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

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M. Mosby and A. Gillman
Motivation

S. Xu, D. Dillard and J. Dillard
Motivation

Cohesive modeling

traction-separation law

Cohesive law based on lower scale physics

\[ \left[ u \right] \]

\[ \left[ \dot{u} \right] \]

\[ \left[ \ddot{u} \right] \]

\[ \left[ \dddot{u} \right] \]

\[ L \gg l_c > d > l_\mu > h \]
Critical assumption: \( l_c \ll \mathcal{O}(L) \)

**Adherends**

\[
0 \varphi(X) = X + 0u(X) \in \Omega_0^+ \\
0 F = 1 + \nabla_X 0u(X) \in \Omega_0^\pm
\]

**Macro Interface: Average Deformation Gradient**

\[
\left[ 0 \varphi(X) \right] = 0 \varphi^+ - 0 \varphi^- = \left[ 0 u(X) \right] \quad \text{on } \Gamma_0 \\
0 F = 1 + \frac{1}{l_c} \left[ 0 u(X) \right] \otimes 0 N \quad \text{on } \Gamma_0
\]

**Micro Interface**

\[
1 \varphi(X, Y) = 0 F(X) Y + 1 u(Y) \in \Theta_0 \\
F = 0 F + \nabla_Y 1 u(Y) \\
= 1 + \frac{1}{l_c} \left[ 0 u(X) \right] \otimes 0 N + \nabla_Y 1 u(Y) \in \Theta_0
\]

Matouš et al., 2008
Mosby and Matouš, 2014
### Strong and Weak Forms

#### Macroscale Strong Form

\[ \nabla_X \cdot 0\, P + f = 0 \quad \in \, \Omega_0^\pm \]

\[ 0\, P = \frac{\partial^0 W}{\partial^0 F} \quad \in \, \Omega_0^\pm \]

#### Boundary Conditions

\[ 0\, P \cdot N = t^p \quad \text{on } \partial\Omega_0^t \]

\[ 0\, u = 0\, u^p \quad \text{on } \partial\Omega_0^u \]

\[ t^+ + t^- = 0 \quad \text{on } \Gamma_0 \]

#### Macroscale Weak Form

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

#### Microscale Strong Form

\[ \nabla_Y \cdot 1\, P = 0 \quad \in \, \Theta_0 \]

\[ 1\, P = \frac{\partial^1 W}{\partial F} \quad \in \, \Theta_0 \]

\[ F = 1 + \frac{1}{l_c} \left[ 0\, u(X) \right] \otimes 0\, N + \nabla_Y 1\, u(Y) \]

#### Hill-Mandel Lemma

- Microscale weak form
- Yields closure on \( 0\, t \)
- Restrictions on BC
**Hill-Mandel Lemma**

\[
\inf_{\lbrack 0 u \rbrack} 0 W(\lbrack 0 u \rbrack) = \inf_{0 F} \inf_{1 u} \frac{l_c}{|\Theta_0|} \int_{\Theta_0} 1 W(0 F(0 u) + \nabla_Y 1 u) \, dV
\]

\[
1 P = \frac{\partial^1 W}{\partial F} \bigg|_{F=0 F+\nabla_Y 1 u}
\]

\[
0 t = \frac{\partial^0 W}{\partial \lbrack 0 u \rbrack}
\]

\[
1 R = \frac{l_c}{|\Theta_0|} \int_{\Theta_0} 1 P : \nabla_Y (\delta^1 u) \, dV = 0
\]

\[
\lbrack 0 u \rbrack R = \left(0 N \cdot \frac{1}{|\Theta_0|} \int_{\Theta_0} 1 P \, dV - 0 t \right) \cdot \left[\delta^0 u\right] = 0
\]

At microscale equilibrium \(0 t = 0 N \cdot \frac{1}{|\Theta_0|} \int_{\Theta_0} 1 P \, dV\) \(\bullet\) No assumption on form of \(0 t\)

**Microscale Boundary Condition Admissibility**

\[
\frac{1}{|\Theta_0|} \int_{\Theta_0} \nabla_Y 1 u \, dV = \frac{1}{|\Theta_0|} \int_{\partial\Theta_0} 1 u \cdot N_{\Theta} \, dA = 0
\]

\[
\begin{cases}
1 u = 0 & \text{on } \partial\Theta \\
1 u^+ = 1 u^- & \text{on } \partial\Theta \\
\dot{t} = 0 & \text{on } \partial\Theta
\end{cases}
\]
Constitutive Response of Adhesive Layer

• Isotropic damage law

\[ 1W(F, \omega) = (1 - \omega)1W(F) \]

• Damage surface

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

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

• Irreversible dissipative evolution equations

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

\[ \dot{\chi}^t = \kappa H \quad \rightarrow \quad \dot{\chi}^t = \mu \langle \phi(g) \rangle \]

1/µ ≈ τ [s]

Epoxy τ-Θ(10^-6-10^-2)

viscous regularization

Different constitutive laws can be used
High Performance Computing - Weak Scaling

Highly scalable finite strains

\[ \text{PGFem3D solver} \]

\[ N_n = 23,841,057 \quad N_e = 123,168,768 \]

- four nonlinear steps
- four iterations
Hierarchically Parallel Multiscale Solver

\[
0 \mathcal{R} = \int_{\Omega_0^+} 0 P : \nabla x (\delta^0 u) \, dV - \int_{\Omega_0^-} f \cdot \delta^0 u \, dV - \int_{\partial \Omega_0^0} t^p \cdot \delta^0 u \, dA + \int_{\Gamma_0} 0 t \cdot [\delta^0 u] \, dA = 0
\]

In this section, we present two numerical examples using the hierarchically parallel multiscale solver for modeling nonlinear response of a heterogeneous layer. The first example is a simple verification problem and convergence study. The second example shows the solver's ability to perform large and detailed simulations that would unlikely be possible by DNM with the same computational resources. In particular, we perform a multiscale simulation with \( \sim 1.1 \) Billion elements and \( \sim 575 \) million nonlinear equations on only 1,552 computing cores. Similarly sized simulations presented in the literature [4] are typically computed on several thousand computing cores.

**Figure 4.** The hierarchically parallel implementation of the estimated solution procedure given in Algorithm 2. Macroscale and microscale computations are overlaid with non-blocking communication patterns. Note that there are \( N_s \) microscale servers that simultaneously compute microscale contributions for the \( N_p \) macroscale clients.

**Table I.** Material properties for all numerical examples.

<table>
<thead>
<tr>
<th>Material</th>
<th>Young's modulus ( E ) [MPa]</th>
<th>Shear modulus ( G ) [MPa]</th>
<th>Poisson's ratio ( \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adherends</td>
<td>( 15 \cdot 10^4 )</td>
<td>( 6 \cdot 10^4 )</td>
<td>0.25</td>
</tr>
<tr>
<td>Interface</td>
<td>( 5 \cdot 10^3 )</td>
<td>( 1 \cdot 10^3 )</td>
<td>0.34</td>
</tr>
</tbody>
</table>

In both examples, we use hyper-elastic material potentials for both macro- and micro-scales given by

\[
W \equiv W = G (\text{tr} \hat{C} - 3) + E (1 - 2\nu) [\exp(J - 1) - \ln(J) - 1],
\]

where \( E \) is Young's modulus, \( G \) is the shear modulus, and \( \nu \) is Poisson's ratio. The Jacobian of the deformation is given by \( J = \det(C) ^{1/2} \), and \( \hat{C} = J^{-2/3} C \) is the deviatoric right Cauchy-Green deformation tensor. Note that the appropriate macro- and micro-deformation gradients \( C_0 \) and \( C \) are used.
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

$N = 500,000$
$2048$ CPUs

$S_{mm}$
$S_{m4}$
$S_{m5}$
$S_{m6}$
$S_{55}$

$S_{rs}$

radius (µm)

$100 µm$

$cp = 53.91\%$

$cp = 55.27\%$

$cp = 54.20\%$

$cp = 53.91\%$

scan - 19123 particles
cell - 1082 particles

scan - 1445x1288x798 µm
cell - 400x400x400 µm

Parallel Genetic Algorithm
Polydisperse Systems

- Rice & Mustard - $c_p=0.667$
- Resolution 69.4 µm
Polydisperse Crystalline Systems

Salt

Sugar

1 mm

1 mm
Image-based (Data-Driven) Modeling

Digital Cell - 1000x1000x200 \( \mu m^3 \)

- \( N_p = 4774 \)
- \( l_c = 200 \mu m \)
- 10% volume fraction
- 20 micron particles

\[
\frac{1}{2} \ l_{RUC} - 70x70x200 \ \mu m^3 \\
\ l_{RUC} - 140x140x200 \ \mu m^3 \\
\ 2 \ l_{RUC} - 280x280x200 \ \mu m^3
\]

\[
\frac{1}{2} \ l_{RUC} - N_p = 23 \\
l_{RUC} - N_p = 93 \\
2 \ l_{RUC} - N_p = 374
\]
**Representative Unit Cell Study**

Mixed mode loading \( [u_n] = [u_{s1}] = [u_{s2}] = 1/\sqrt{2} [u_s] \)

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

Mean element size 1.5 \( \mu m \)

---

\( l_{RUC} \)
- \( Ne \approx 12,317,628 \)
- \( Nn \approx 2,103,957 \)
- \( Dofs \approx 6,280,495 \)

\( 2l_{RUC} \)
- \( Ne \approx 48,537,975 \)
- \( Nn \approx 8,294,617 \)
- \( Dofs \approx 24,758,080 \)

---

Figure 6: Traction-separation laws for the stiff particle and soft matrix under mixed-mode loading with three different strain-rates. Solid lines denote the strain rate prescribed in subsequent studies, while dashed and dot-dashed lines represent response from \( \frac{1}{10} \) and \( 10 \) times the applied strain rate. Note that the materials are only weakly rate-sensitive over a wide range of strain rates. (a) Normal component of mixed-mode response. (b) Shear component of mixed-mode response.

---

Table 3: Mesh identifiers and characteristics for the grid convergence study.

<table>
<thead>
<tr>
<th>Identifiers</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>( h ) ( \mu m )</td>
<td>( \frac{1}{h} ) ( \mu m )</td>
</tr>
<tr>
<td>( h_{avg} ) ( \mu m )</td>
<td>( h_{min} ) ( \mu m )</td>
</tr>
<tr>
<td>6.00</td>
<td>0.167</td>
</tr>
<tr>
<td>3.00</td>
<td>0.333</td>
</tr>
<tr>
<td>1.50</td>
<td>0.667</td>
</tr>
<tr>
<td>0.75</td>
<td>1.333</td>
</tr>
</tbody>
</table>

Figure 7 shows the macroscopic traction-separation laws computed from increasingly finer meshes. Not surprisingly, all discretizations capture the hyperelastic response without any difficulty. Finer meshes transition to a more gradual softening response due to properly capturing the microscale damage features that are linked to morphology and damage properties (e.g., damage viscosity \( \mu \)). We will analyze these microscale damage features in more detail in subsequent studies (see Sections 4.2-4.4).

Figure 8 shows the convergence of the strength and fracture toughness with respect to decreasing mesh size. We define the fracture toughness in the normal and shear directions as...
Mesh Convergence Study

Figure 8: Convergence of macroscopic response with increasing mesh refinement. (a) Convergence of strength (maximum tractions). (b) Convergence of fracture toughness as given by Equation (29).

The dimensions of the cells, number of particles, and the average mesh characteristics for each sized cell are given in Table 4.

Table 4: Microstructure and average mesh characteristics for the RUC convergence study.

<table>
<thead>
<tr>
<th>Cell size</th>
<th>Dimensions [µm]</th>
<th># particles</th>
<th># nodes</th>
<th># elements</th>
<th># DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2 l stat</td>
<td>69.408 × 69.408</td>
<td>69</td>
<td>23</td>
<td>552,086</td>
<td>3,235,854</td>
</tr>
<tr>
<td>l stat</td>
<td>139.569 × 139.569</td>
<td>93</td>
<td>374</td>
<td>8,294,617</td>
<td>48,537,975</td>
</tr>
<tr>
<td>2 l stat</td>
<td>279.887 × 279.887</td>
<td>374</td>
<td>139</td>
<td>8,294,617</td>
<td>48,537,975</td>
</tr>
</tbody>
</table>

Figure 9 shows the macroscopic traction separation law for the different cells. The initial stiffness is identical for each cell, but the limit and softening responses are not. While the two larger unit cells have small and overlapping error bars until the very end of the load history, the smallest cell has a distinctly different softening response with very large error. The deviation between the two larger cells at the end of the loading history is mostly due to large mesh distortions and the associated deterioration of accuracy.

Figure 10 shows the convergence of the maximum traction (strength) and fracture toughness with respect to the side length of the unit cell. We note that the fracture toughness is computed according to Equation (29) with

\[ G_n = \{ 5.485, 7.757 \} \mu m. \]

We will use this failure (final) point for all studies to follow. Figure 10 shows the rapid convergence of both average and standard deviation of macroscopic response with increasing cell size. In our previous study [44], rapid convergence of the mean response was also observed. However, the standard deviation of response remained substantial even for very large unit cells. In this study, rapid convergence of both mean and standard deviation can be attributed to the use of statistically equivalent unit cells.

- **Used mesh**
  - \( h_{\text{min}} = 0.073 \) microns
  - \( h_{\text{mean}} = 1.370 \) microns
  - \( h_{\text{max}} = 2.25 \) microns

- **Finest mesh**
  - \# Nodes = 16,020,086
  - \# Elements = 93,856,013
  - \# DOFs = 47,938,704

Richardson extrapolation max error < 1.05%
In order to quantify the complex microstructural damage, we introduce a number of damage metrics that describe the extent of failure in the microstructure, whereas different morphologies.

We establish the bounds on different values of \( l = 0 \) at failure. As can be observed, the damage metrics in the two larger cells are nearly identical, while the smallest cell has a smaller volume fraction of thinner cracks. Additionally, we obtain \( (33) \) we get, in the case that \( l = 0 \).

Examining Equation (32), it is clear that the limit cases for different sized cells. The cells with equal to some threshold value. Similarly to Equation (30), we define the damage metric \( ! \) cell \( \mu \) is 0. In the case that \( l = 0 \) we get, \( ! \) cell \( \mu \) = \( ! \) cell \( \mu \) \( = 1 \) for any threshold value \( ! \) cell \( \mu \) |\( l \) = 1. For the case of constant failure throughout 1 different sized cells. The different sized cells. The different sized cells.

Finally, we establish the bounds on different values of \( l = 0 \) at failure. As can be observed, the damage metrics in the two larger cells are nearly identical, while the smallest cell has a smaller volume fraction of thinner cracks. Additionally, we obtain \( (33) \) we get, in the case that \( l = 0 \).

Examining Equation (32), it is clear that the limit cases for different sized cells. The cells with equal to some threshold value. Similarly to Equation (30), we define the damage metric \( ! \) cell \( \mu \) is 0. In the case that \( l = 0 \) we get, \( ! \) cell \( \mu \) = \( ! \) cell \( \mu \) \( = 1 \) for any threshold value \( ! \) cell \( \mu \) |\( l \) = 1. For the case of constant failure throughout 1 different sized cells. The different sized cells. The different sized cells.
Multiscale Cohesive Model - Mixed Mode Loading

- 10% volume fraction
- 2 l_{RUC} - N_p = 374
- 20 micron particles

Isocontours of $\omega \geq 0.999$

512 CPUs
Figure 9: Comparison of the average traction-separation law for different sized cells consisting of 10% volume fraction of 20 µm diameter particles. Error bars represent one standard deviation from five realizations. (a) Normal component of mixed-mode response. (b) Shear component of mixed-mode response.

Figure 11 compares the damage patterns at the failure points for the different sized cells. The two larger cells have a more-distributed damage pattern, whereas the cell with \( l_{\text{cell}} \approx \frac{1}{2} l_{\text{stat}} \) has a single dominant crack at the top of the cell.

In order to quantify the complex microstructural damage, we introduce a number of damage metrics. To motivate these metrics, let us consider a single crack of finite thickness, \( l_{\mu} \), with the volume, \( V_{|!} \), consisting of points with \( ! \) greater or equal to some threshold value as shown in Figure 12(a). First, we define

\[
M_{1|!} = \frac{V_{|!}}{V_{\text{cell}}},
\]

which is the volume fraction of damage in the microstructure, where \( V_{\text{cell}} \) is the volume of the cell.

Now let us consider a single discrete crack, as shown in Figure 12(b), given by the contour of points with \( ! \) equal to some threshold value. Similarly to Equation (30), we define the damage metric

\[
M_{2|!} = \frac{A_{|!}}{V_{\text{cell}}},
\]

which is the area density of cracks in the microstructure for a given value of \( ! \). Note that \( A_{|!} \) is the...
Particle Diameter Effect

10 % volume fraction

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

Figure 14: Damage in the microstructure at points A, B, and C, in the macroscopic response curve.

Table 8: Microstructure and average mesh characteristics for the particle diameter study.

<table>
<thead>
<tr>
<th>d [μm]</th>
<th>Dimensions [μm] × [μm]</th>
<th># particles</th>
<th># nodes</th>
<th># elements</th>
<th># DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>64.982 × 64.982</td>
<td>64</td>
<td>1,292</td>
<td>1,696,876</td>
<td>9,836,031</td>
</tr>
<tr>
<td>10</td>
<td>99.883 × 99.883</td>
<td>381</td>
<td>1,420,119</td>
<td>8,272,851</td>
<td>4,242,575</td>
</tr>
<tr>
<td>20</td>
<td>139.569 × 139.569</td>
<td>93</td>
<td>2,103,957</td>
<td>12,317,628</td>
<td>6,280,495</td>
</tr>
</tbody>
</table>

Figure 19: Comparison of traction-separation laws for RUCs with 10% volume fraction of different sized particles. Error bars show one standard deviation of the response for five realizations of each RUC. (a) Normal component of the mixed-mode response. (b) Shear component of the mixed-mode response.

Figure 20 compares the strength and fracture toughness of the different mixtures. There is a monotonic decrease in the strength with increasing particle diameter, which is often observed in experiments [32, 33]. However, the fracture toughness with relation to particle diameter is non-monotonic and attains a maximum for 10 μm diameter particles. This non-monotonic trend is also observed in experiments for fixed volume fractions [10, 34], and our work shows the ability to capture this particle size effect. We note that the particle size effect is captured because we have sufficiently resolved discretizations (h_{min} = 0.073 μm and h_{avg} ≥ 1.50 μm), and the value of damage viscosity, μ, is within the range of realistic material properties. Previous numerical studies using a similar damage model were not able to capture the particle size effect due to the highly viscous damage behavior (with thick cracks often on the order of particle diameters) and under resolved computations [26].

Figure 21 shows the damage pattern at failure in the RUCs with different diameter particles. The 5 μm particle RUC (Figure 21(a)) has very small arrested cracks around the particles. The damage localizes at the matrix-rich top and bottom surfaces, leading to adhesive failure. The mixture with 10 μm particles (Figure 21(b)) has a well distributed network of thin interconnecting cracks, leading to cohesive failure with multiple dominant cracks. This multiplicity of dominant cracks...
Particle Diameter Effect

10% volume fraction

- Smaller particles - higher strength
- Non-monotonic fracture toughness
Hierarchically Parallel Multiscale Solver

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

<table>
<thead>
<tr>
<th></th>
<th>Nodes</th>
<th>Elements</th>
<th>DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Macroscale</td>
<td>731</td>
<td>2,684</td>
<td>1,878</td>
</tr>
<tr>
<td>Microscale</td>
<td>193,873,920</td>
<td>1,098,283,920</td>
<td>574,612,560</td>
</tr>
<tr>
<td>TOTAL</td>
<td>193,874,651</td>
<td>1,098,286,604</td>
<td>574,614,438</td>
</tr>
</tbody>
</table>

- 16 Clients
- 12 Servers @ 128 cores
- 1552 cores
- 370,241 DOFs / core

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...
Figure 9. Multiscale solution of the DCB problem with heterogeneous interface. (a) shows contours of the
opening experience tensile loading. Figure 10(b) also shows that the peak compressive traction
decreases at the far end from the opening.

Figure 10. Macroscopic response of the interface. (a) shows the interface discretization with locations of elements 1, 3, and 4 in (a) as a function of the prescribed displacement.

Figure 11 shows the effective Eulerian/Almansi strain, \( \varepsilon^{\text{eff}} \), showing the normal and shear components of the traction computed from RUCs associated with the interface.

We note that strains in cells 4 and 6 are not symmetric to the marked interface elements in Figure 10(a). The high levels of strain (80%) are detected due to mixed-mode loading. As expected, the strains increase for cells closer to the leading edge.
Hierarchically Parallel Multiscale Solver
Macro-scale
- No-slip on top/bottom
- \( h = 10 \text{ mm}, d = 20 \text{ mm} \)
- \( E = 15 \text{ GPa}, \nu = 0.25 \)
- 15K elements in Macro

Micro-scale
- 250 x 250 x 125 \( \mu \text{m}^3 \)
- 40 voids, 40 \( \mu \text{m} \) diameter
- \( E = 5 \text{ GPa}, \nu = 0.34 \)
- 5M elements in RUC
Multi-scale Simulations, *PGFem3D* - GCTH

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

\[ \sigma \] GPa

\[ t \] GPa

\[ e \]

\[ h_e(\text{min}) = 60 \text{ nm} \]

> LLNL Vulcan
Hierarchically Parallel Multiscale Solver

- **LLNL Vulcan**

- **Total**
  - 16.1M Elements
  - 3.6M Nodes
  - 8.6M 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

Real material

Surrogate medium

Model reduction

microscale/mesoscale

statistical equivalence

multiscale analysis

Mesoscale Validation

Testing inside scanner

Macroscale Validation

Numerical analysis
**Microtomography In Situ Testing**

\[ N_v = 17,008 \]

- **Force vs. Displacement**
  - Blue line: Loading/Unloading 1
  - Green line: Loading/Unloading 2
  - Red dot: Image

- **Three-dimensional image**
  - Scale bar: 5 mm

- **Histogram**
  - PDF of radius distribution
  - \( r_{\text{max}} = 106 \, \mu m \)
  - \( r_{\text{avg}} \approx 25 \, \mu m \)

- ** VOIDs after debonding**

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Department of Aerospace and Mechanical Engineering

University of Notre Dame
“Virtual” FE² Micro-computer Tomography

1x1x1 mm³ = $\mathcal{O}(10^9)$ elem.
mean element size ~ 1 micron

1000 RUCs
Trillion number of elements
Billion number of equations

1x1x1 cm³ = $\mathcal{O}(10^{12})$ voxels
detectability ~ 1 micron

3μm resolution
Karel Matouš
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