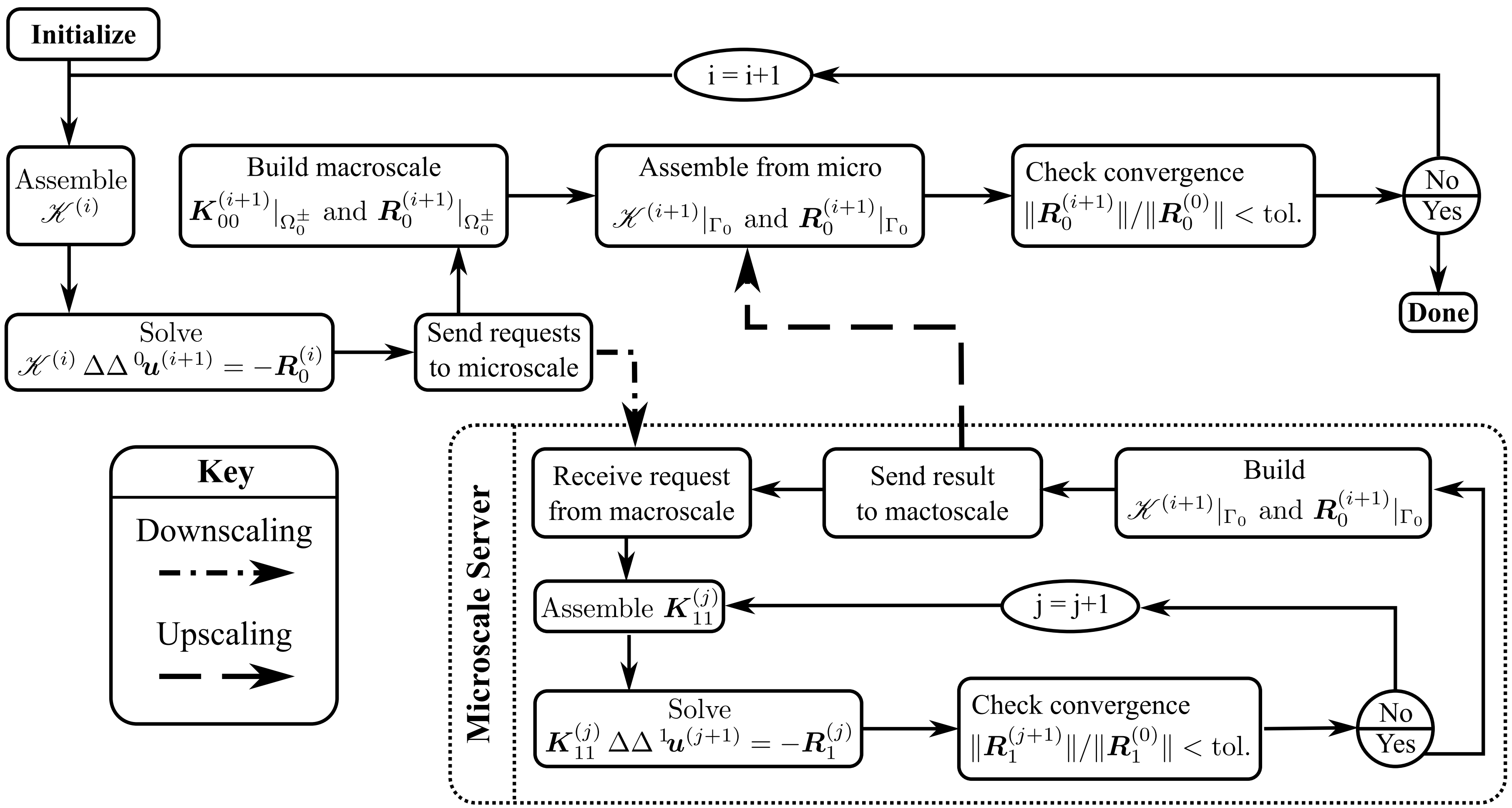
Hierarchically Parallel Multiscale Solver

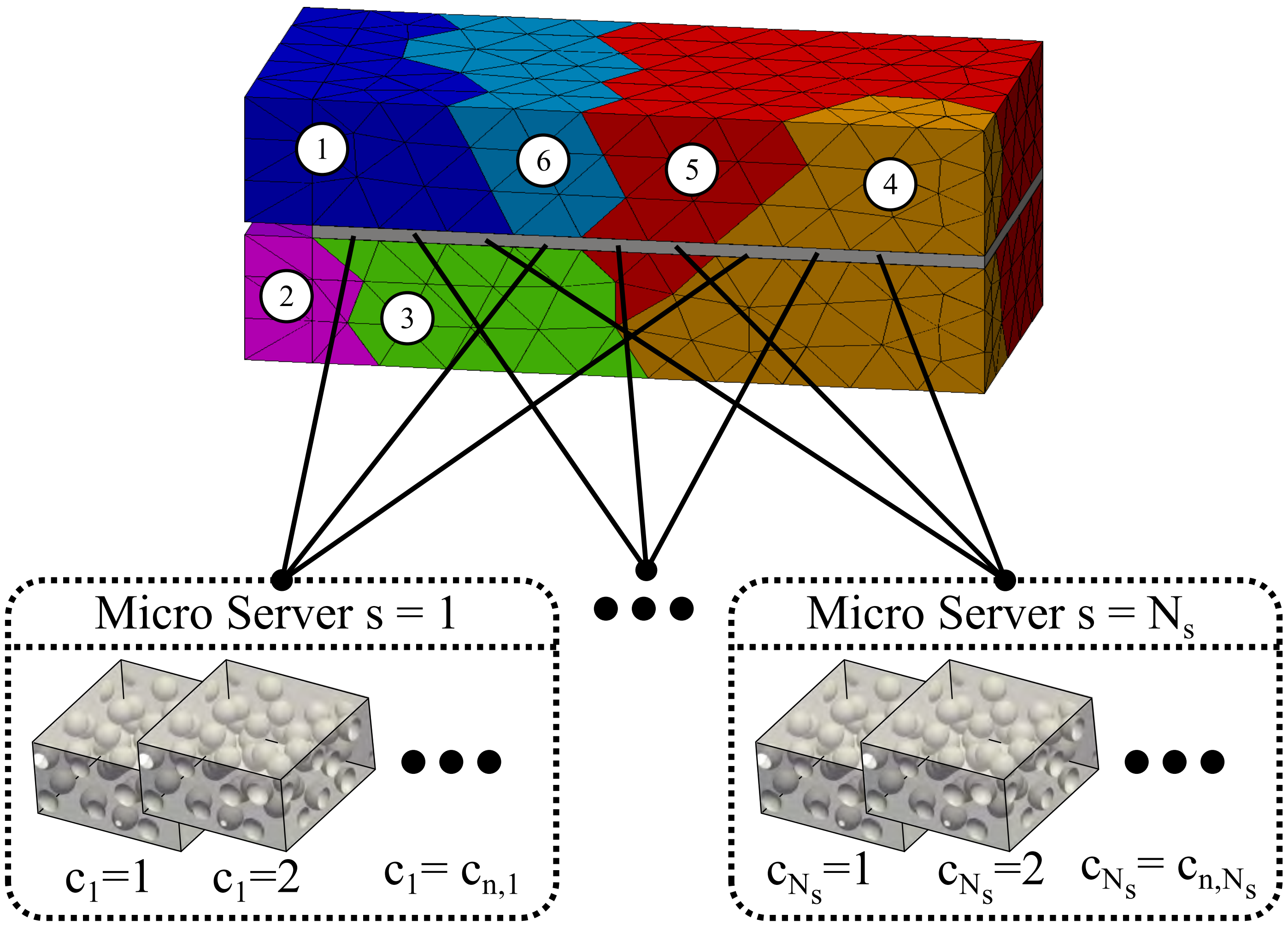
$$ {}^0\mathcal{R} = \int_{\Omega_0^\pm} {}^0\boldsymbol{P} : \nabla_{\boldsymbol{X}}(\delta^0\boldsymbol{u})\,\mathrm{dV} - \int_{\Omega_0^\pm} \boldsymbol{f}\cdot\delta^0\boldsymbol{u}\,\mathrm{dV} - \int_{\partial\Omega_0^{\mathrm{t}}} \boldsymbol{t}^{\mathrm{p}}\cdot\delta^0\boldsymbol{u}\,\mathrm{dA} + \int_{\Gamma_0} {}^0\boldsymbol{t}\cdot[\![\delta^0\boldsymbol{u}]\!]\,\mathrm{dA} = 0 $$

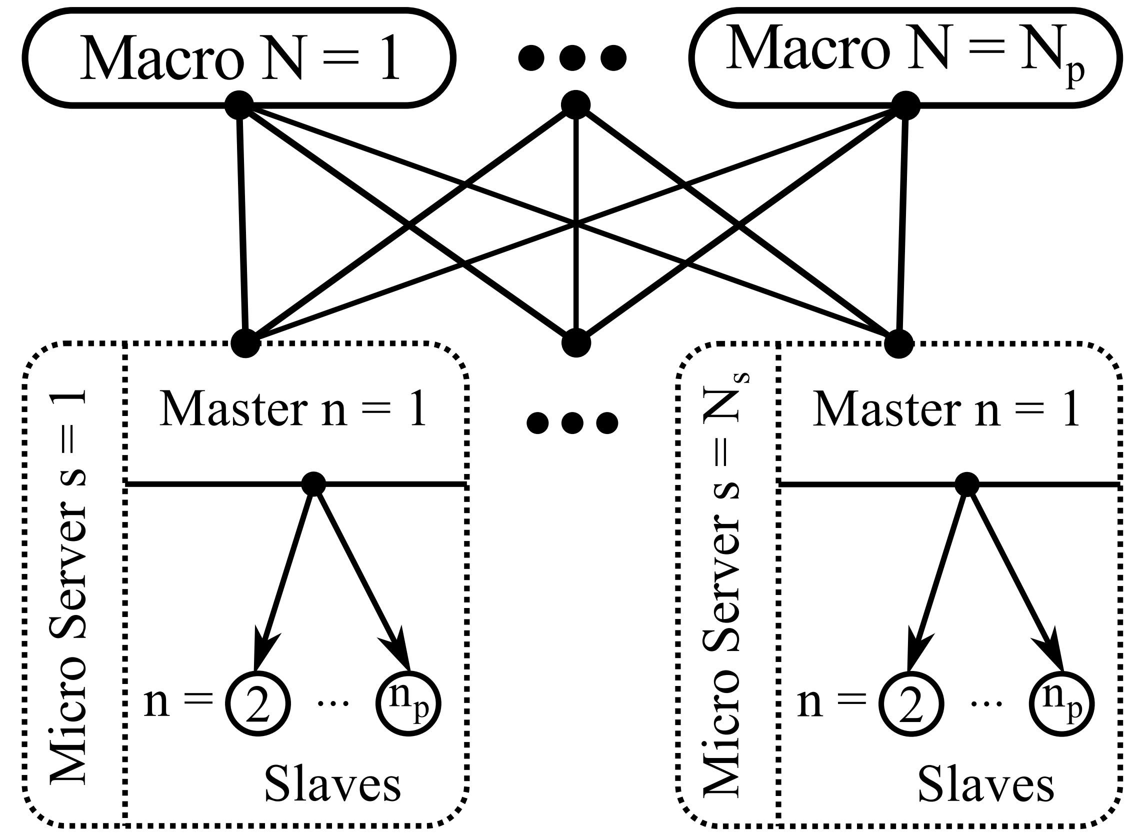


$$ {}^1\mathcal{R} = \frac{l_c}{|\Theta_0|}\int_{\Theta_0} {}^1\boldsymbol{P} : \nabla_{\boldsymbol{Y}}(\delta^1\boldsymbol{u})\,\mathrm{dV} = 0 $$

$$ {}^{[\![^0\boldsymbol{u}]\!]}\mathcal{R} = \left({}^0\boldsymbol{N}\cdot\frac{1}{|\Theta_0|}\int_{\Theta_0} {}^1\boldsymbol{P}\,\mathrm{dV} - {}^0\boldsymbol{t}\right)\cdot[\![\delta({}^0\boldsymbol{u})]\!] = 0 $$

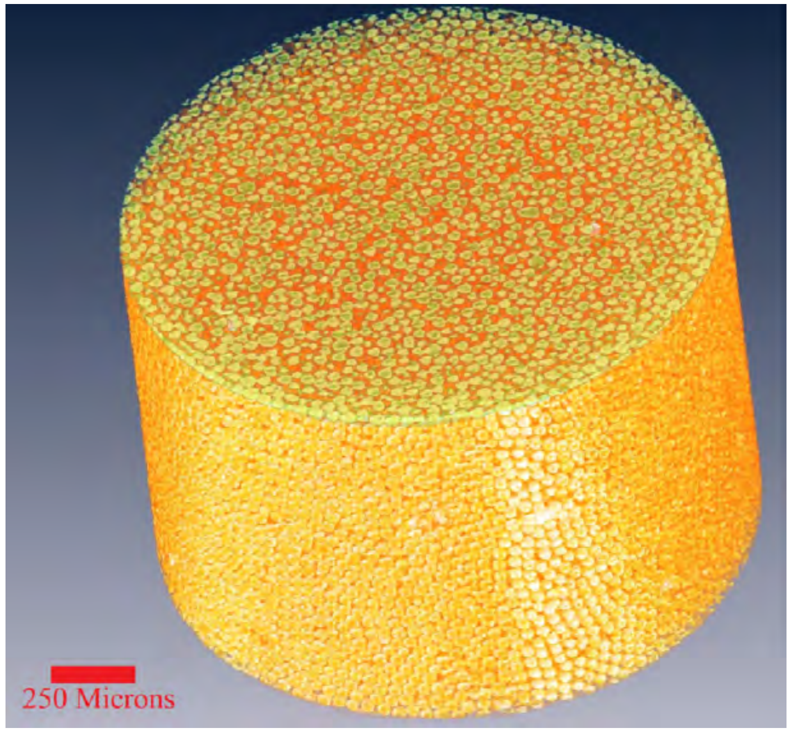
Hierarchically Parallel Multiscale Solver



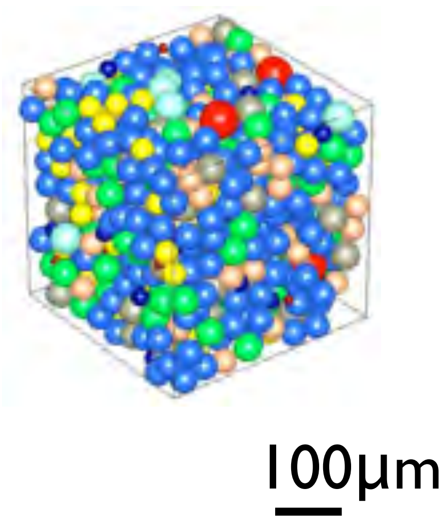


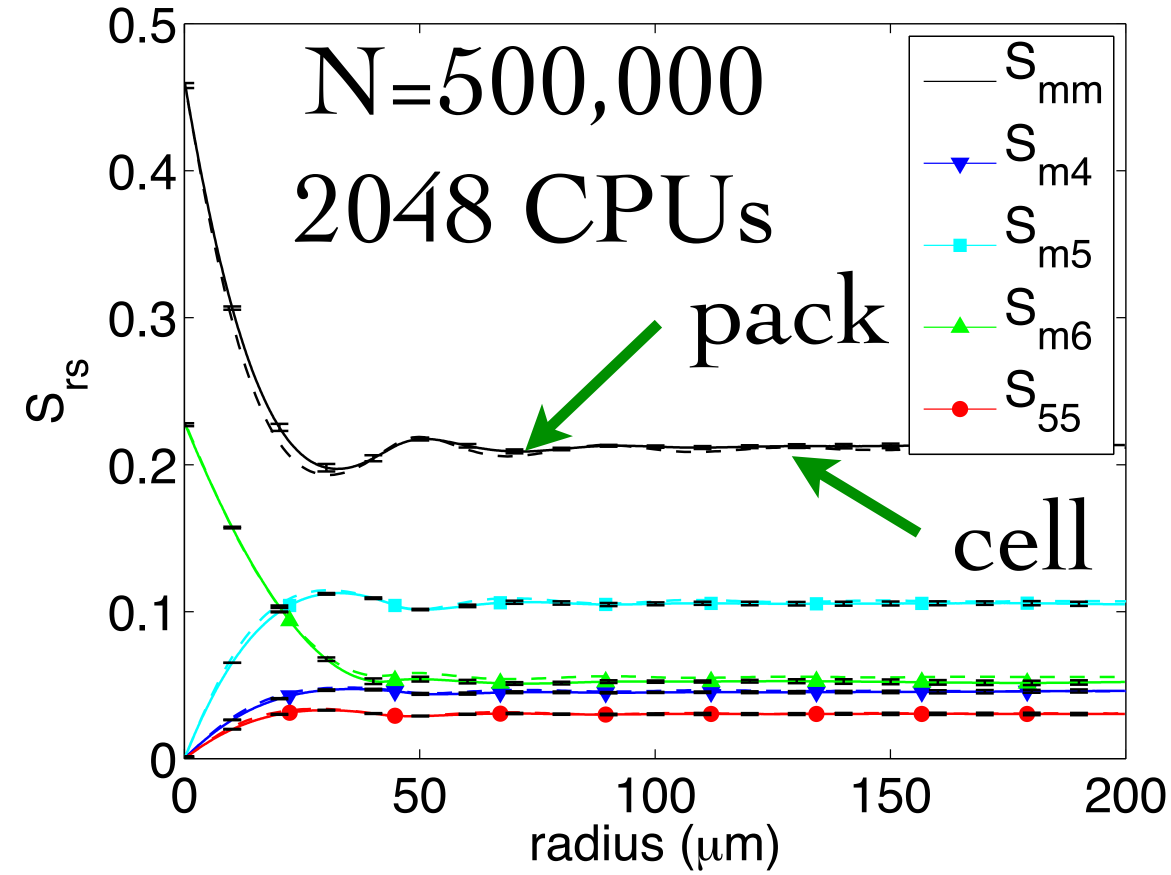
- Client-server communication structure
- Point-to-point, non-blocking communication structure
- Load balancing based on round-robin scheduling

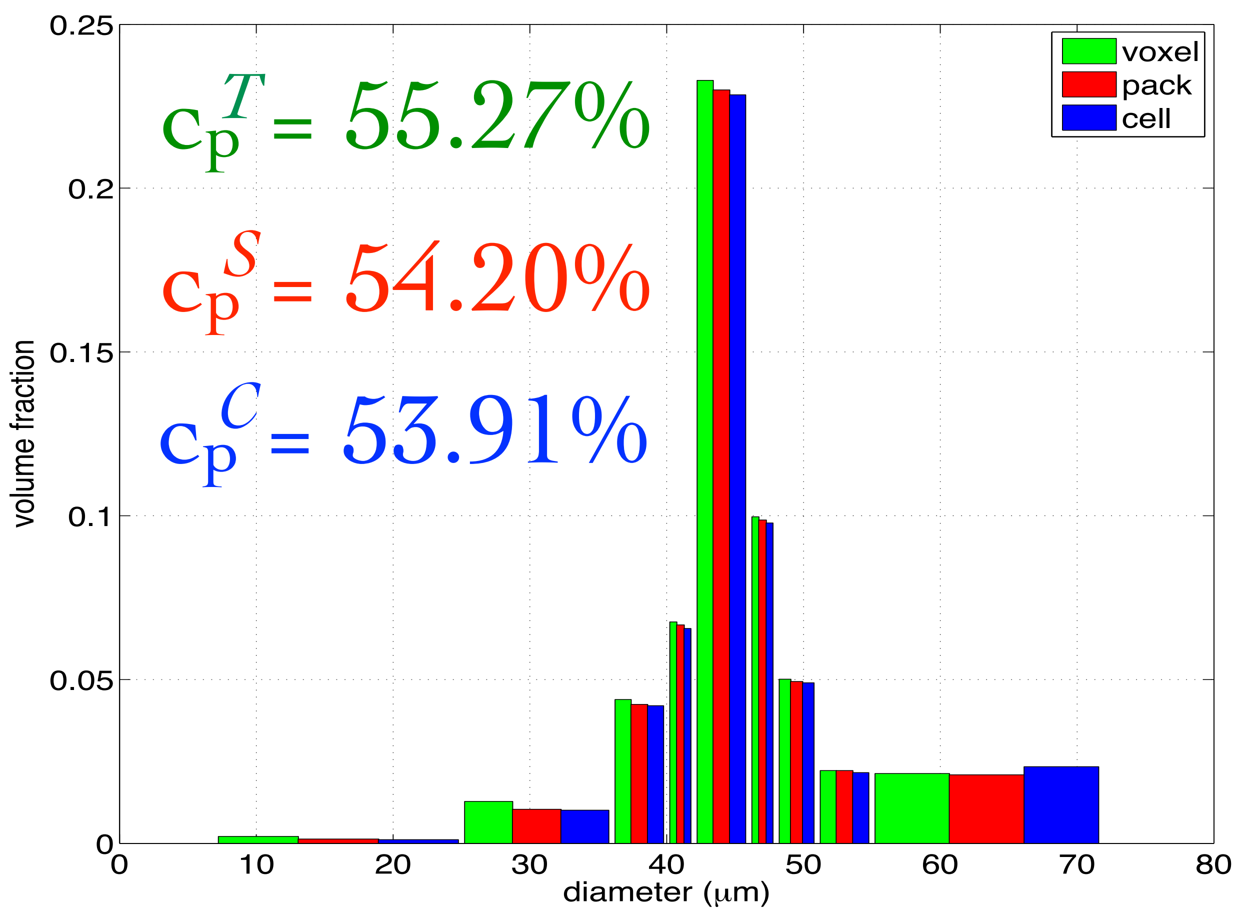
Image-based (Data-Driven) Modeling



9- bins







scan - 19123 particles
cell - 1082 particles

scan - 1445x1288x798 μm
cell - 400x400x400 μm

Parallel Genetic Algorithm

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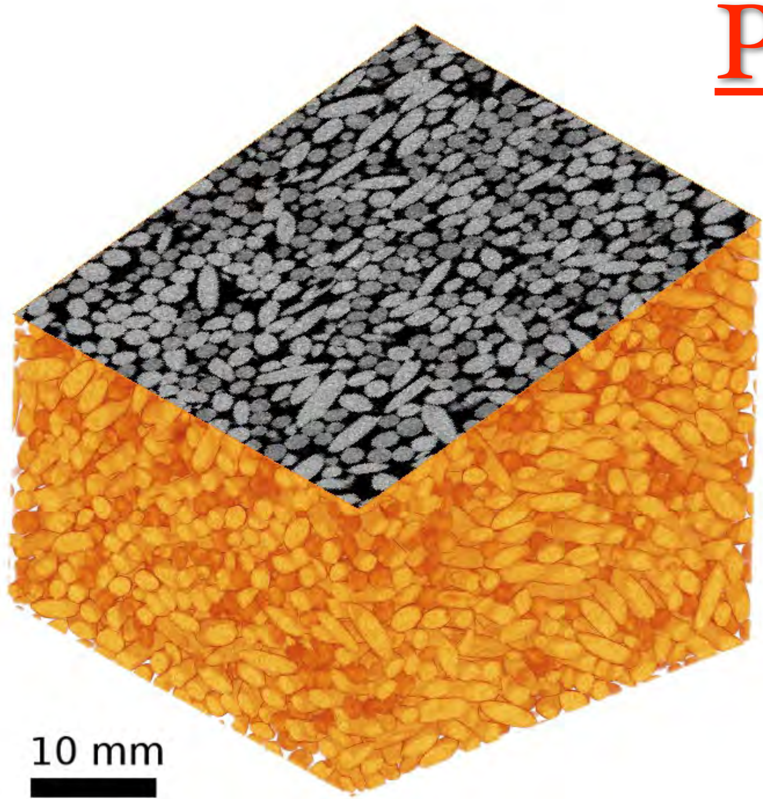
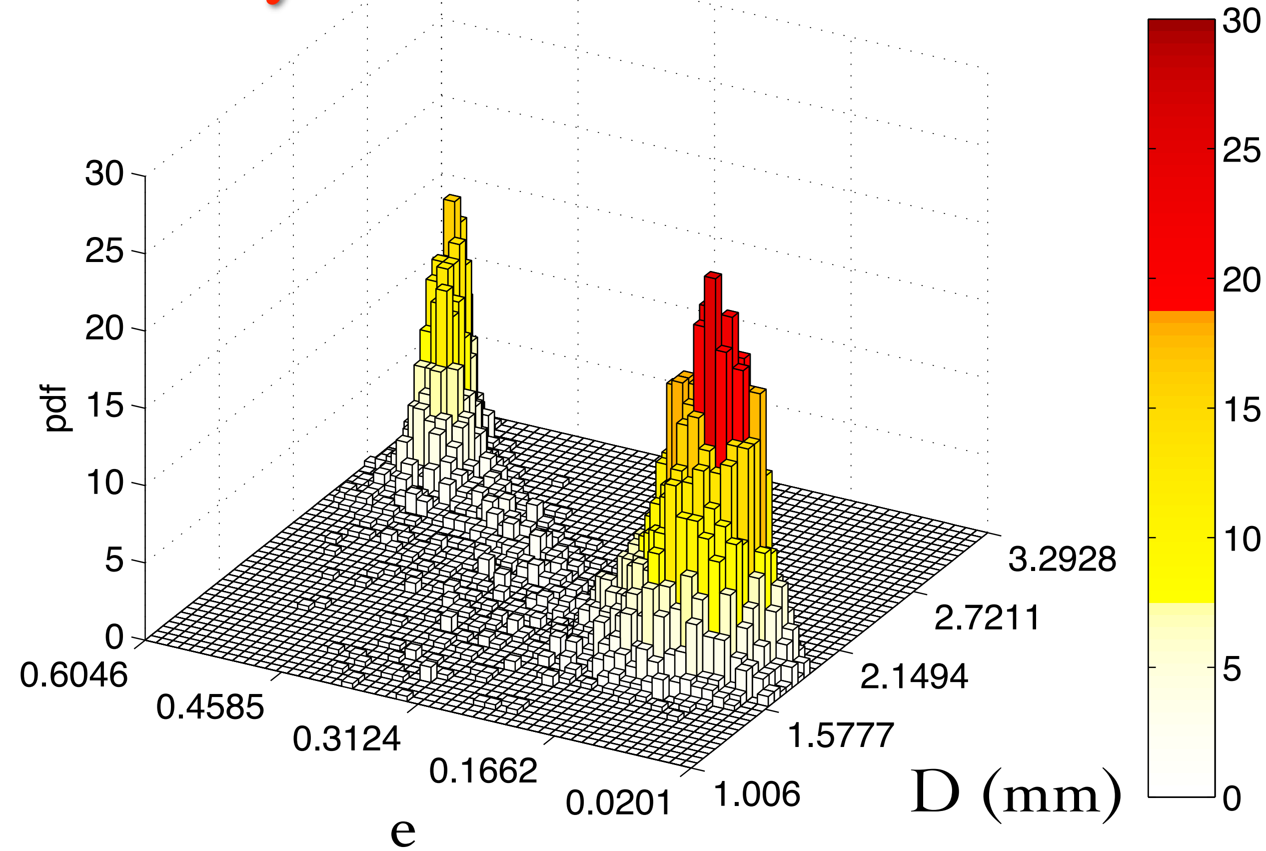
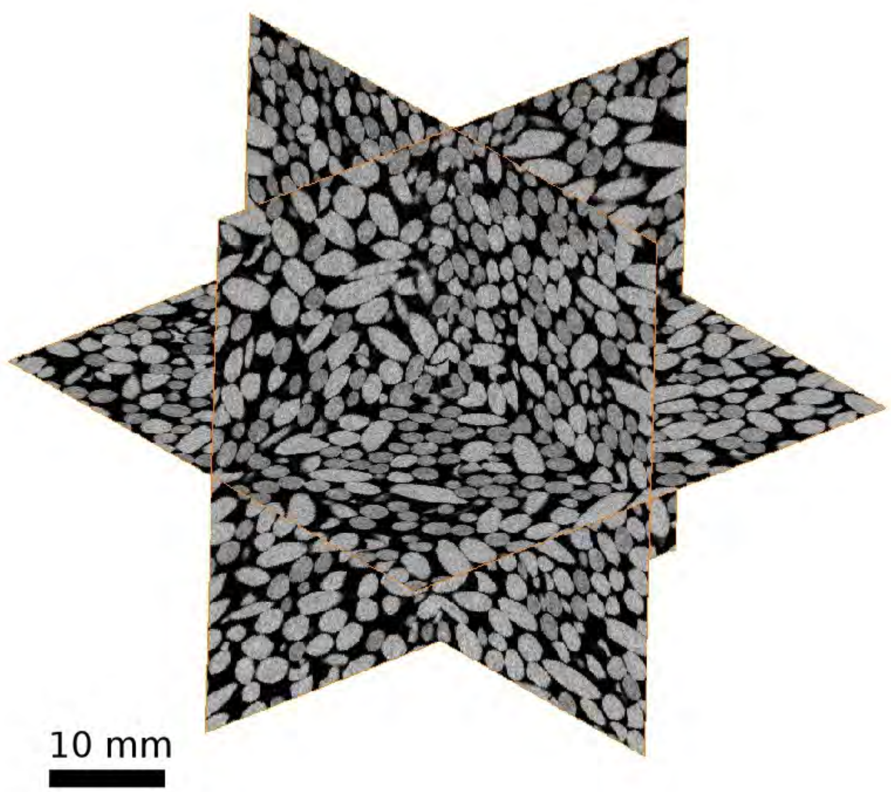
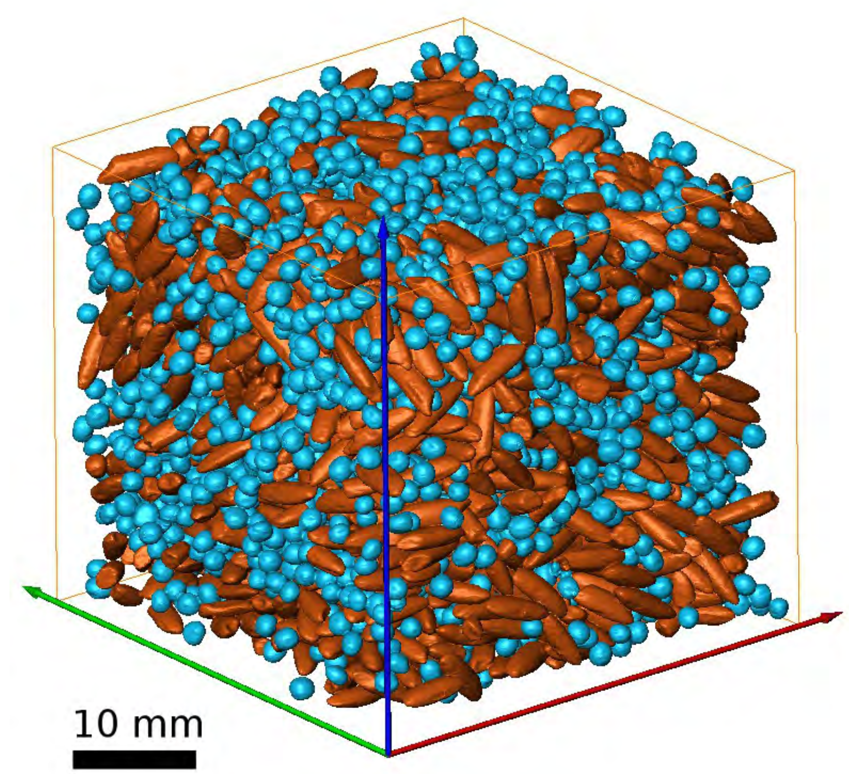
Polydisperse Systems



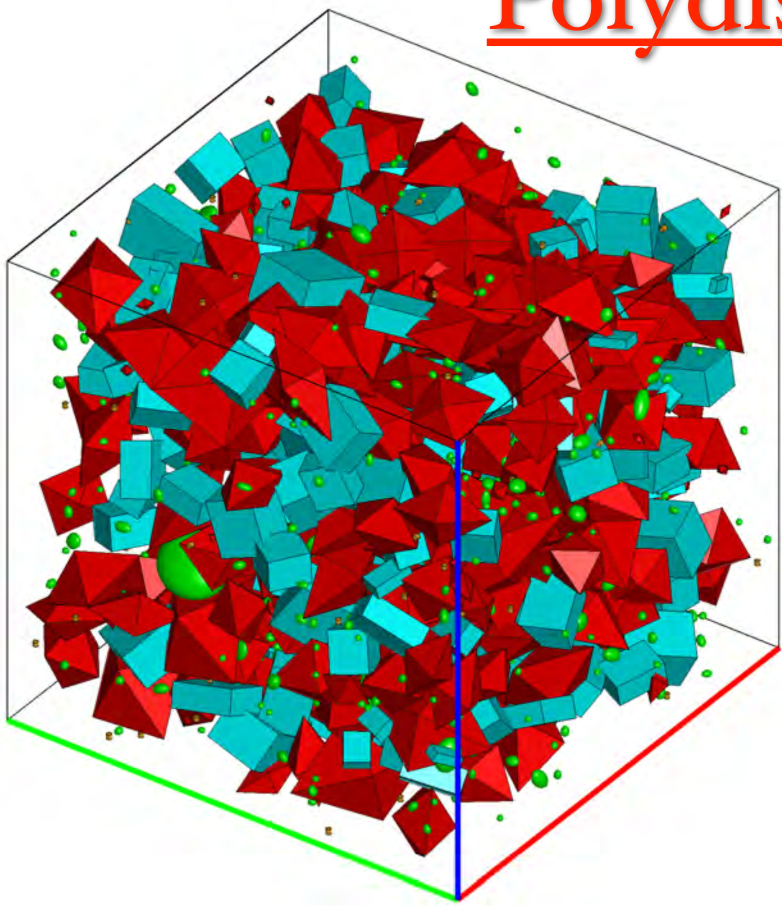




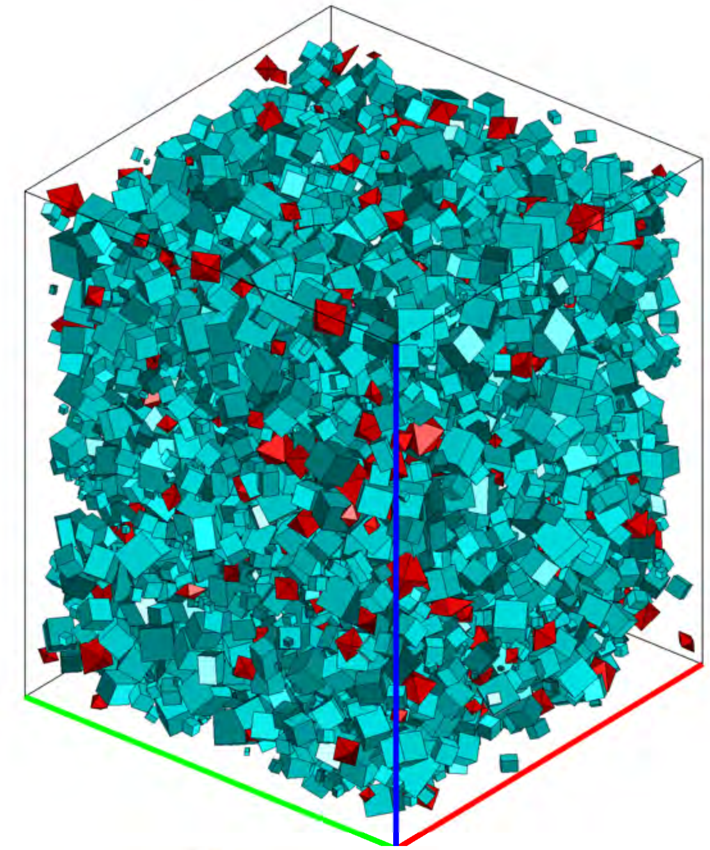


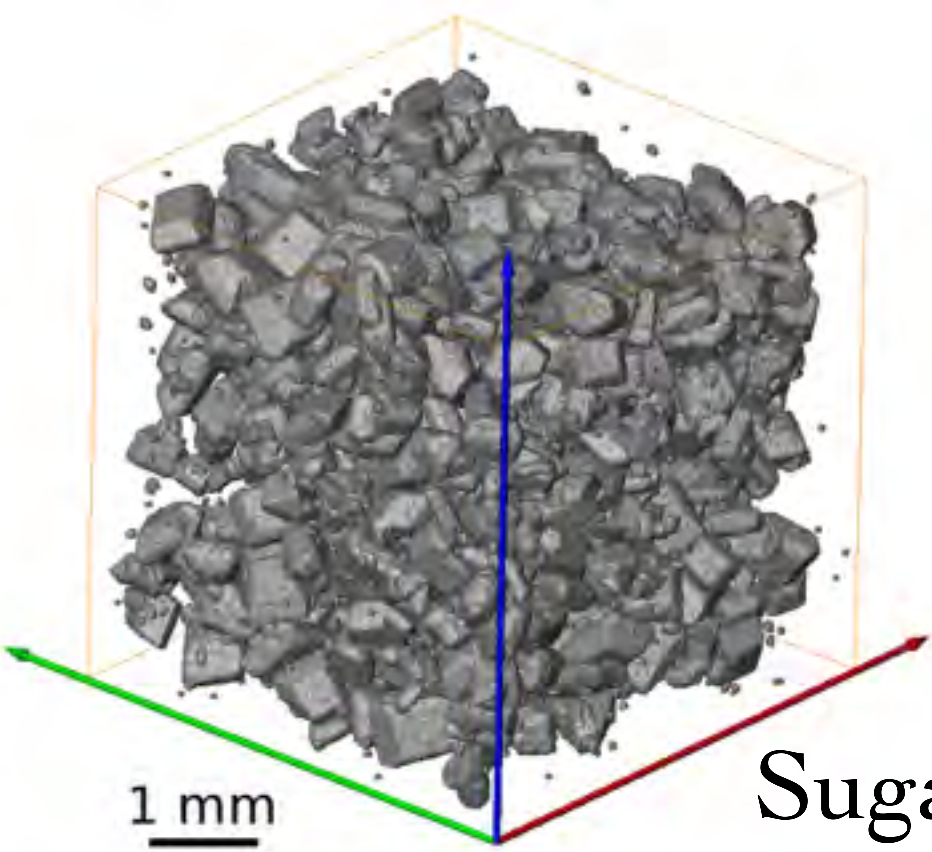
- Resolution 69.4 μm
- Rice & Mustard - c_p=0.667

Polydisperse Crystalline Systems



Salt





Sugar

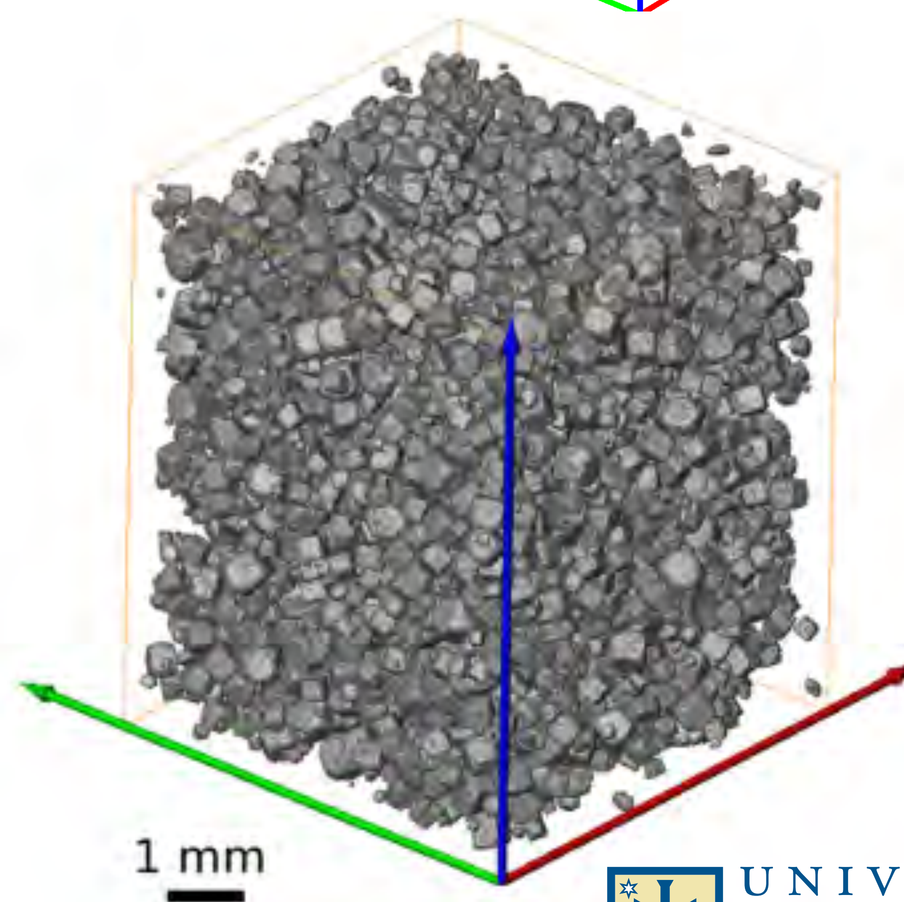
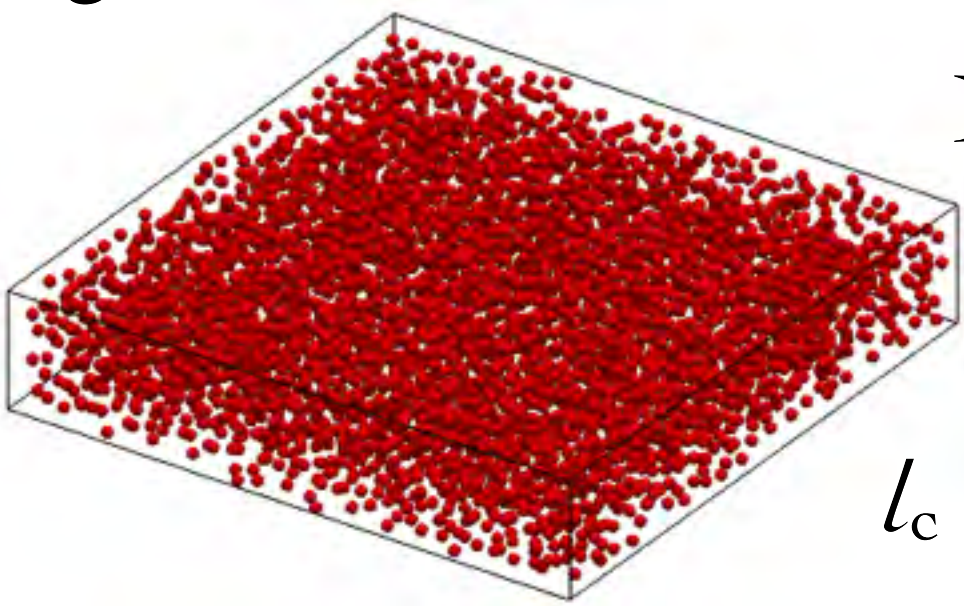


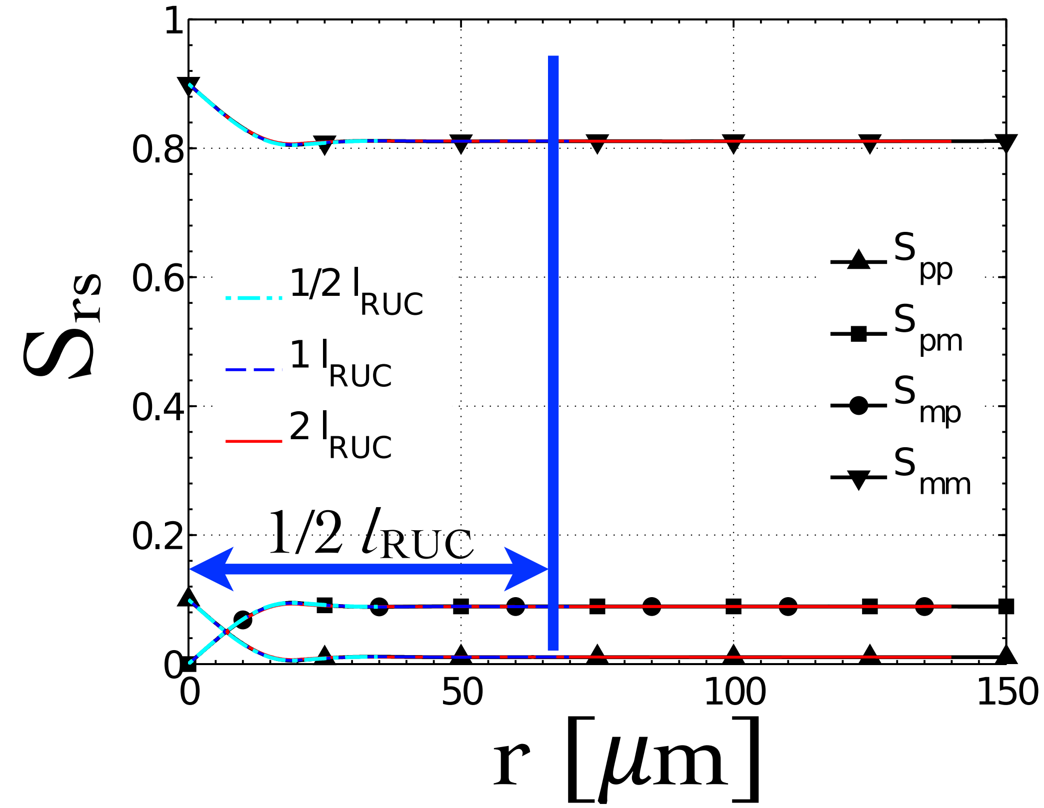
Image-based (Data-Driven) Modeling

- Digital Cell - 1000x1000x200 μm^3



Np = 4774

l_c = 200 μm

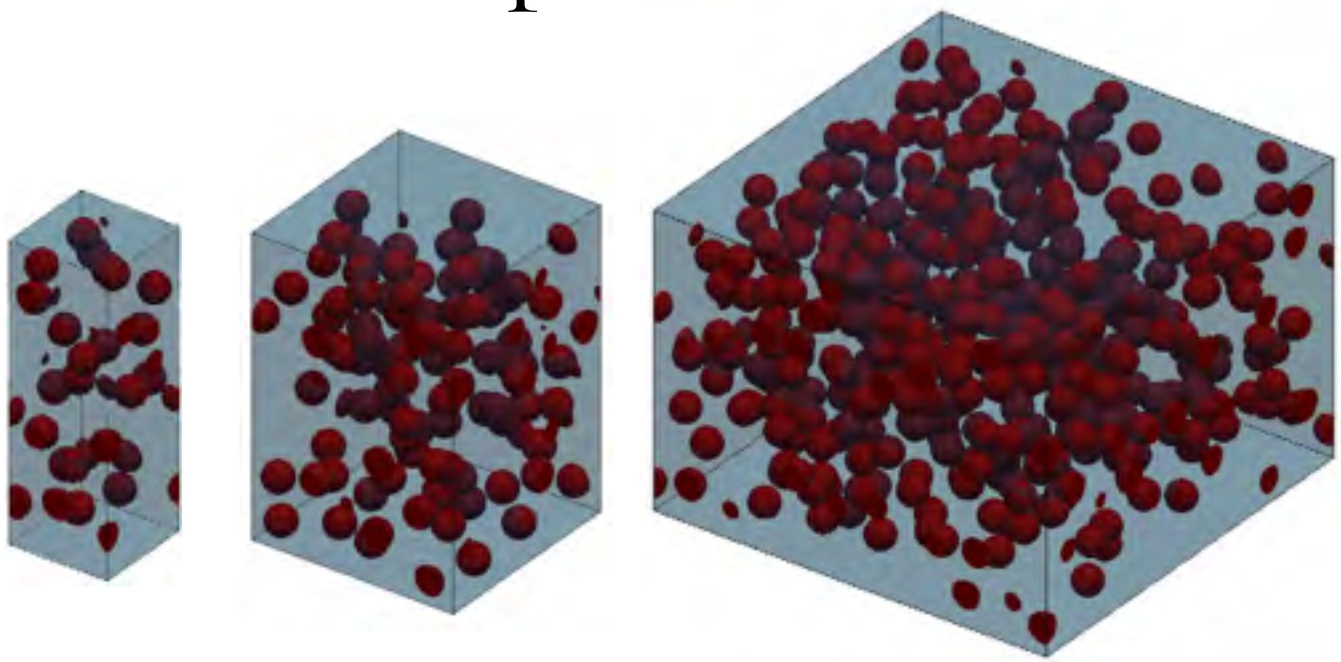


- 10 % volume fraction
- 20 micron particles

1/2 l_{RUC} - 70x70x200 μm^3

l_{RUC} - 140x140x200 μm^3

2 l_{RUC} - 280x280x200 μm^3



1/2 l_{RUC} l_{RUC} 2 l_{RUC}

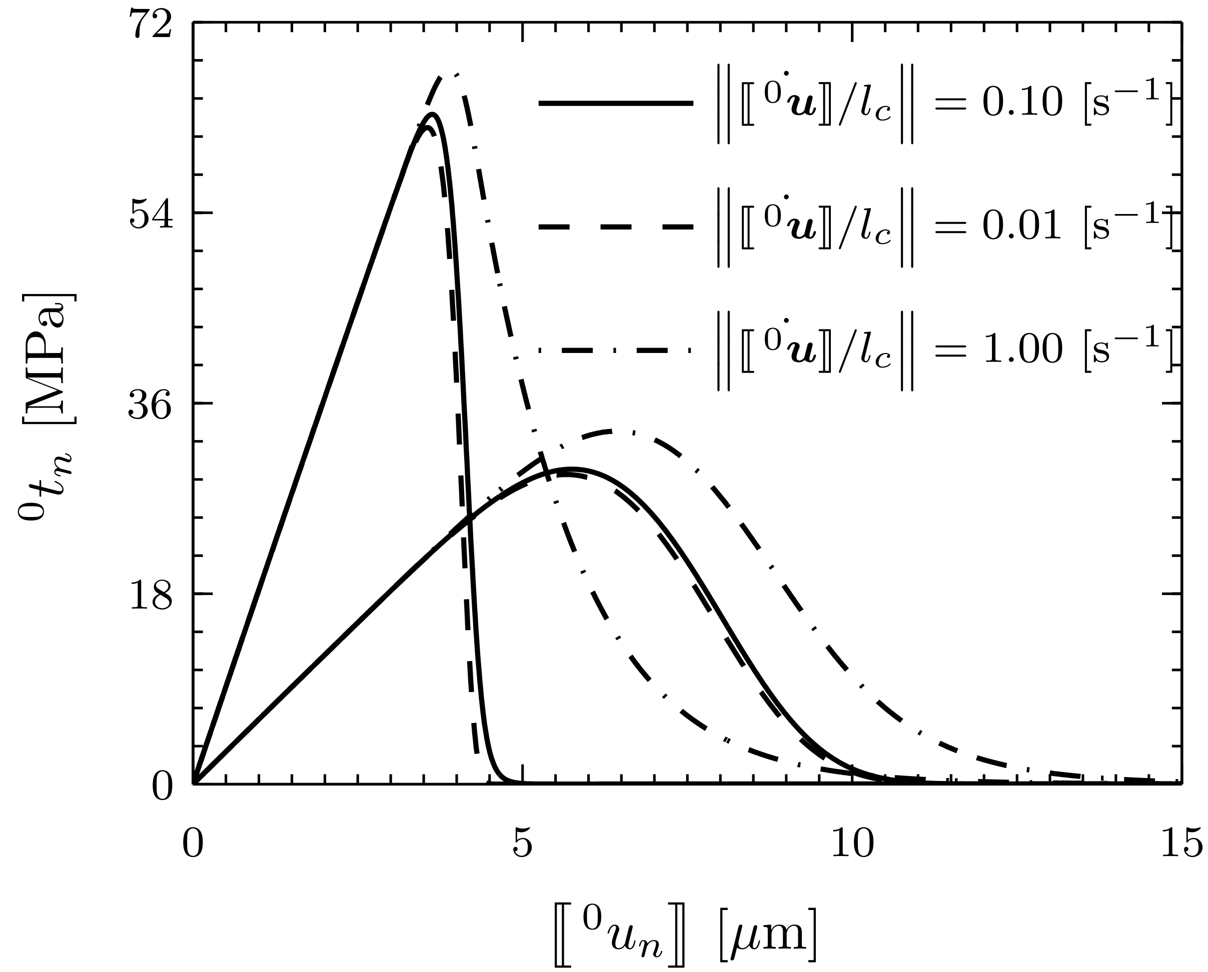
1/2 l_{RUC} - Np = 23

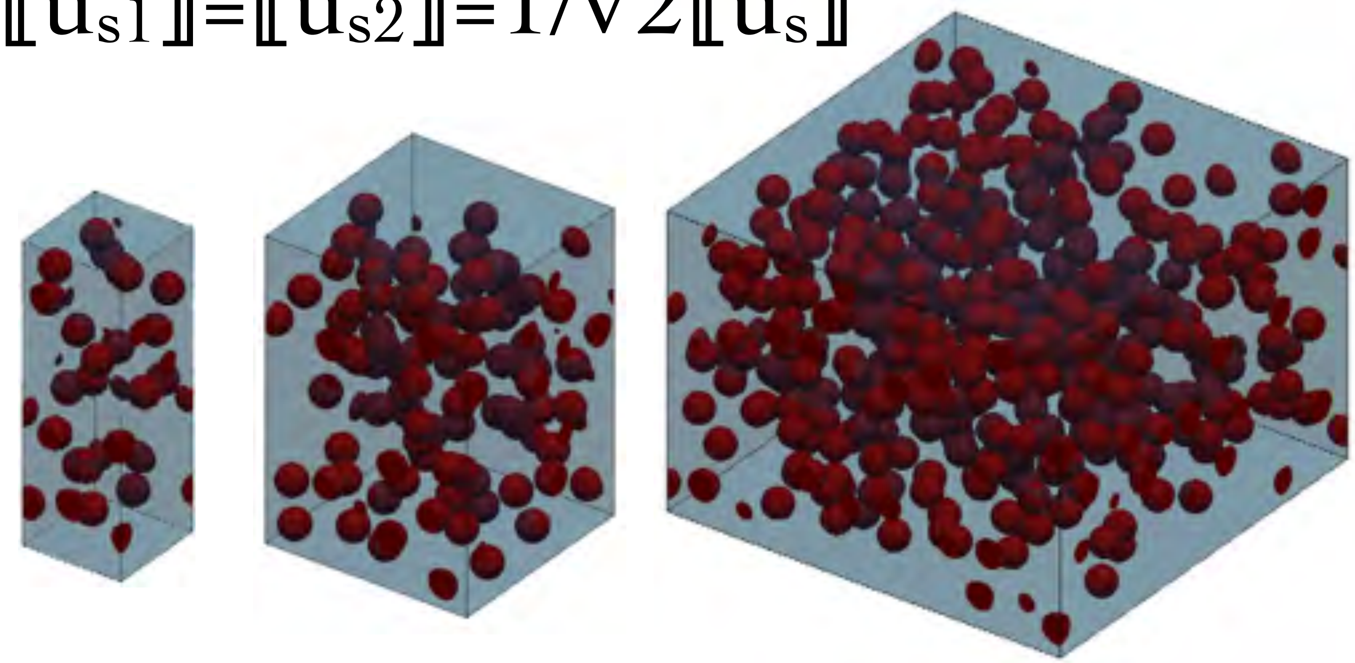
l_{RUC} - Np = 93

2 l_{RUC} - Np = 374

Representative Unit Cell Study

- Mixed mode loading $[\![u_n]\!]=[\![u_{s1}]\!]=[\![u_{s2}]\!]=1/\sqrt{2}[\![u_s]\!]$





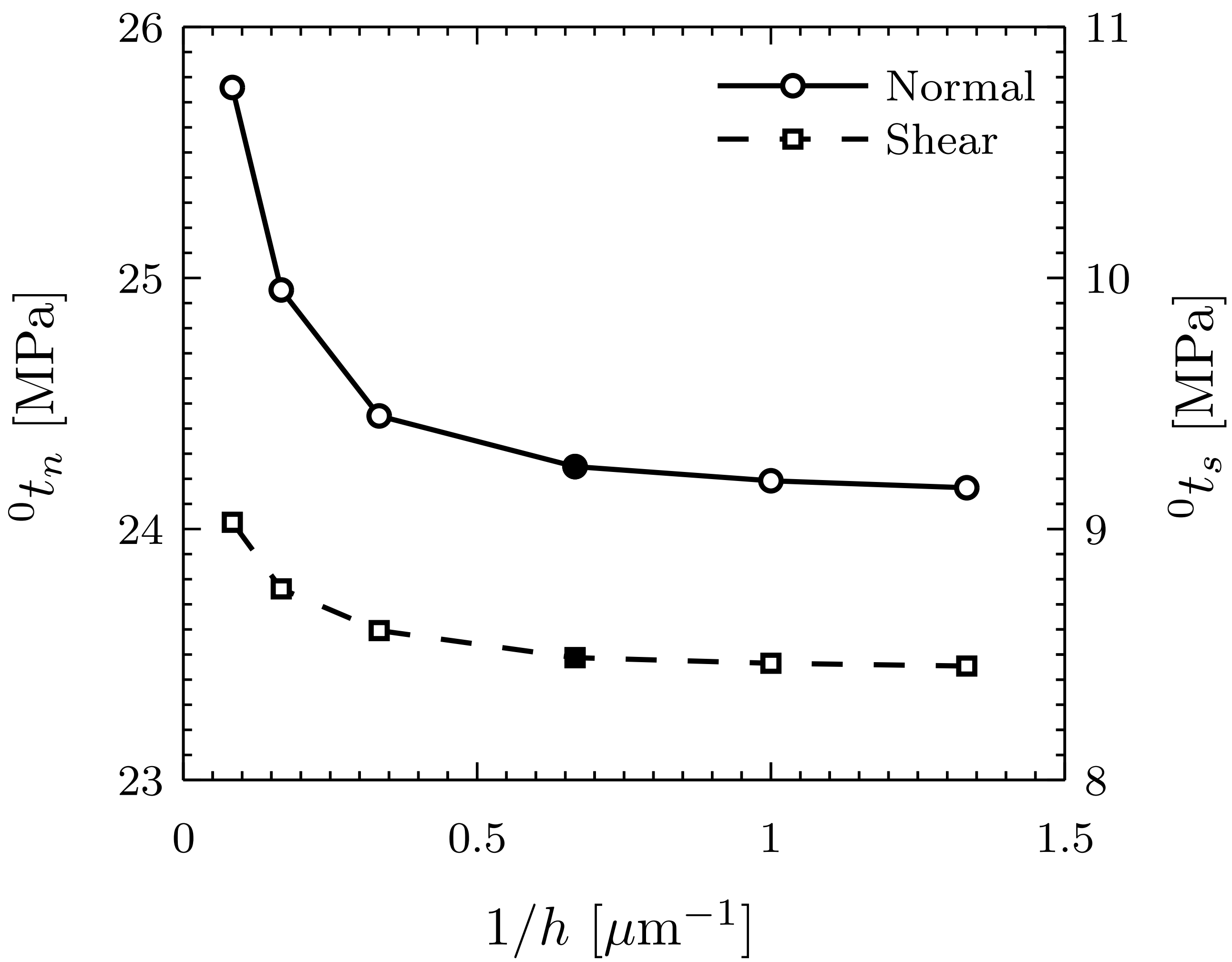
l_{RUC}
- Ne≃12,317,628
- Nn≃2,103,957
- Dofs≃6,280,495

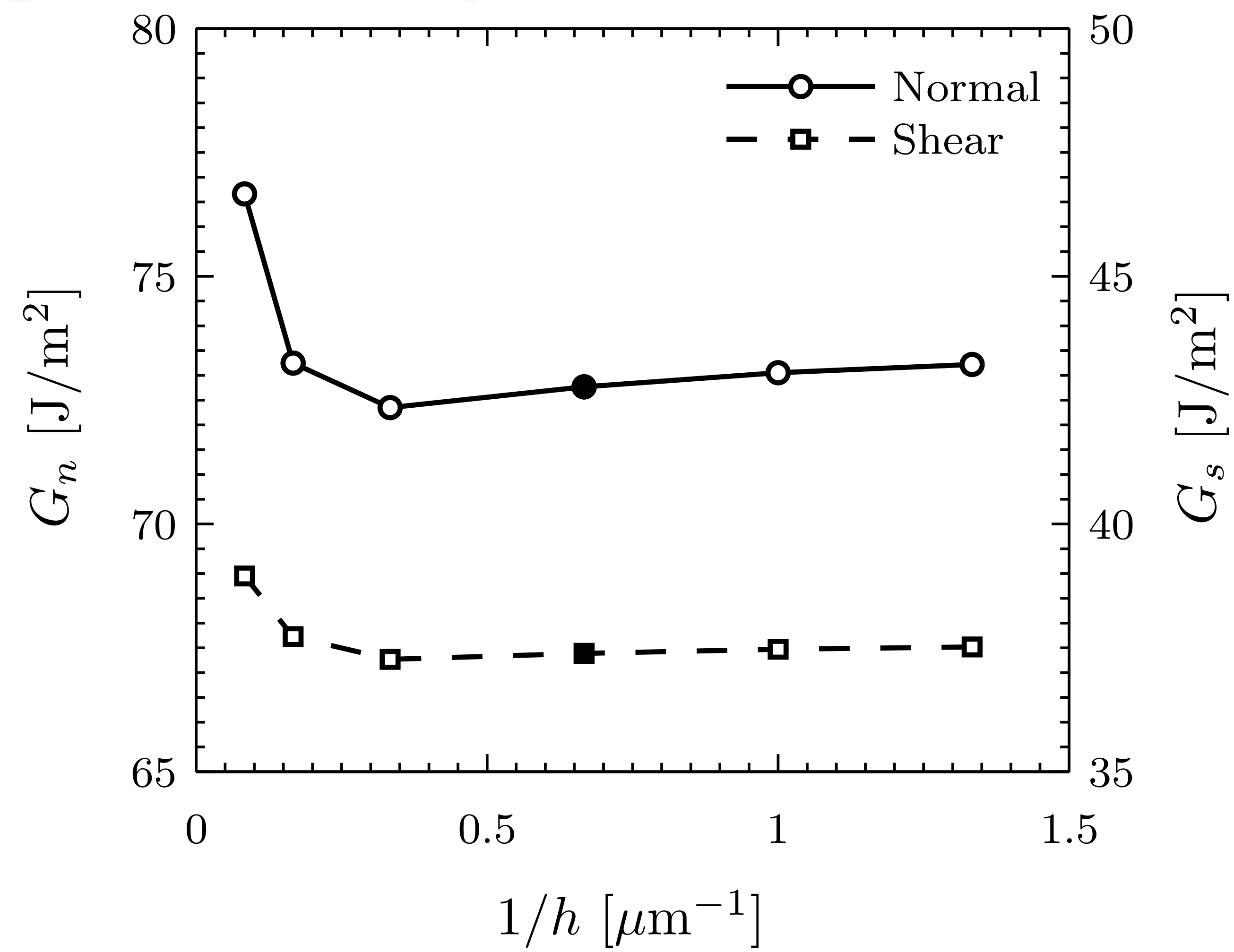
$2\ l_{\text{RUC}}$
- Ne≃48,537,975
- Nn≃8,294,617
- Dofs≃24,758,080

$$[\![u_s]\!] = \sqrt{[\![u_{s1}]\!]^2 + [\![u_{s2}]\!]^2}$$

- Mean element size 1.5 μm

Mesh Convergence Study





● Used mesh

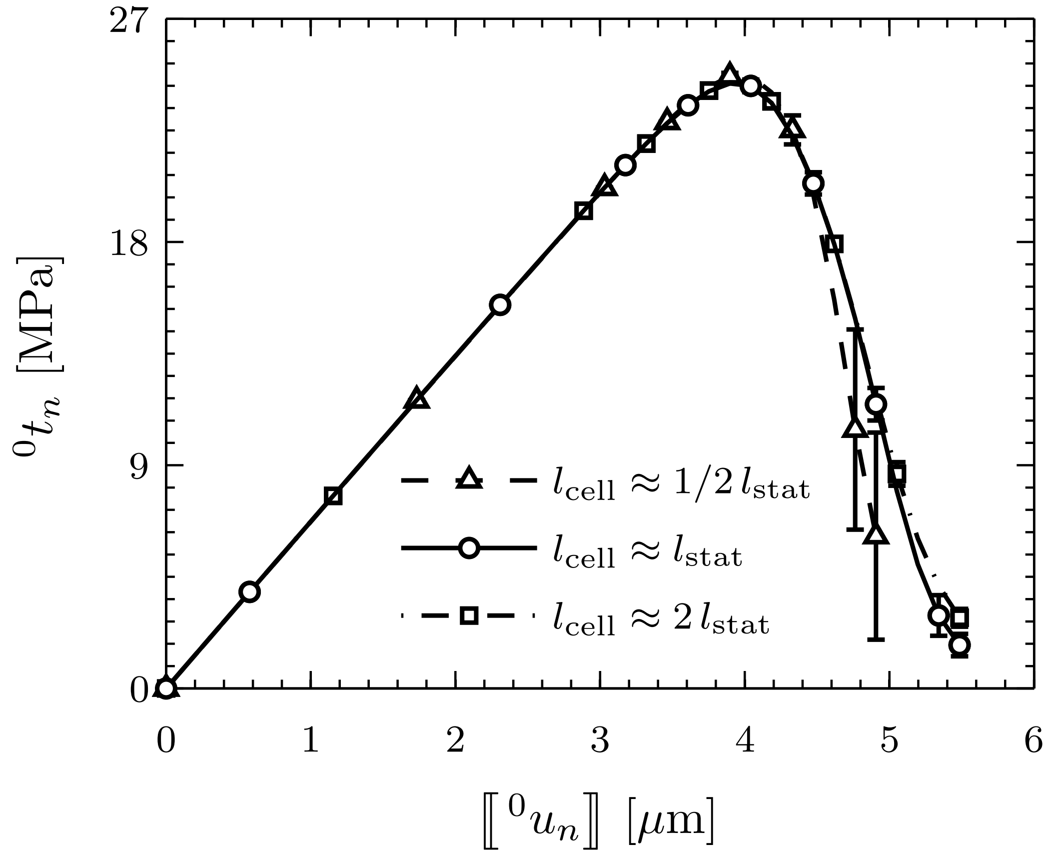
● Finest mesh

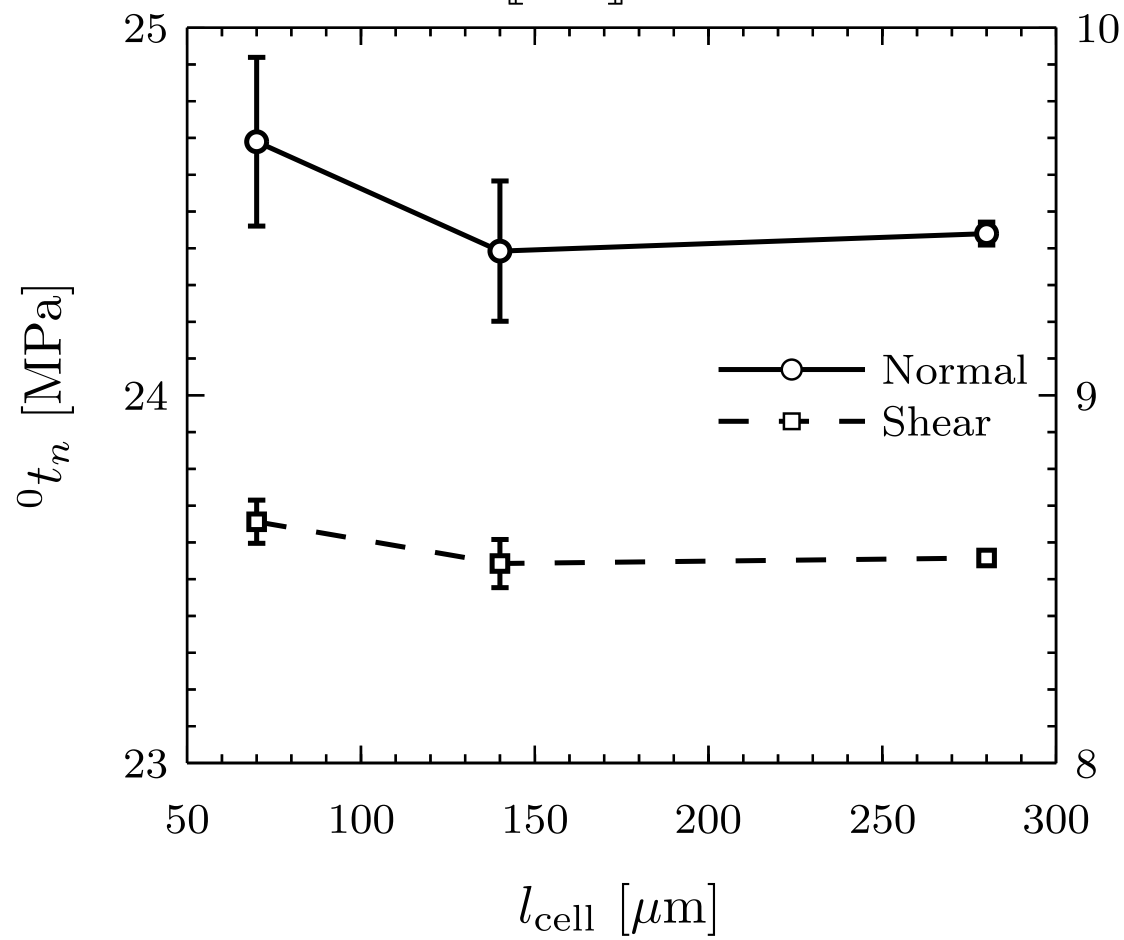
h_{min} = 0.073 microns
h_{mean} = 1.370 microns
h_{max} = 2.25 microns

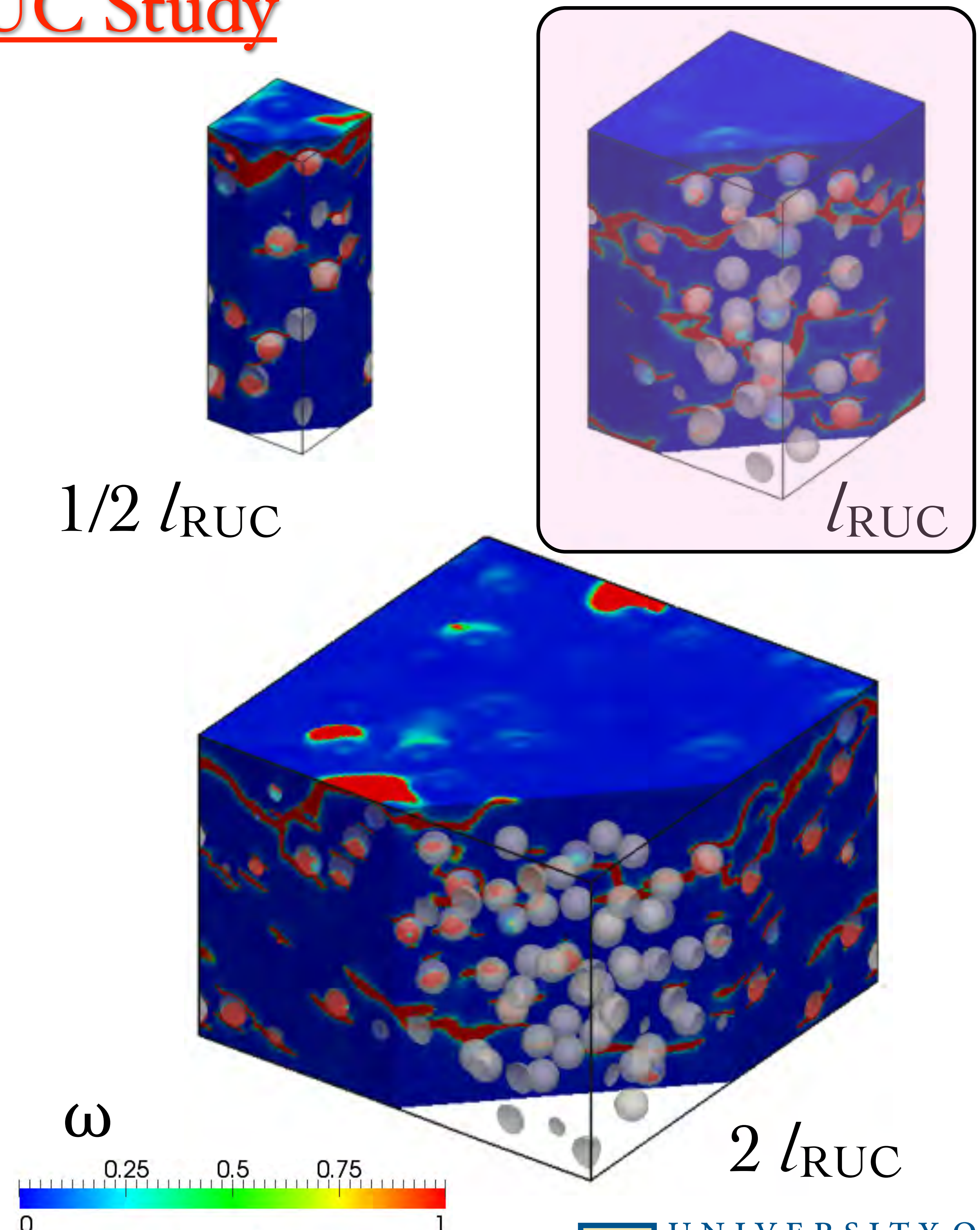
Nodes = 16,020,086
Elements = 93,856,013
DOFs = 47,938,704

- Richardson extrapolation max error < 1.05%

RUC Study







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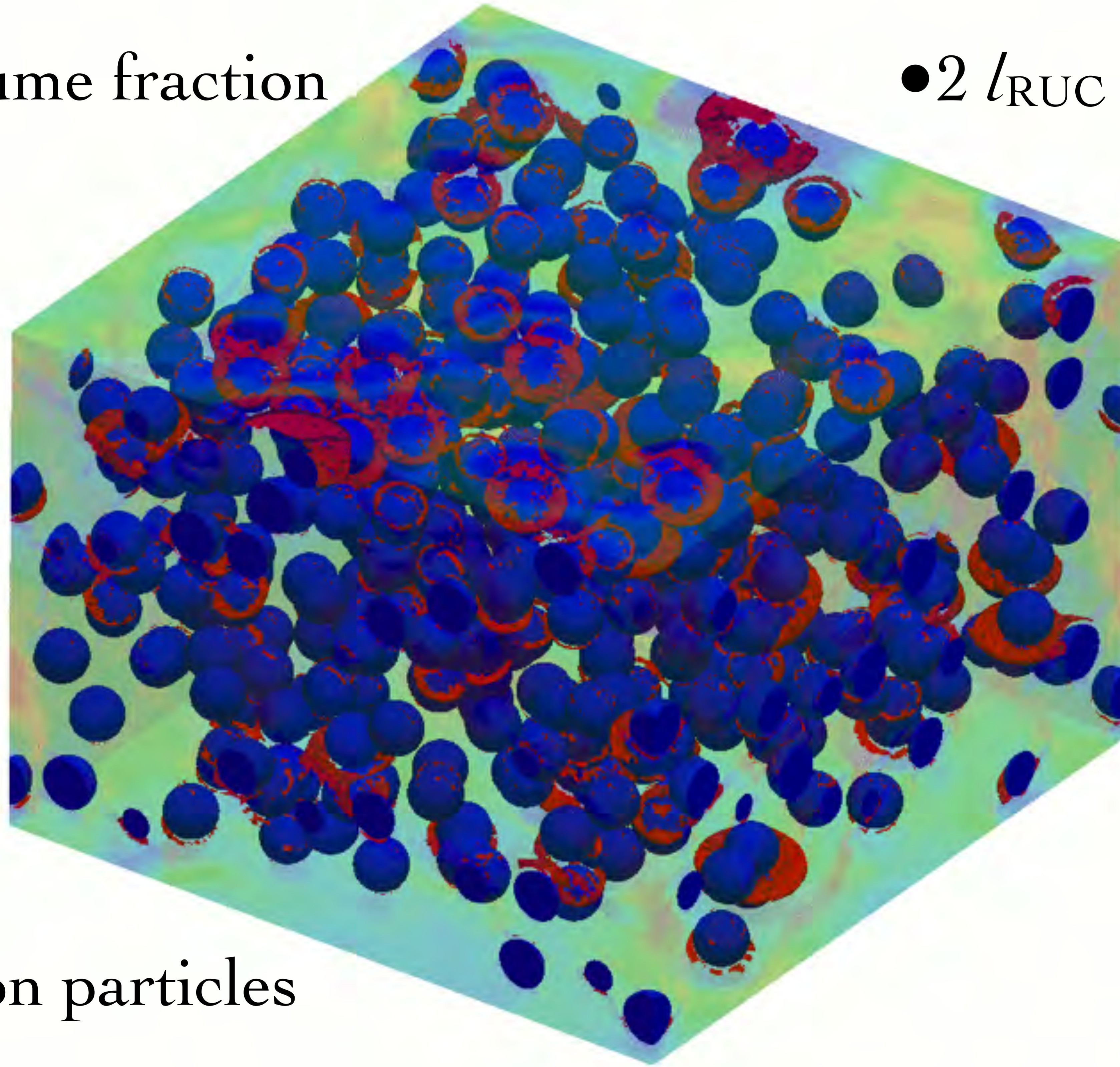
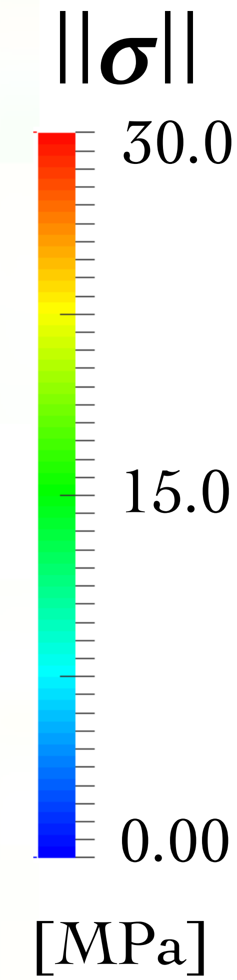
Multiscale Cohesive Model - Mixed Mode Loading

- 10 % volume fraction
- 2 l_{RUC} - Np = 374

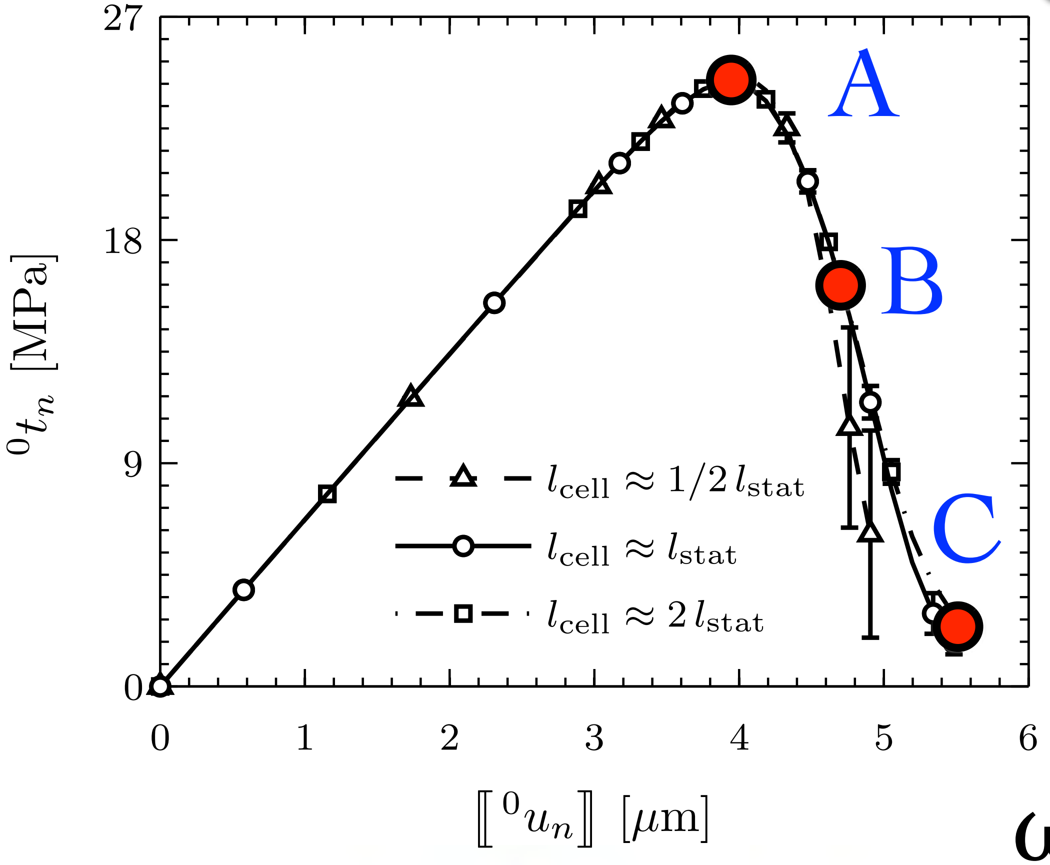




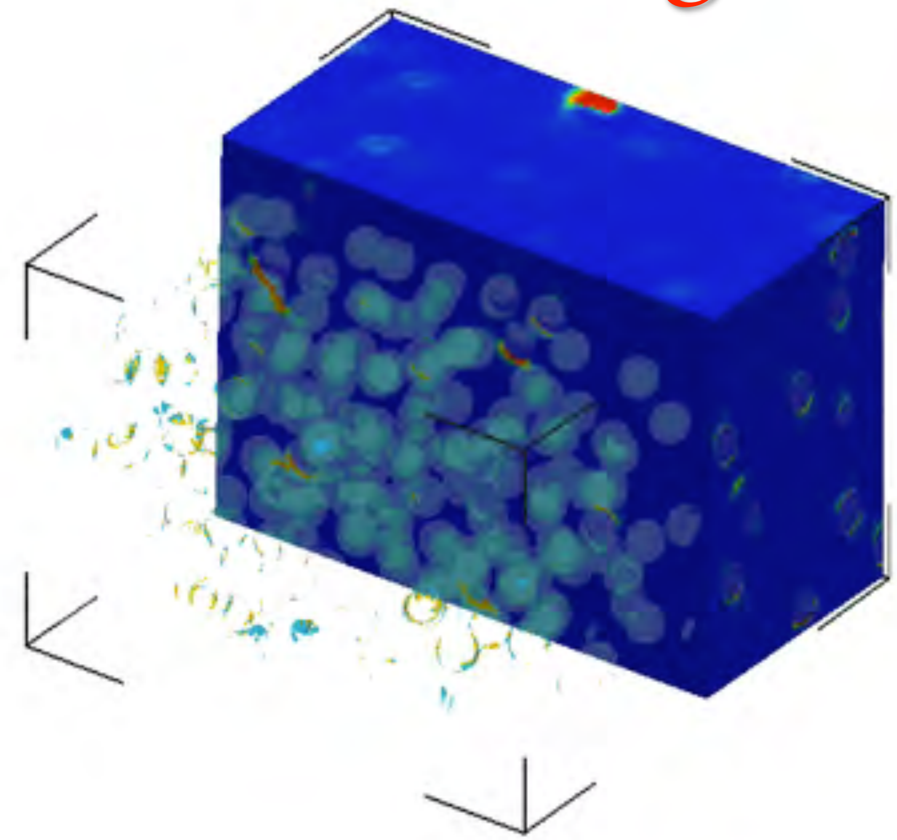
- 20 micron particles

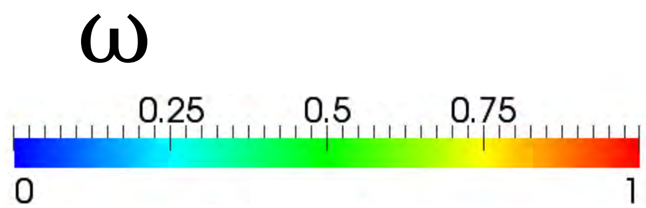
- Isocontours of $\omega \geq 0.999$
- 512 CPUs

Extent of Damage - Mixed Mode Loading

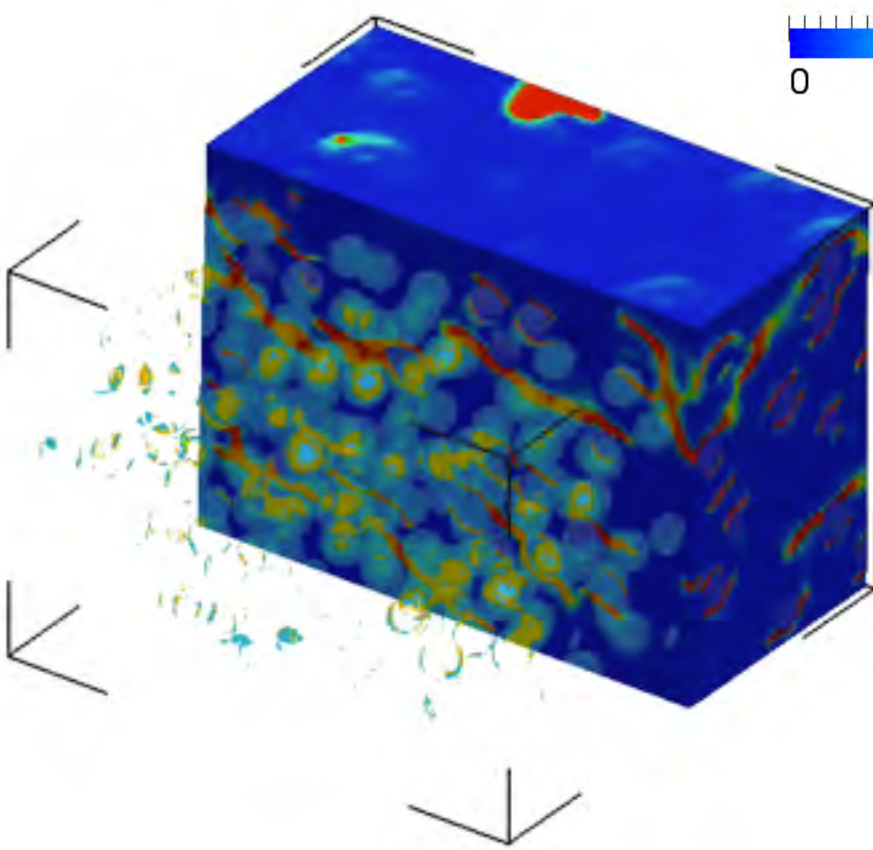


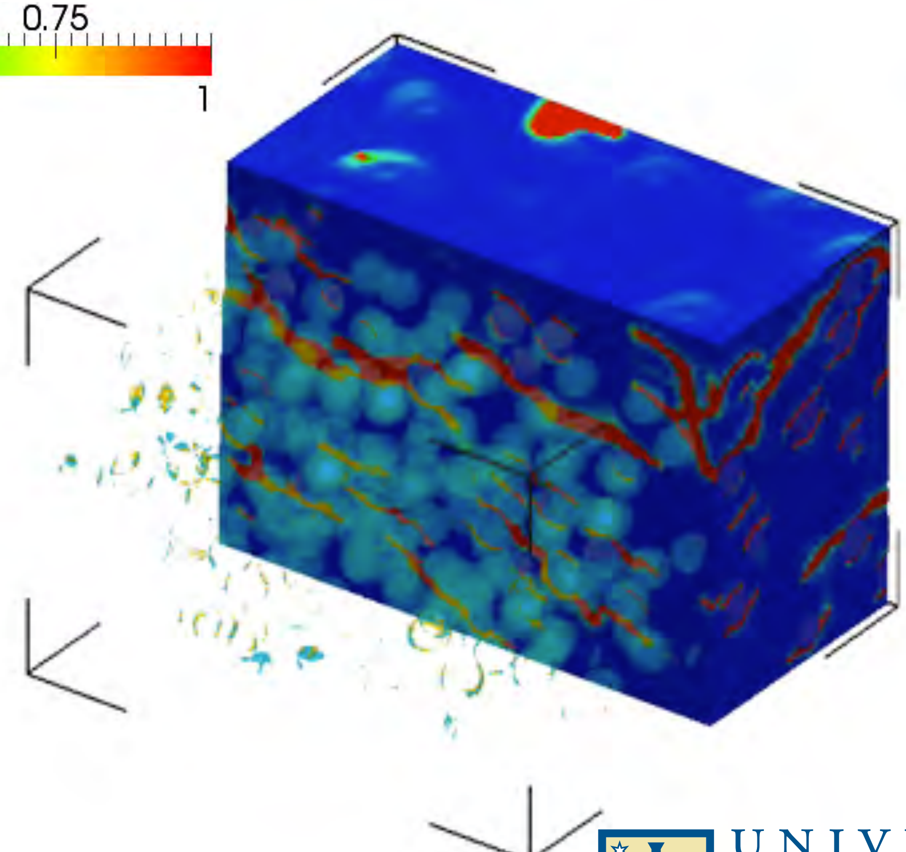
A





B

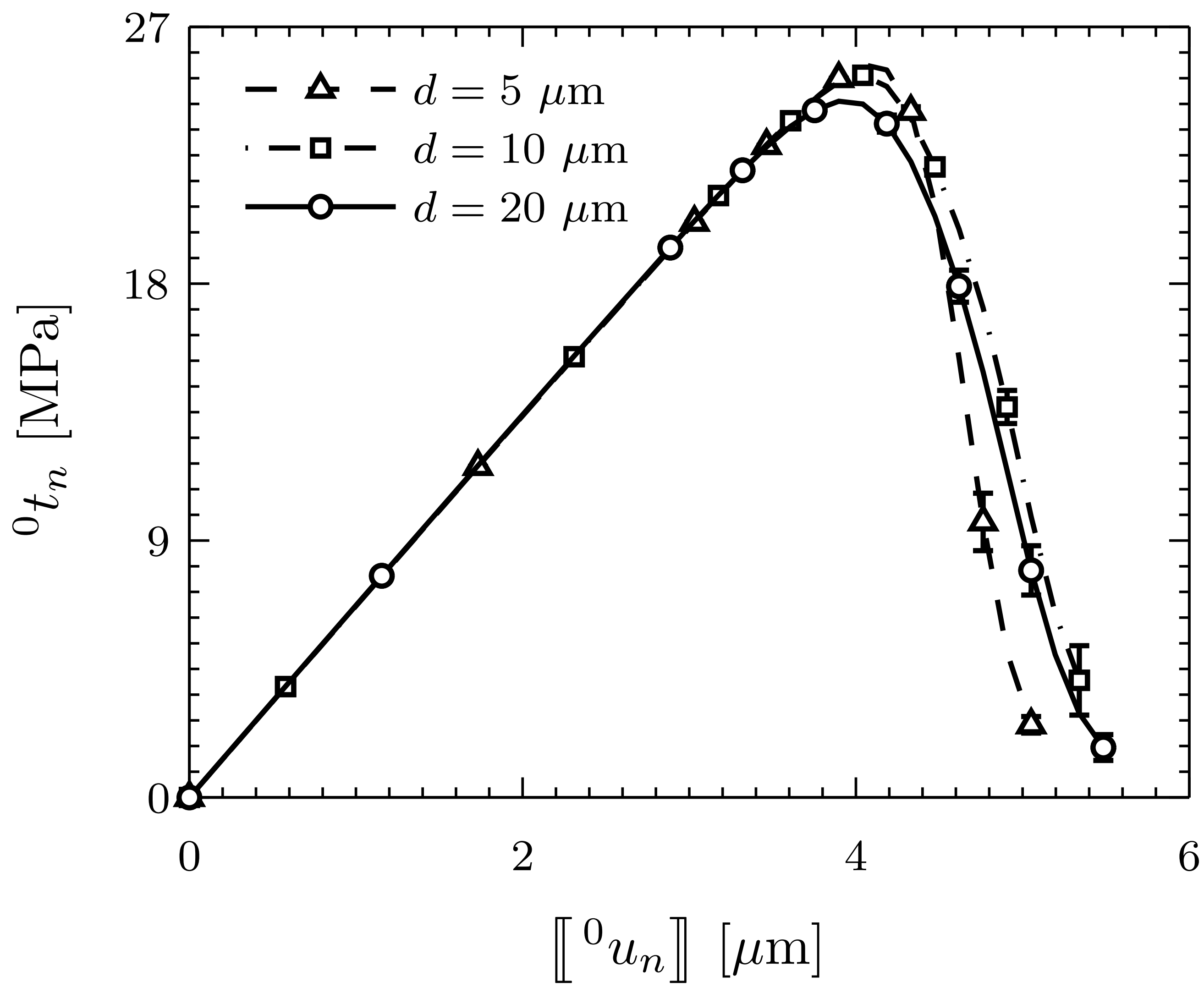




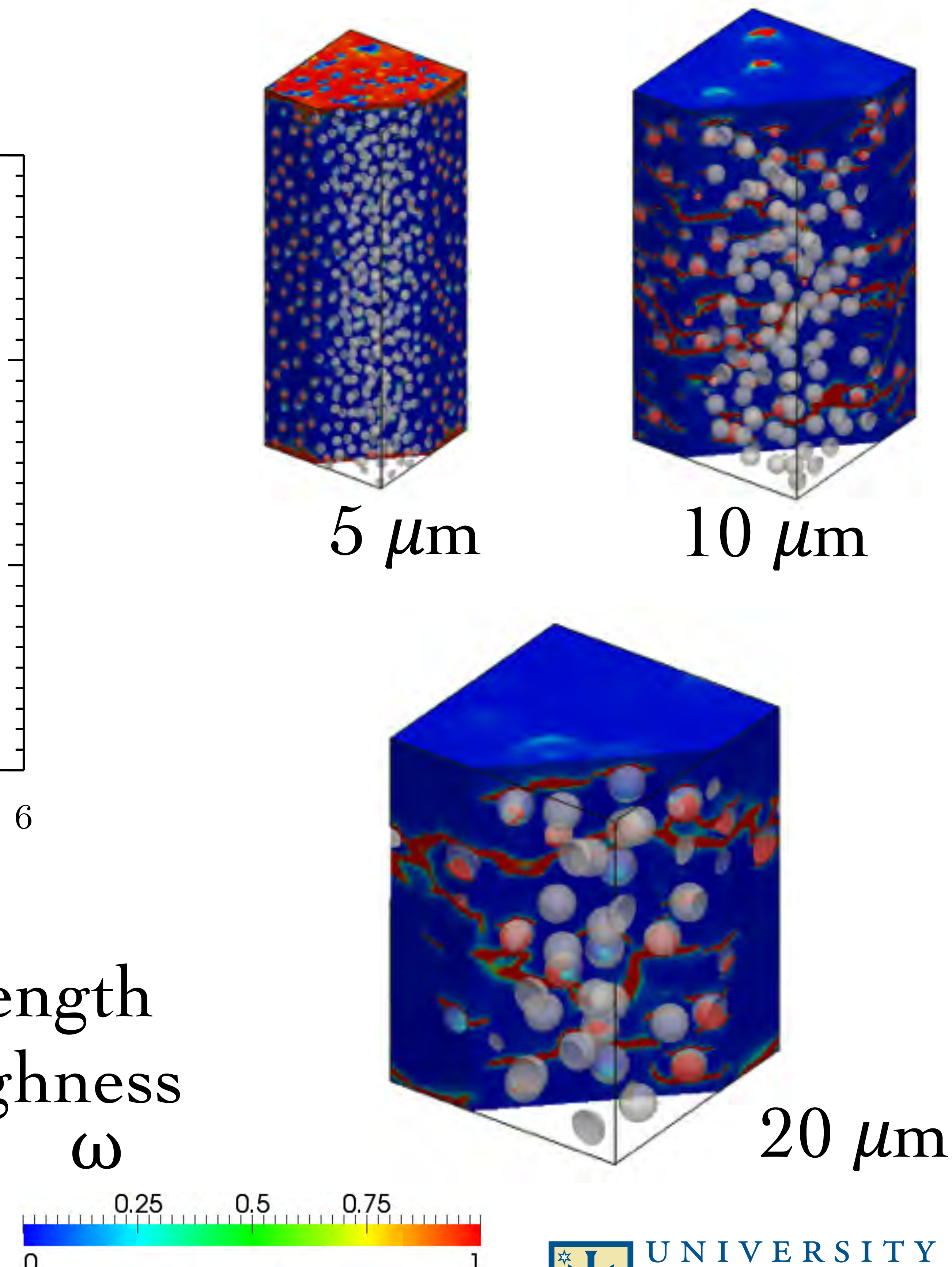
C

Particle Diameter Effect

- 10 % volume fraction

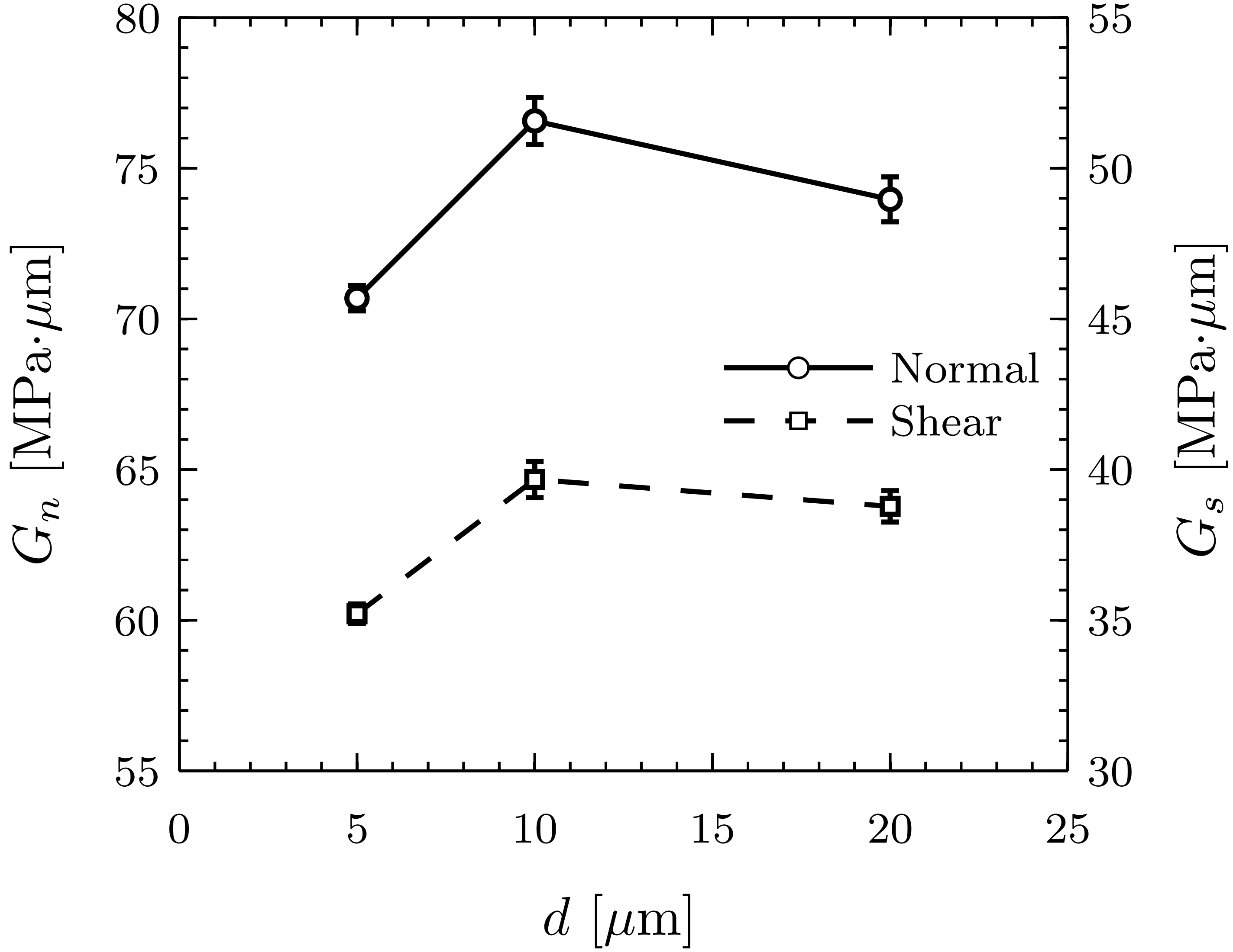


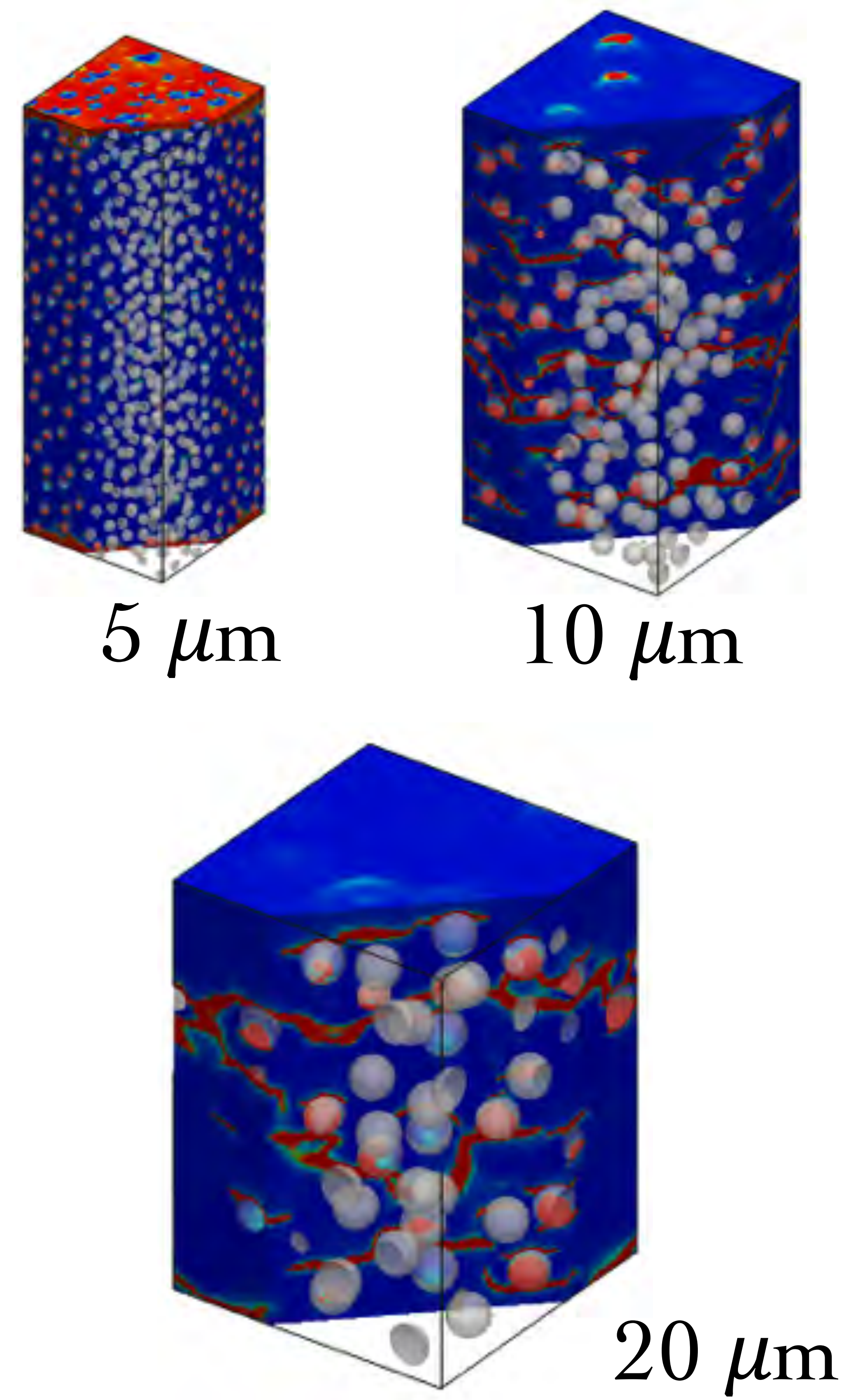
- Smaller particles - higher strength
- Non-monotonic fracture toughness



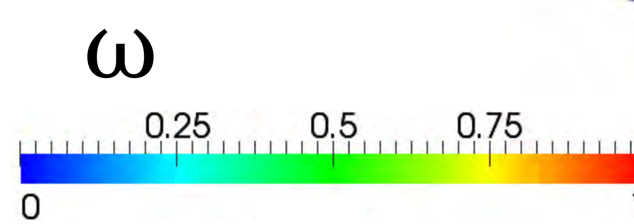
Particle Diameter Effect

10 % volume fraction

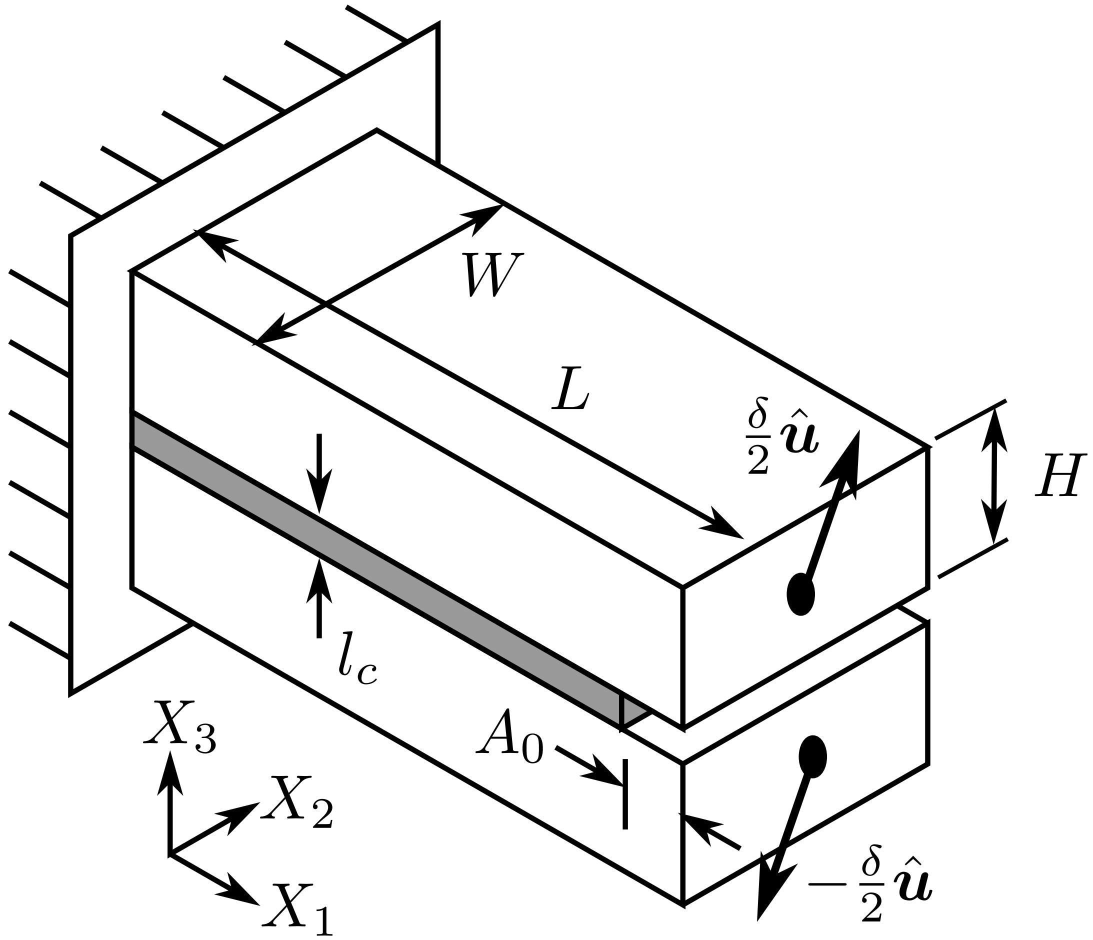




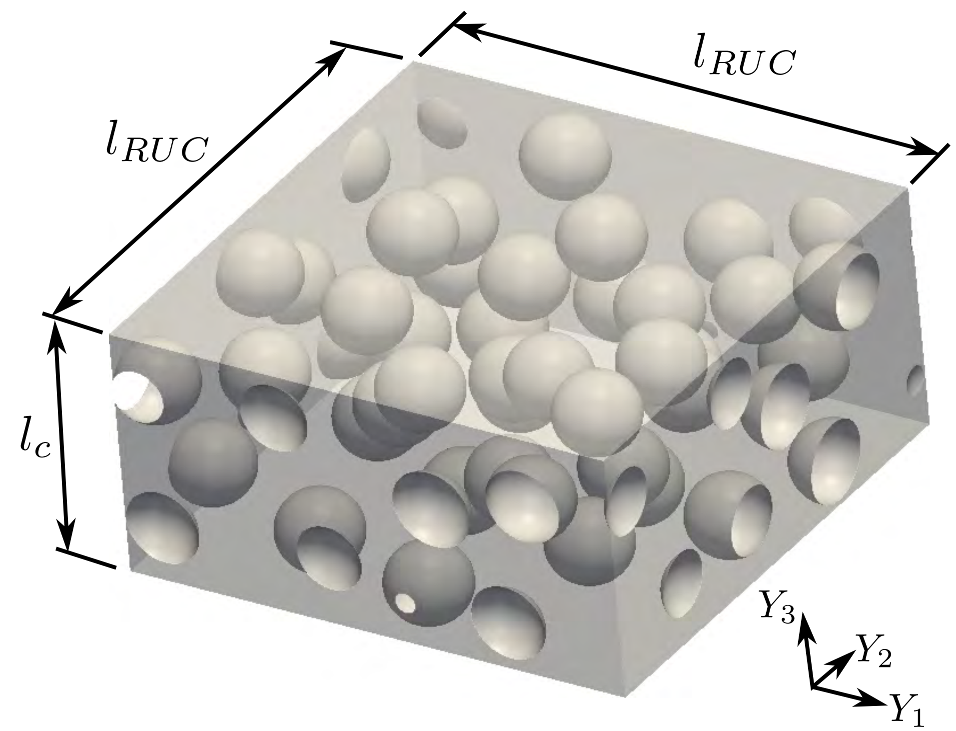
- Smaller particles - higher strength
- Non-monotonic fracture toughness



Hierarchically Parallel Multiscale Solver



- 40 voids
- 40 µm



- L=22 mm, W=10 mm, H=5 mm
- l_c=0.125 mm, l_{RUC}=0.25 mm

- 16 Clients
- 12 Servers @ 128 cores

	Nodes	Elements	DOFs
Macroscale	731	2,684	1,878
Microscale	193,873,920	1,098,283,920	574,612,560
TOTAL	193,874,651	1,098,286,604	574,614,438

- 1552 cores
- 370,241 DOFs / core

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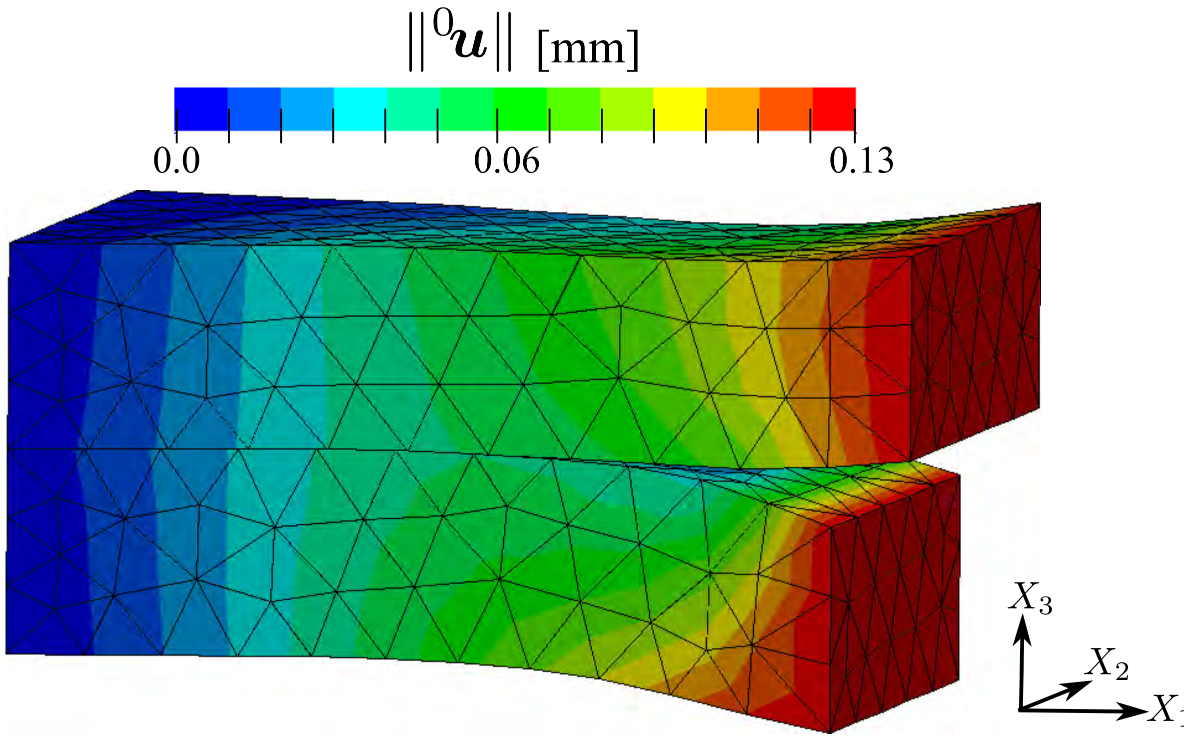
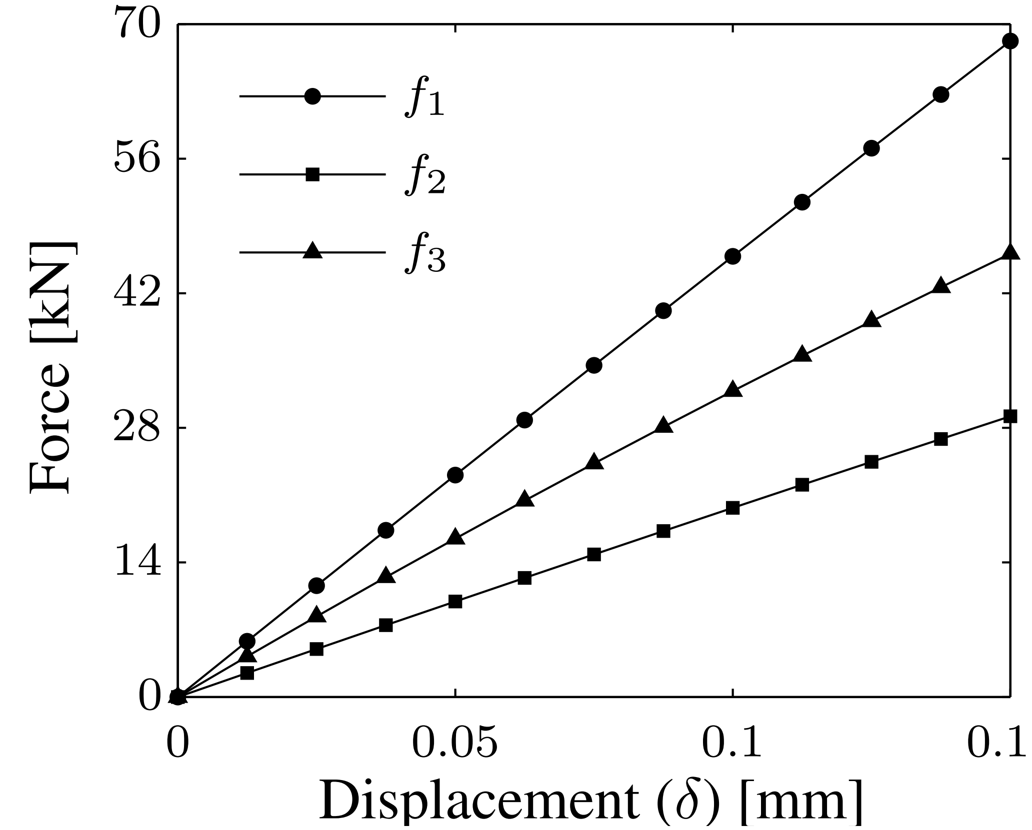
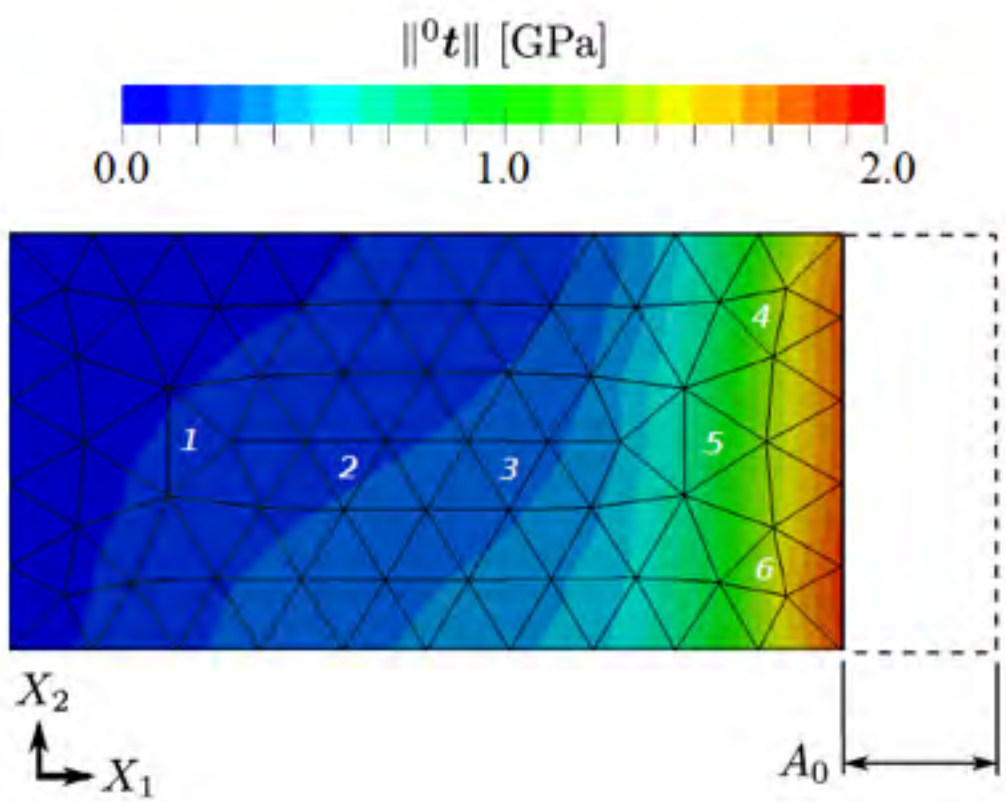
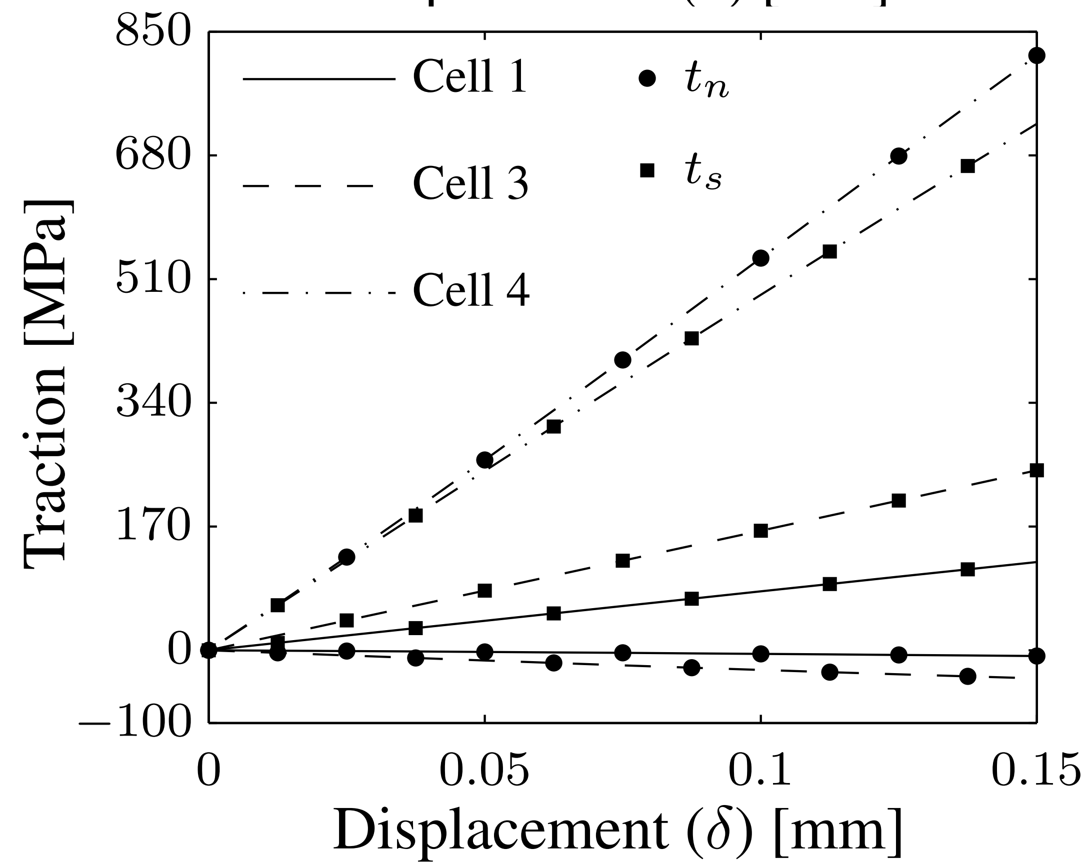
Hierarchically Parallel Multiscale Solver









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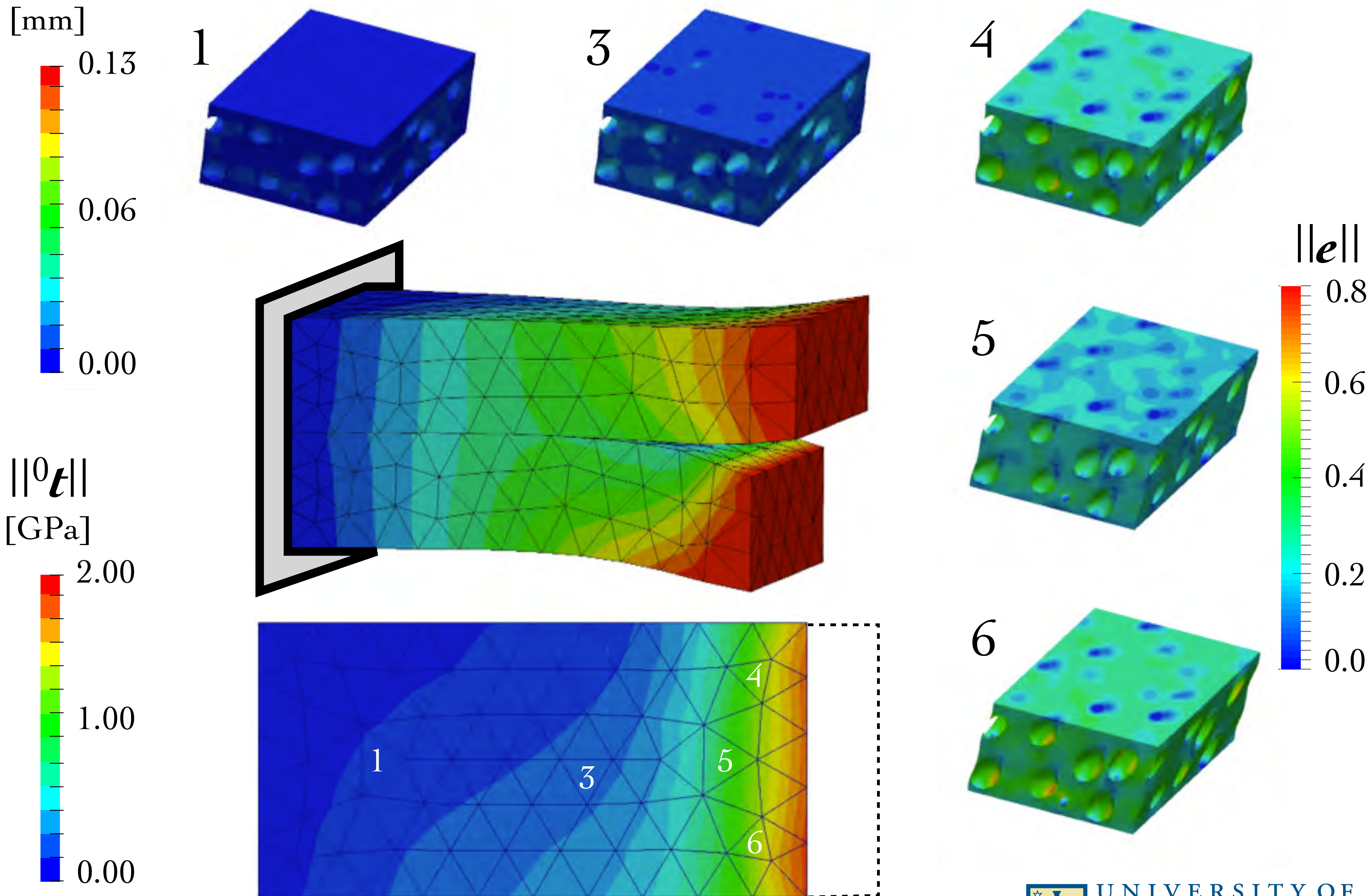
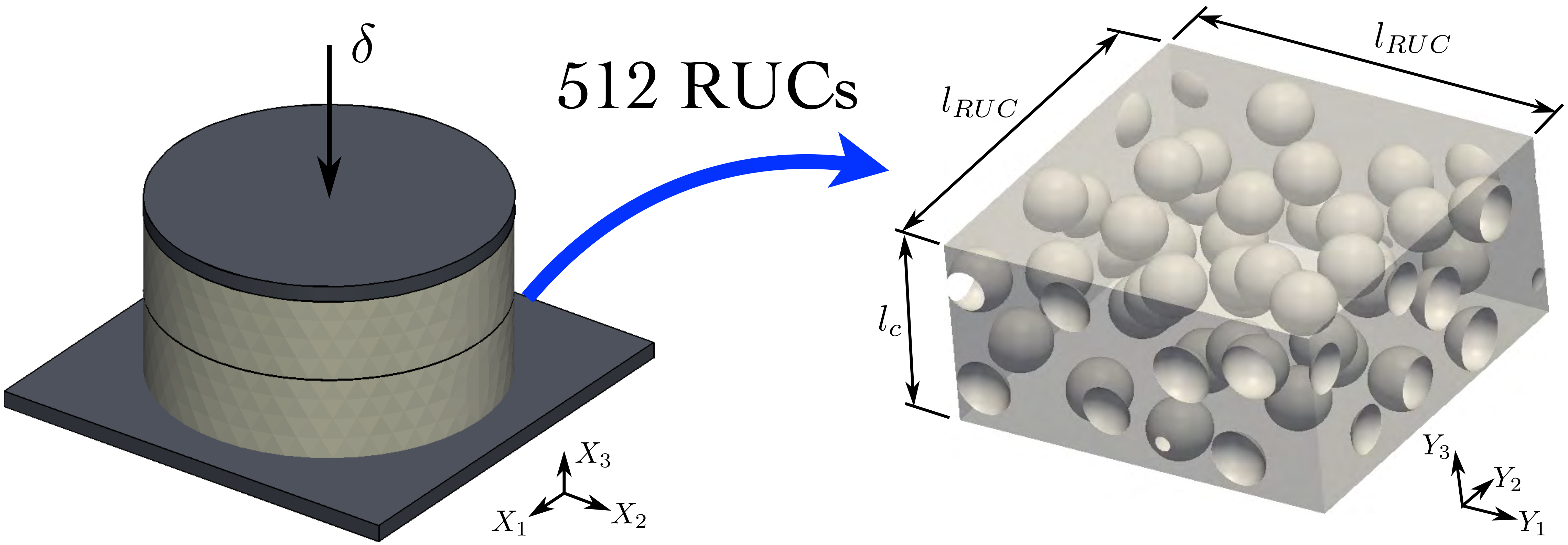
Hierarchically Parallel Multiscale Solver



Hierarchically Parallel Multiscale Solver

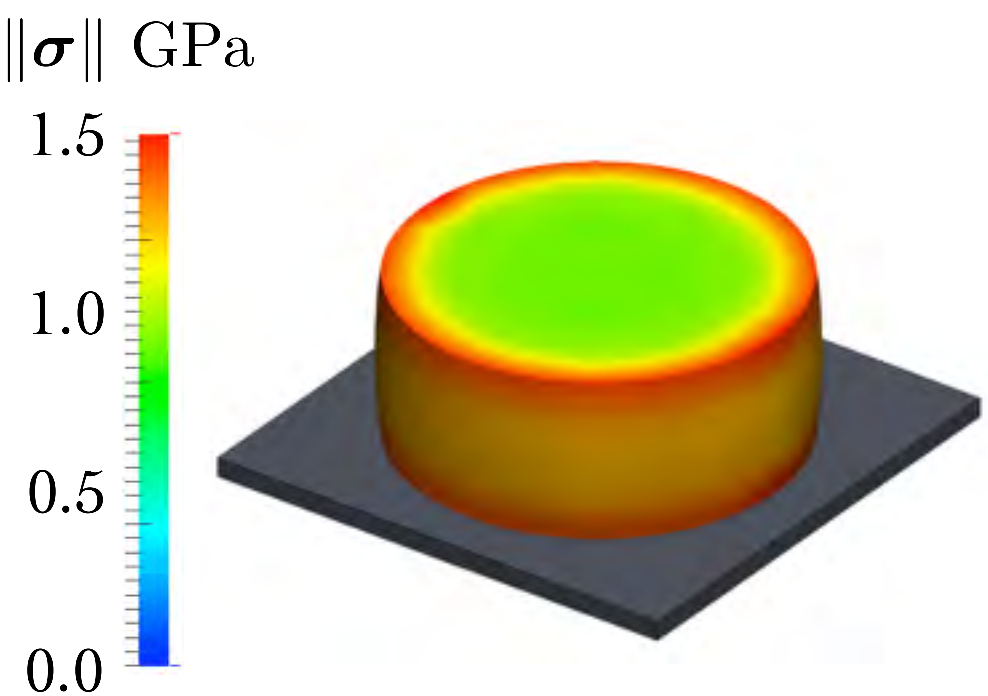


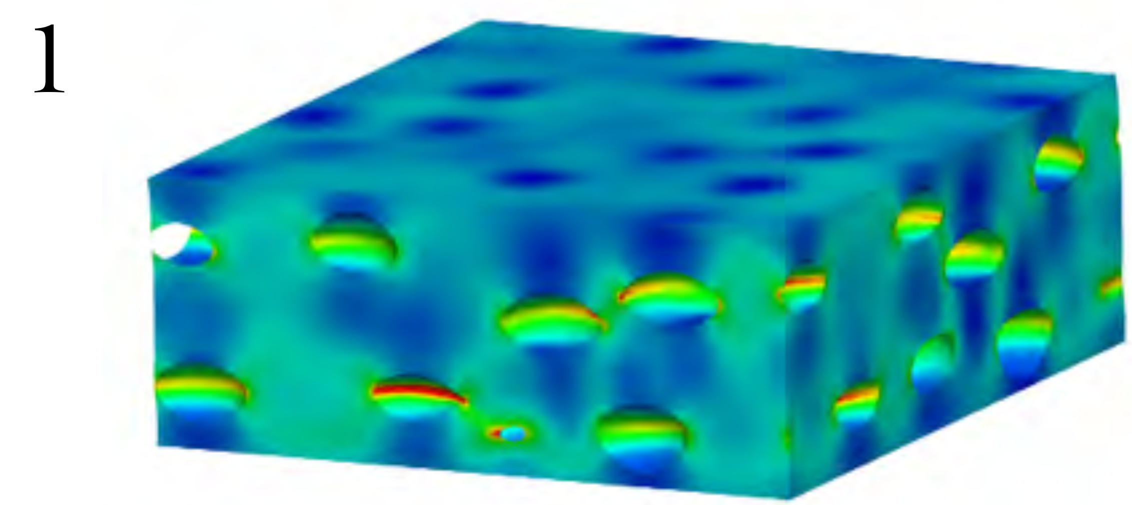
- Macro-scale
  - No-slip on top/bottom
  - h= 10 mm, d = 20 mm
- E = 15 GPa, ν = 0.25
- 15K elements in Macro

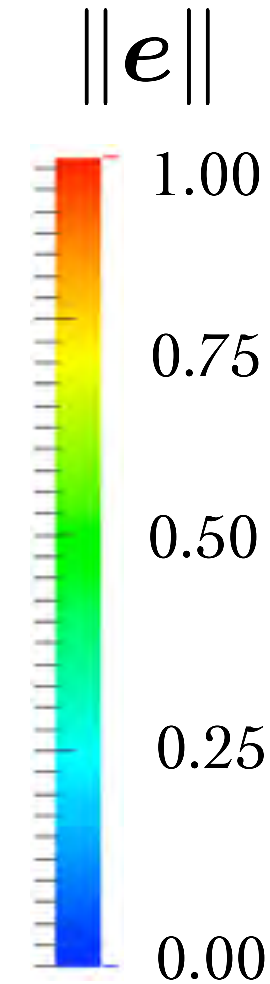
- Micro-scale
  - 250 x 250 x 125 μm^3
  - 40 voids, 40 μm diameter
- E = 5 GPa, ν = 0.34
- 5M elements in RUC

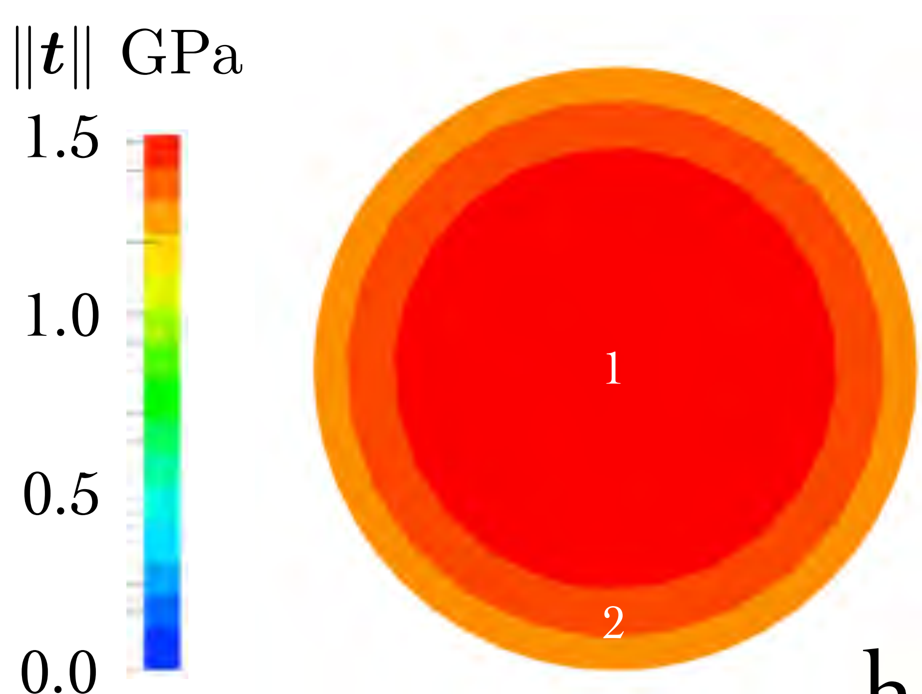
Multi-scale Simulations, *PGFem3D* - GCTH

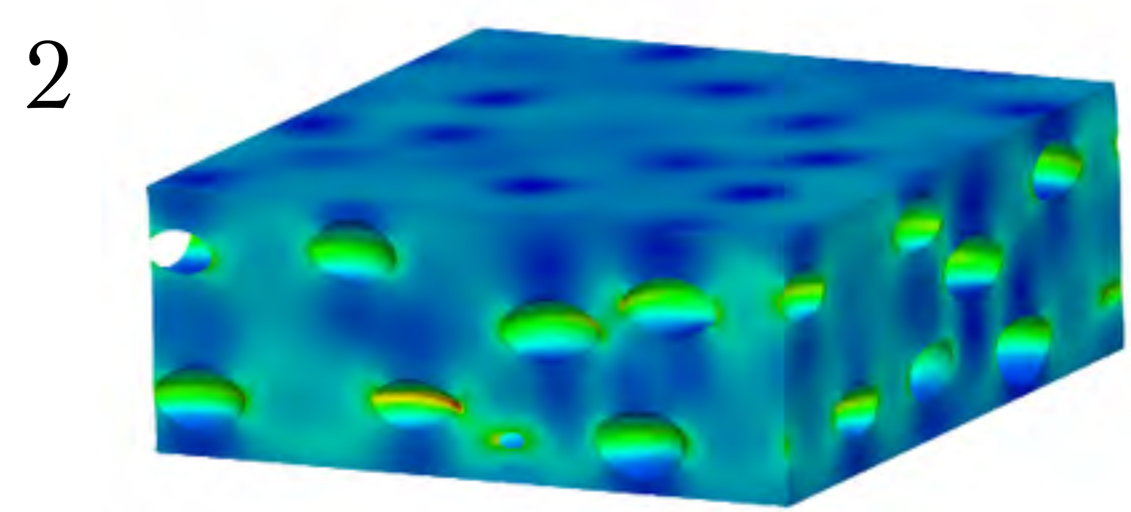
- 487M Node, 2.65B Elements, 1.39B DOF, 64K cores
  - LLNL Vulcan







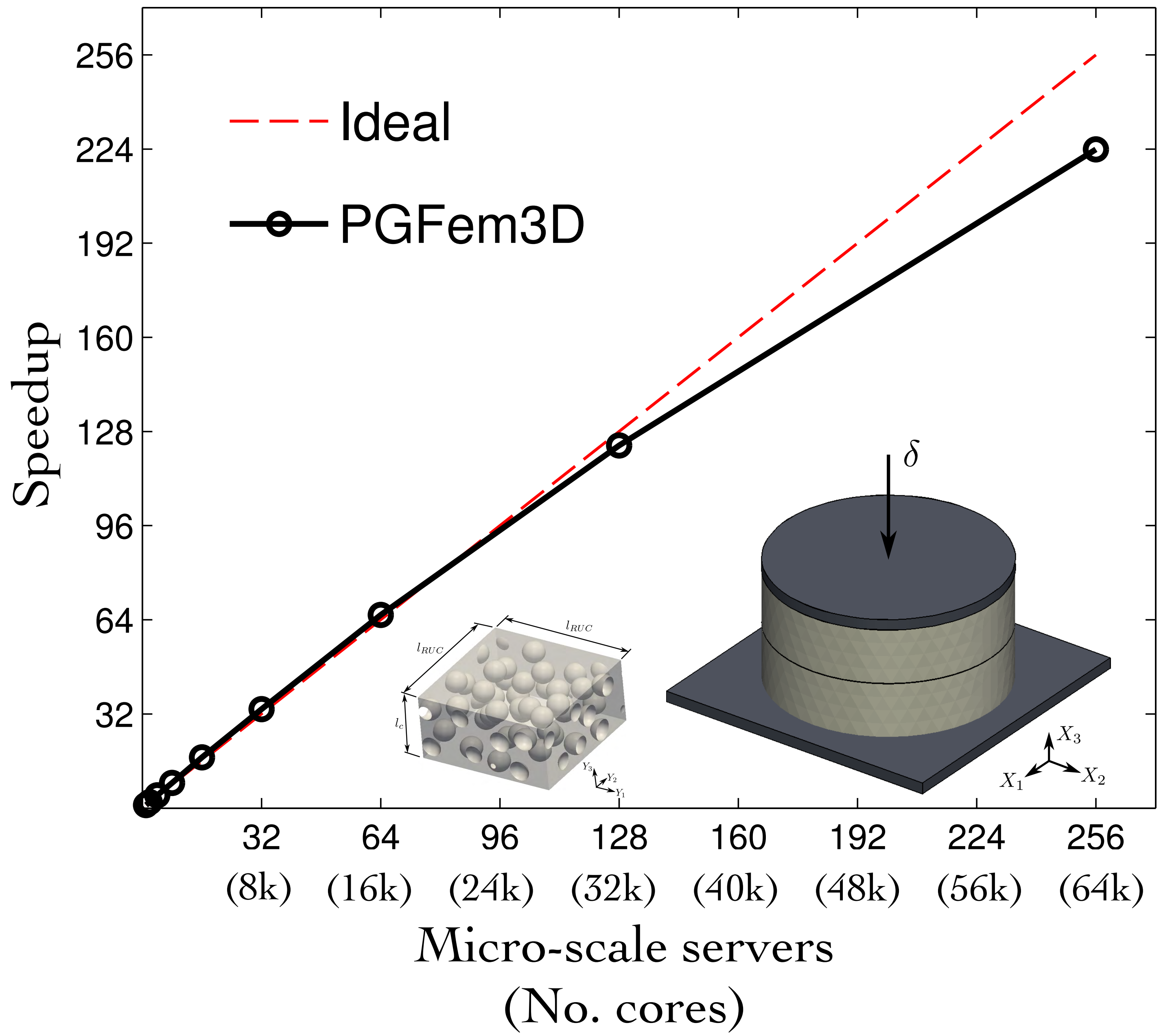




$h_e(\min)=60$ nm

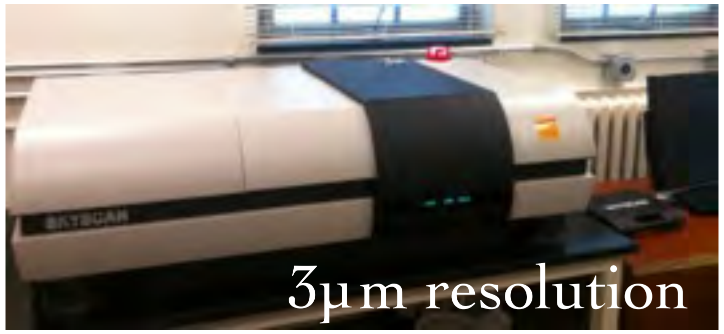
Hierarchically Parallel Multiscale Solver

- LLNL Vulcan



- Total
  - 16.1*M* Elements
  - 3.6*M* Nodes
  - 8.6*M* DOF
- Macro-scale (16 core)
  - 15,164 Elements
  - 3,338 Nodes
  - 8,328 DOF
- RUC (256 core each)
  - 31,392 Elements
  - 7,074 Nodes
  - 16,758 DOF

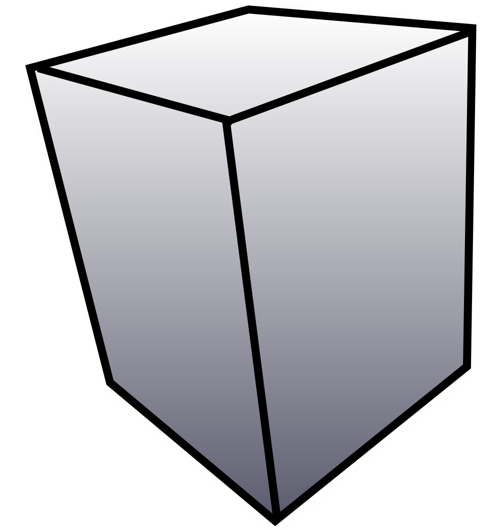
Modeling with Co-Designed Experiments



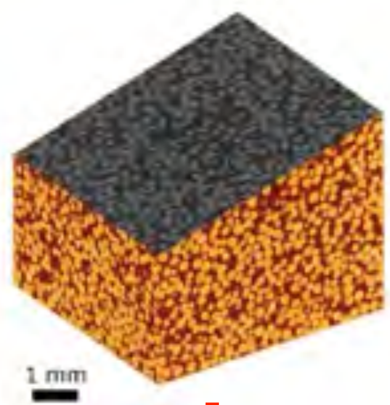
Model reduction

microscale/mesoscale

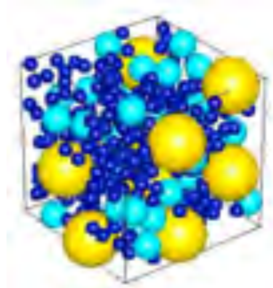
Surrogate medium



Real material



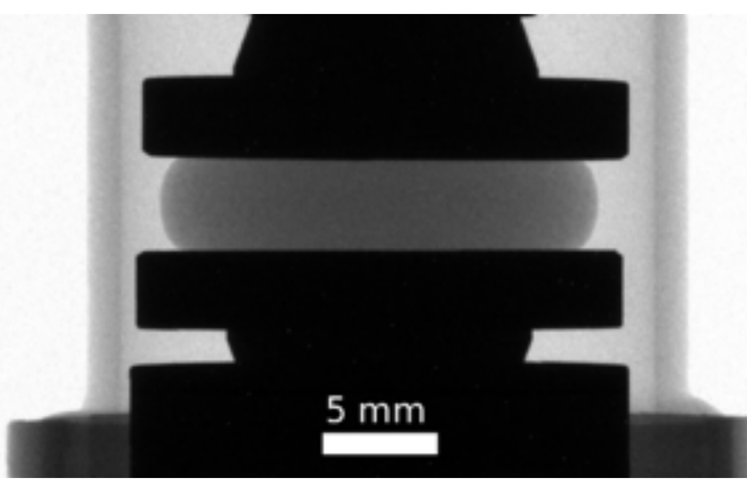
statistical equivalence



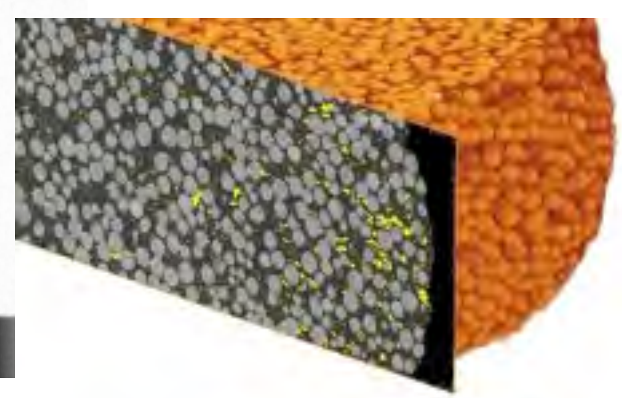
multiscale analysis

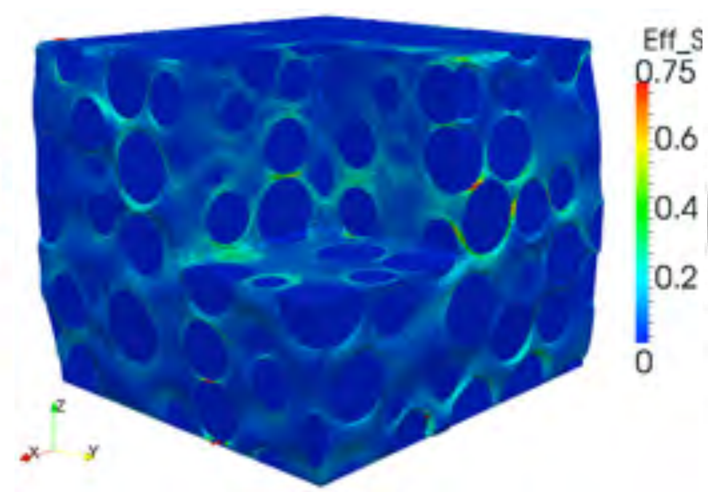
macroscale

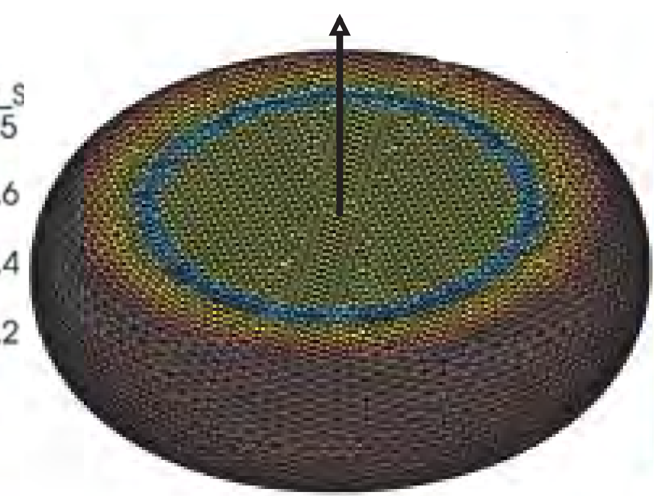
Mesoscale Validation



Testing inside scanner



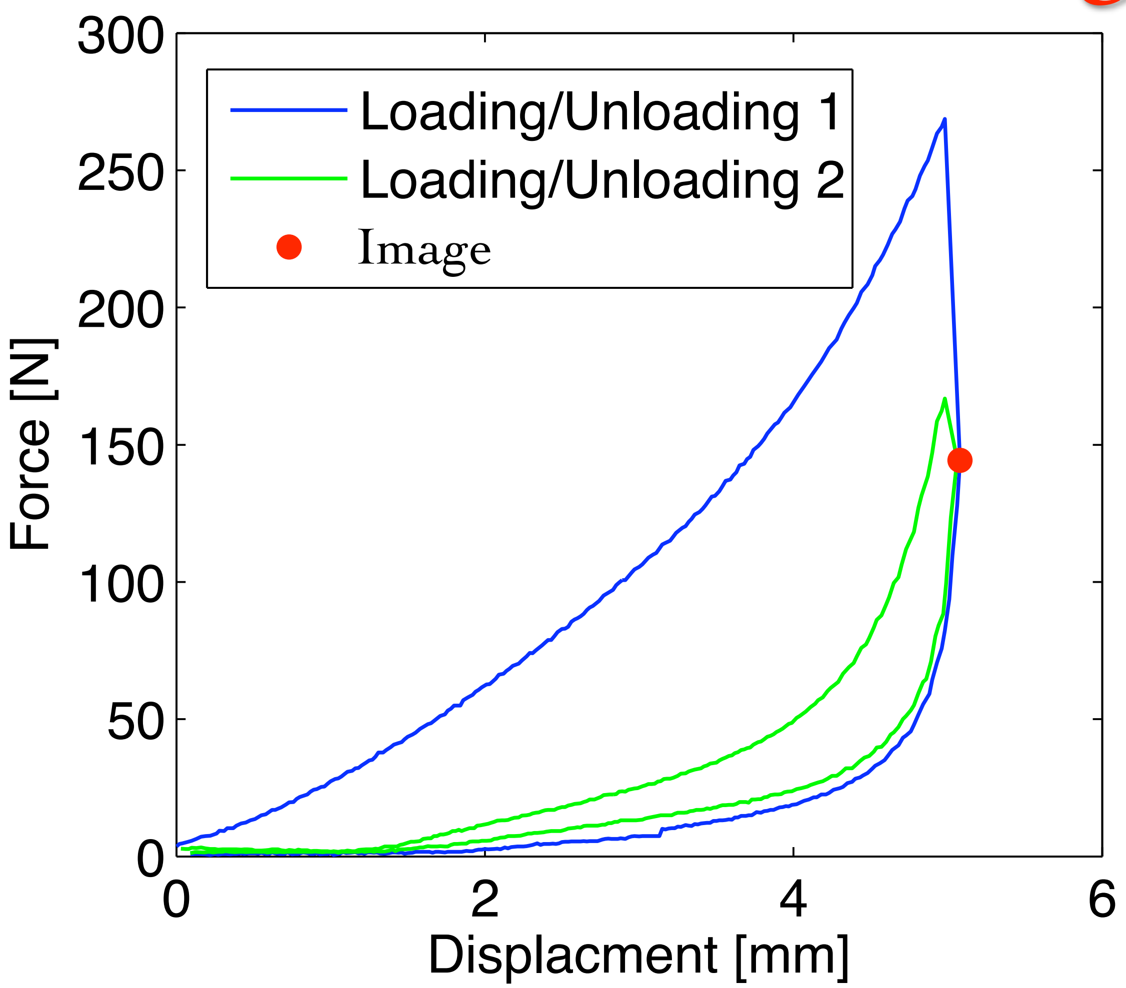




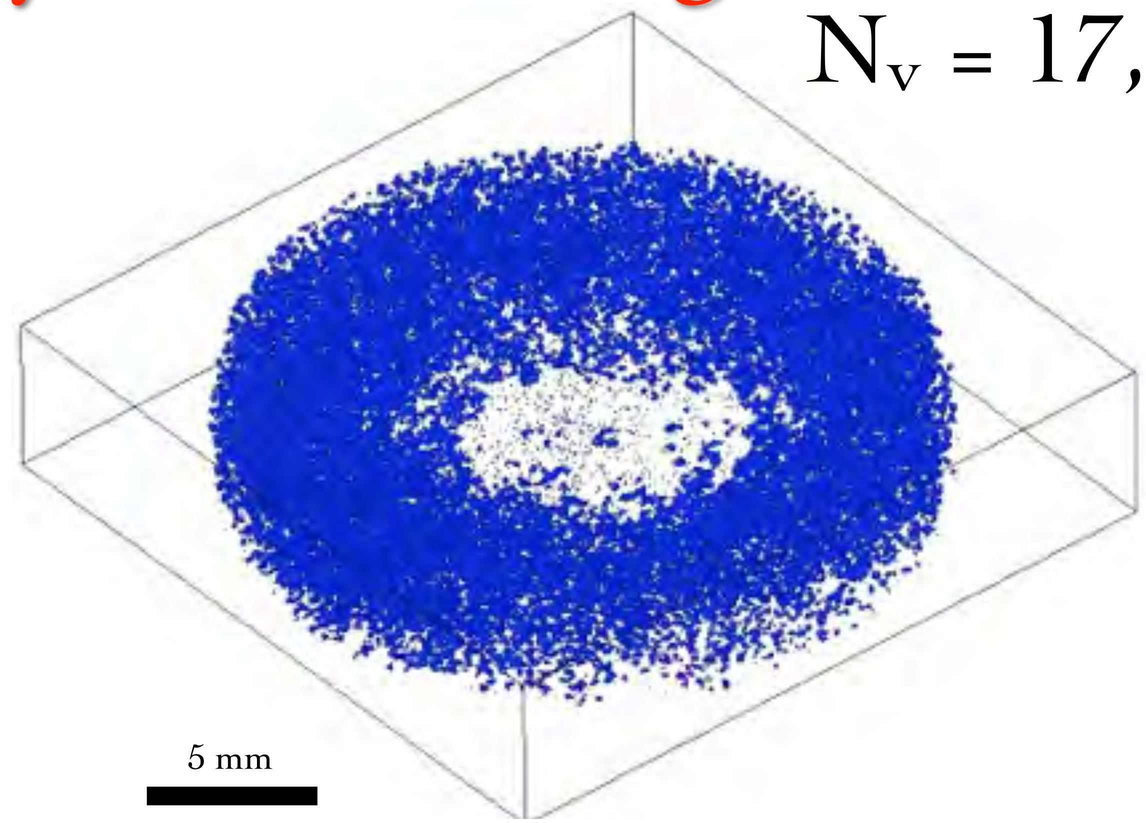
Numerical analysis

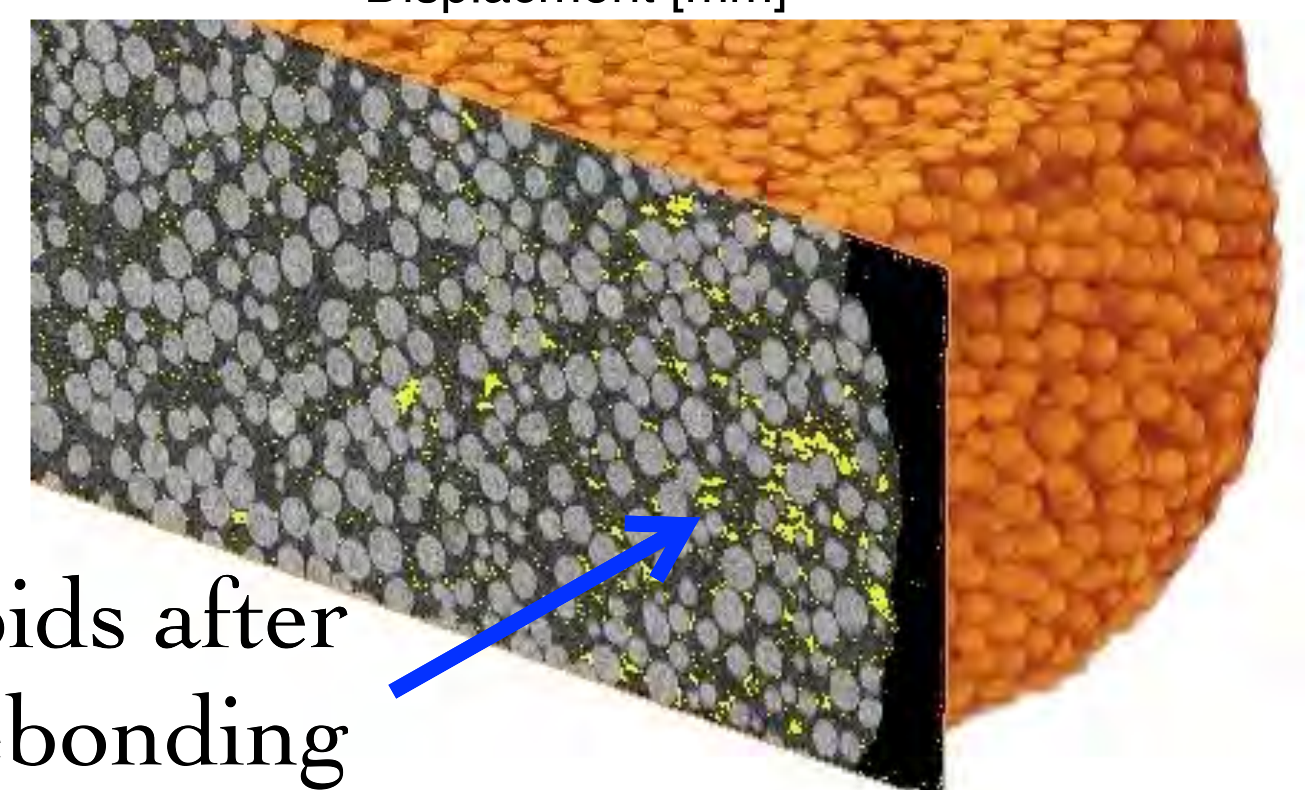
Macroscale Validation

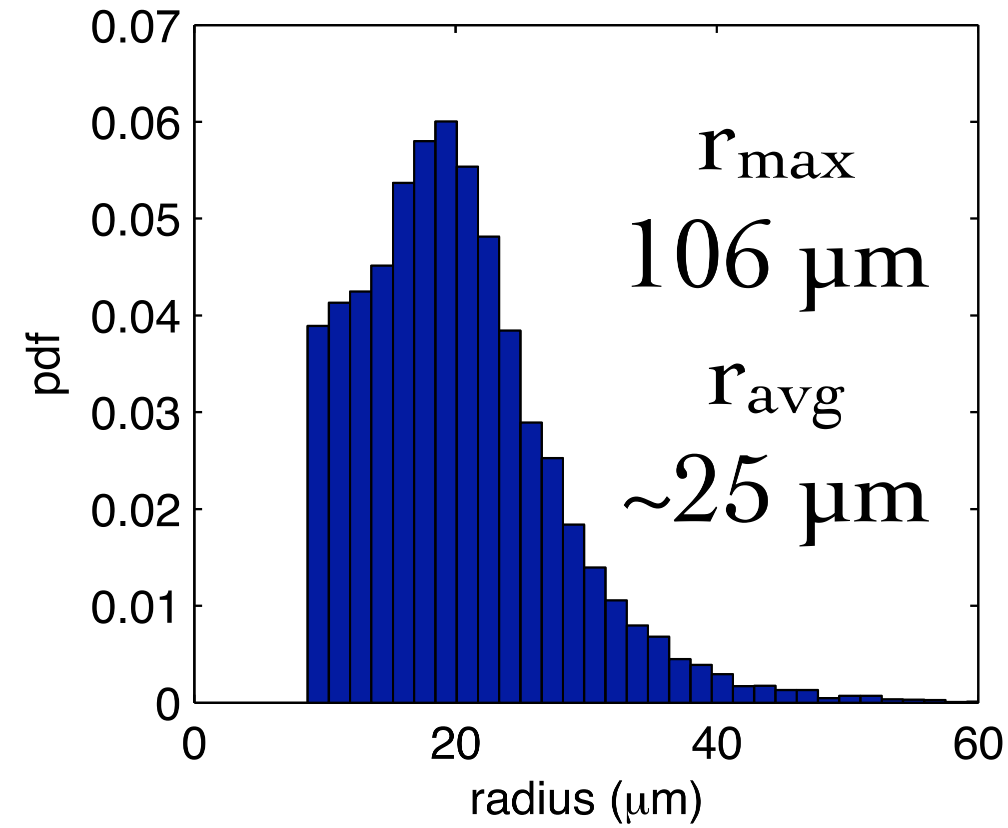
Microtomography *In Situ* Testing



N_v = 17,008







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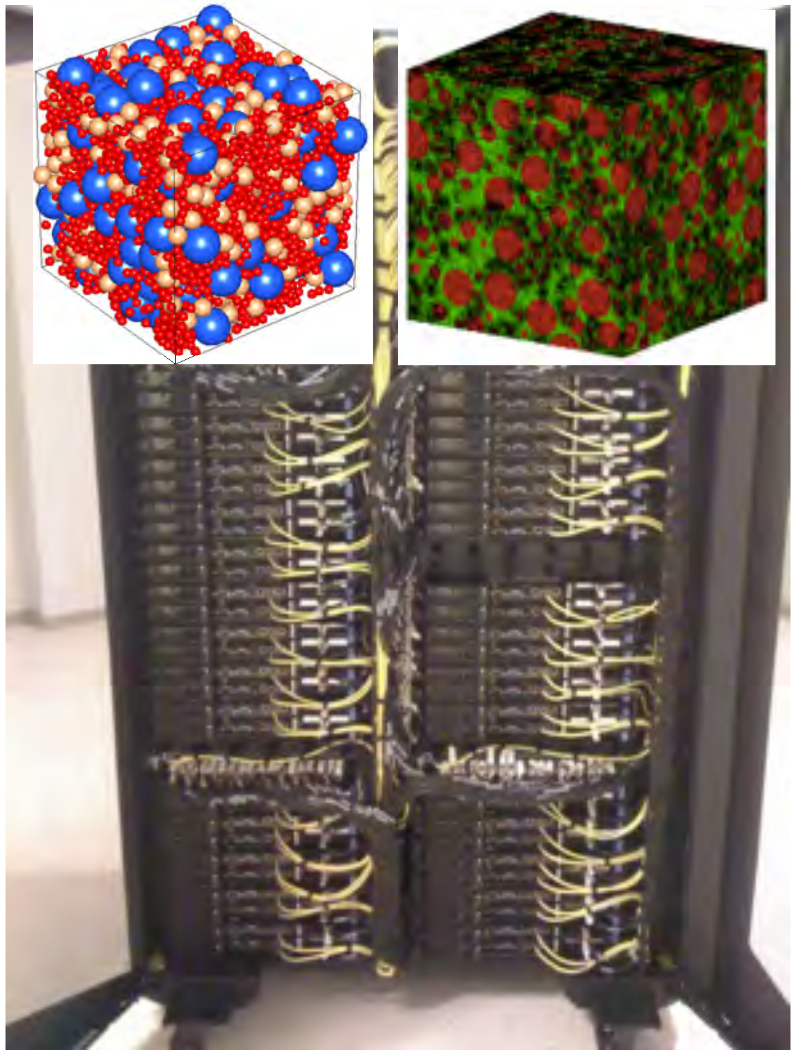
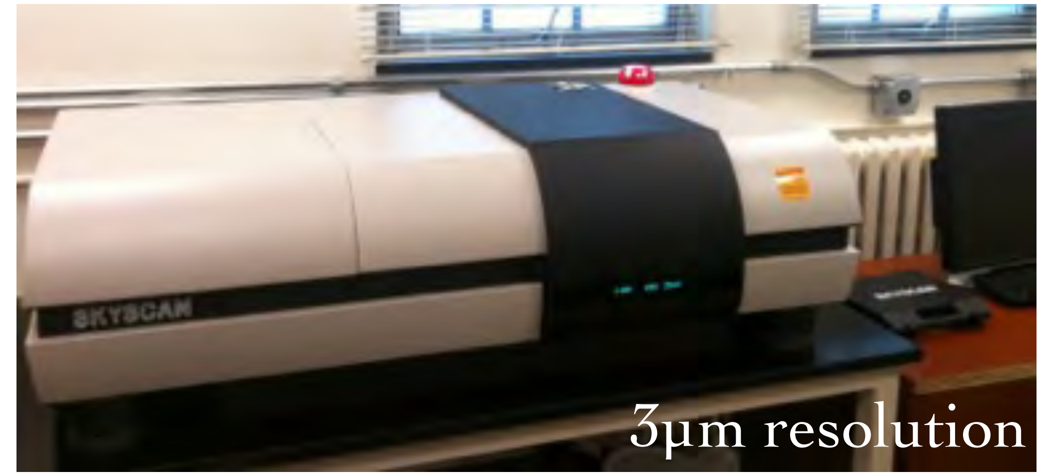
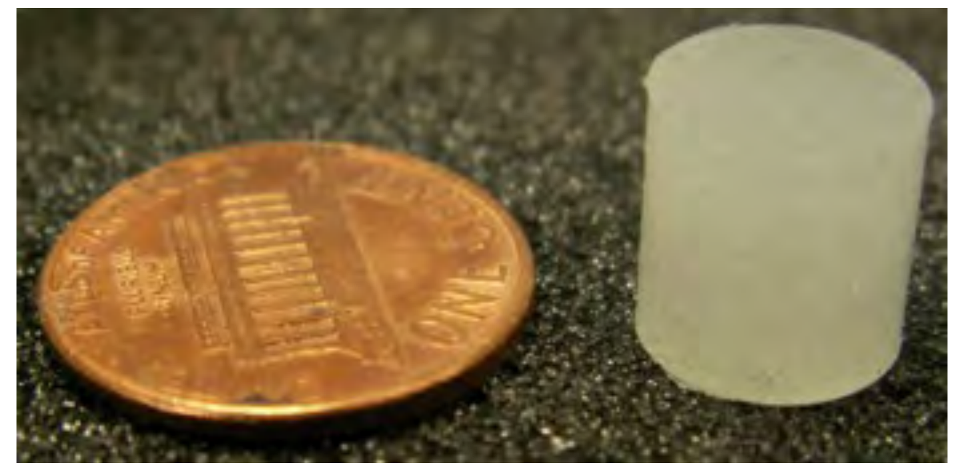
"Virtual" FE^2 Micro-computer Tomography







1x1x1 $mm^3 = \mathcal{O}(10^9)$ elem.
mean element size ~ 1 micron

1x1x1 $cm^3 = \mathcal{O}(10^{12})$ voxels
detectability ~ 1 micron

- 1000 RUCs
- Trillion number of elements
- Billion number of equations

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