Application of Numerical Methods to Study Arrangement and Fracture of Lithium-Ion Microstructure

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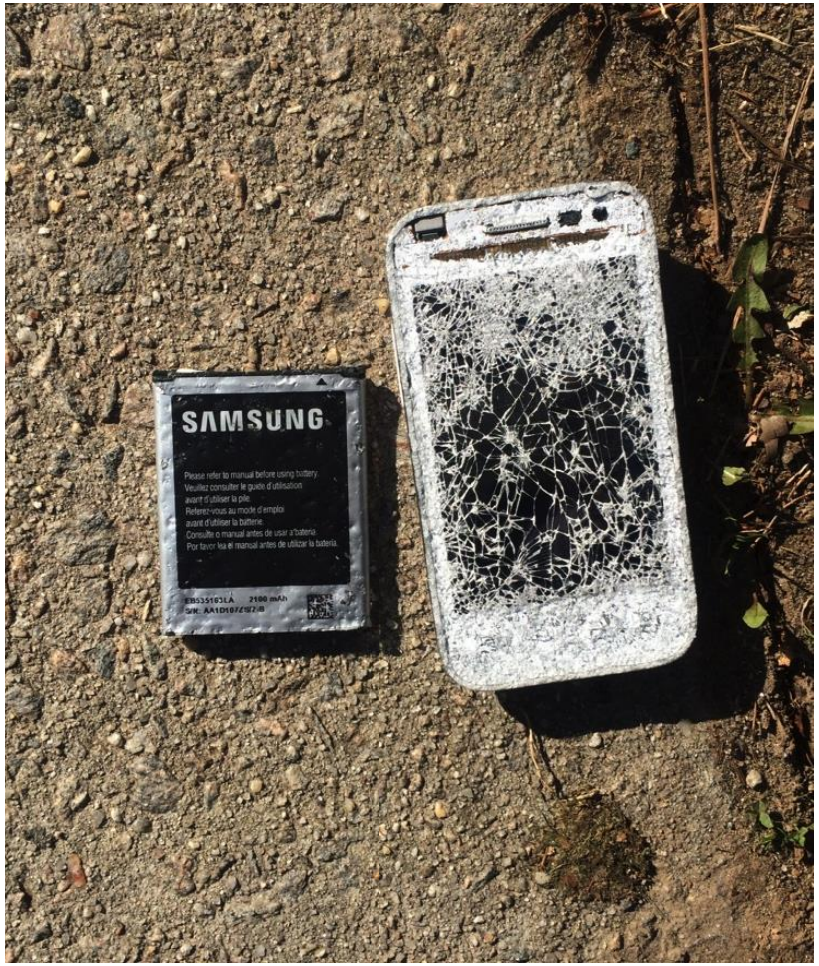
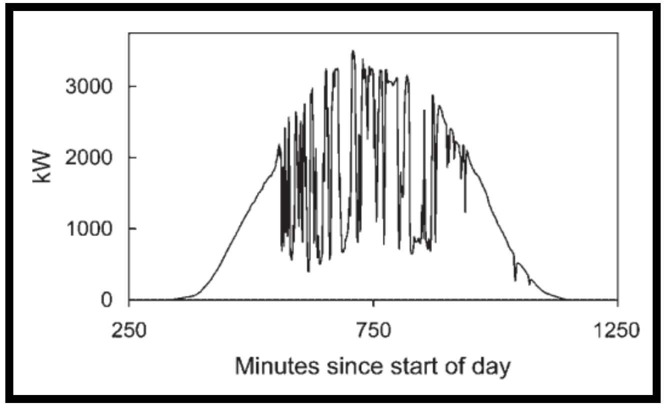
Motivation





Solar Farm Output, Springerville, Ariz.
(Curtright et al., 2008)

Tesla Battery File, Seattle, Wash.
(http://images.dailytech.com)

- Increasing societal demand for energy storage
- Lithium-ion batteries play an increasing role for meeting storage needs
  - Personal vehicles
  - Consumer electronics
  - Renewable energy production smoothing
  - Grid-scale storage

Motivation

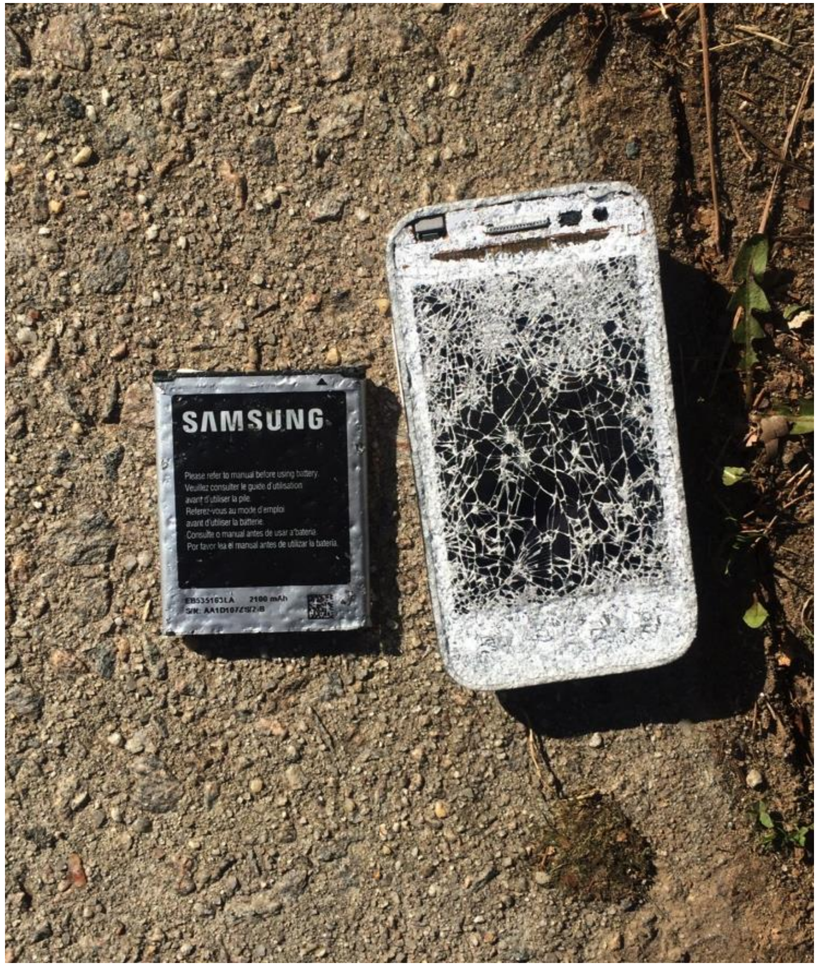
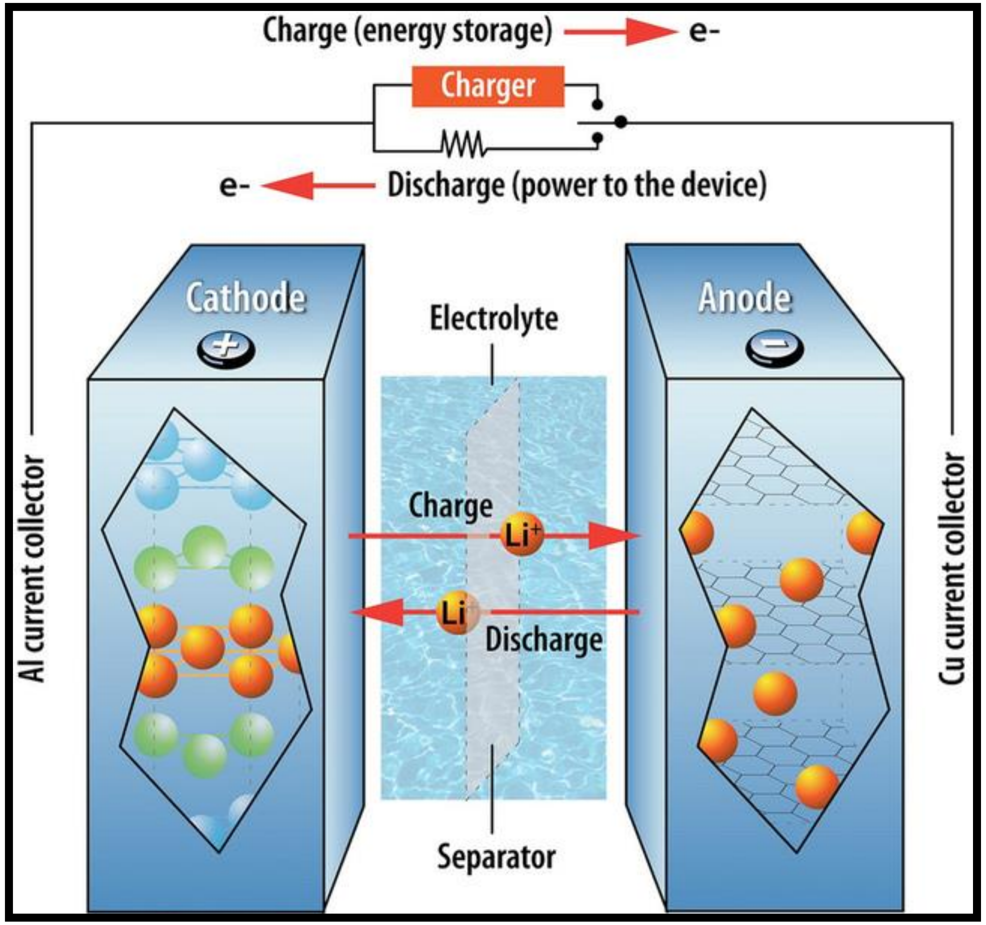
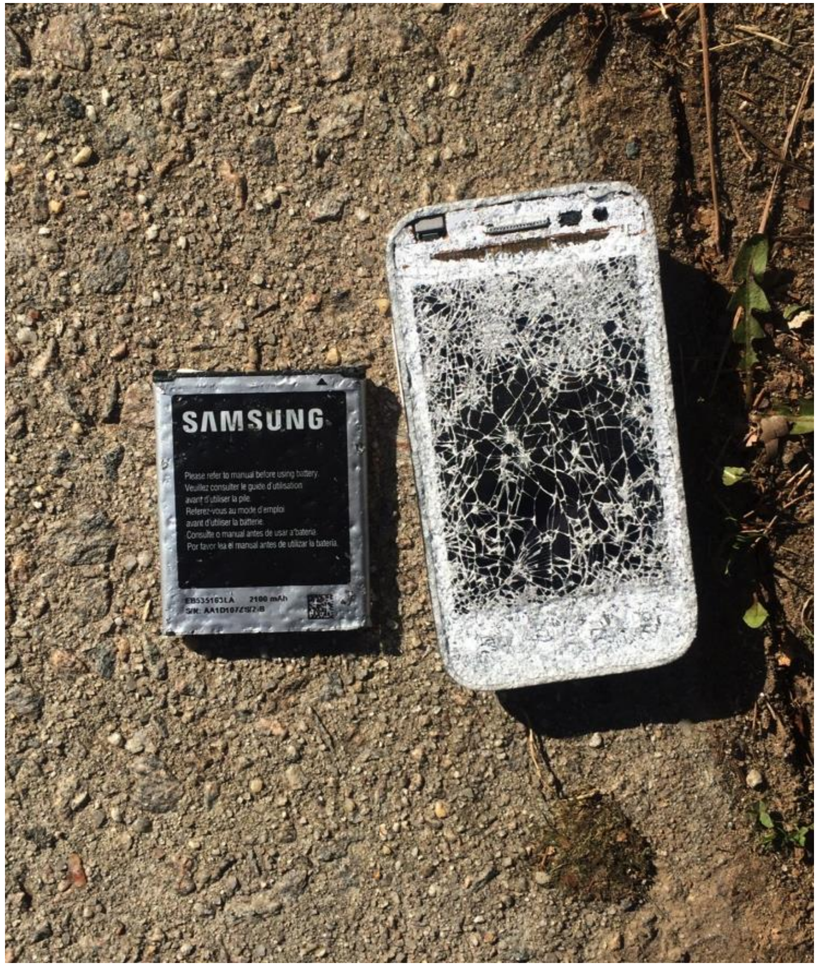


Diagram of Lithium-Ion Battery “Innards”

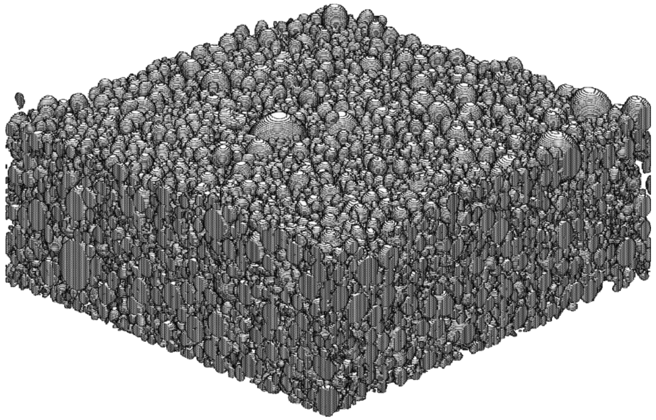


(Argonne National Laboratory)

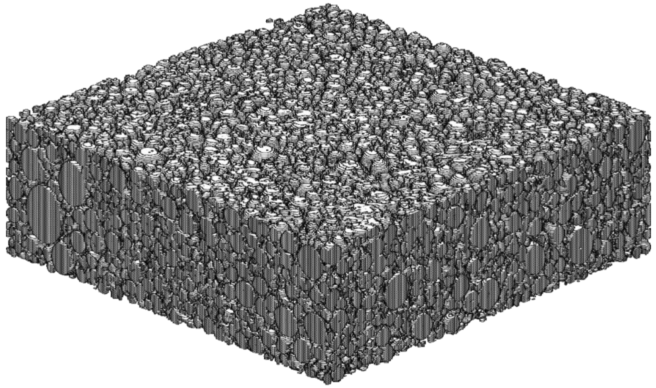
Motivation



Electrode Compaction in Manufacturing



Before Compaction



After Compaction @ 2000 bar ≈ 29ksi

Contact network serves as pathway for:

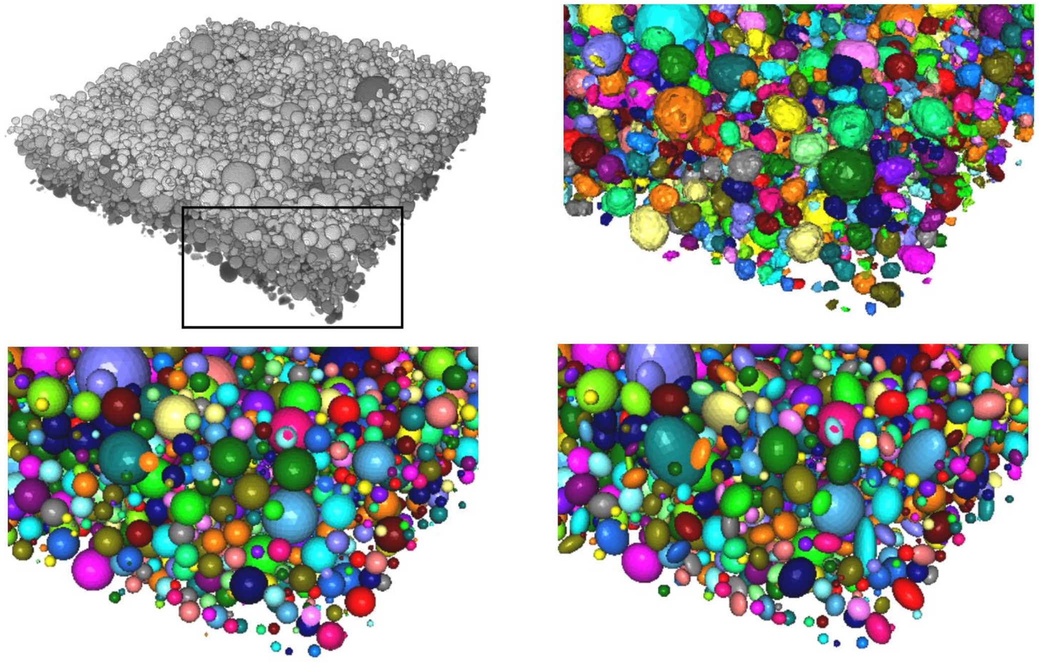
- electronic transport
- thermal transport
- mechanical forcing

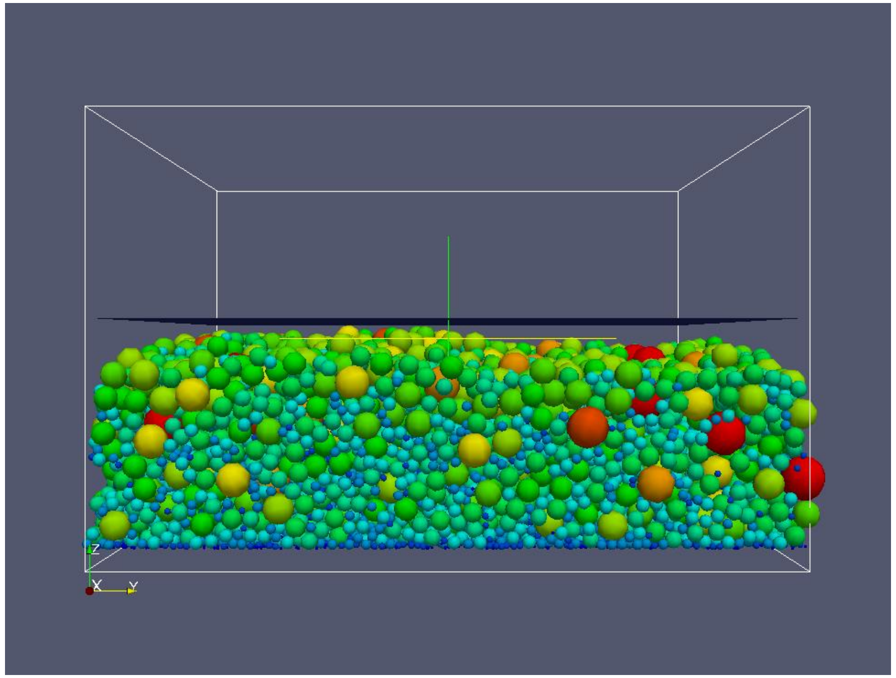
Important to develop accurate approximation!

Contact Network Study

<u>Goal</u>:

- Employ the fabric tensor as a directional measure of contact distribution

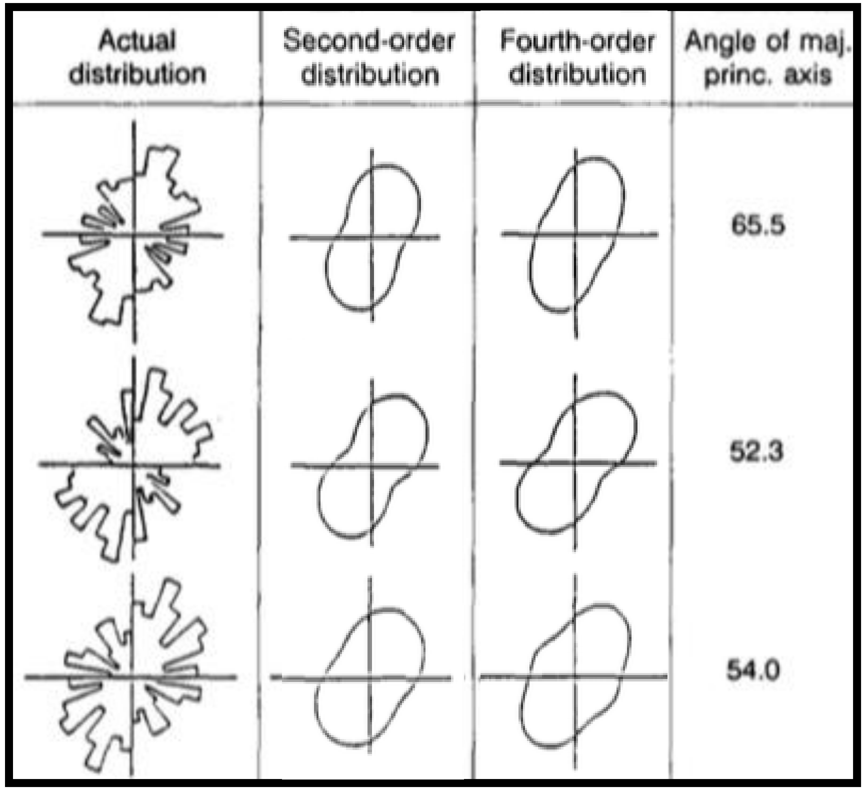




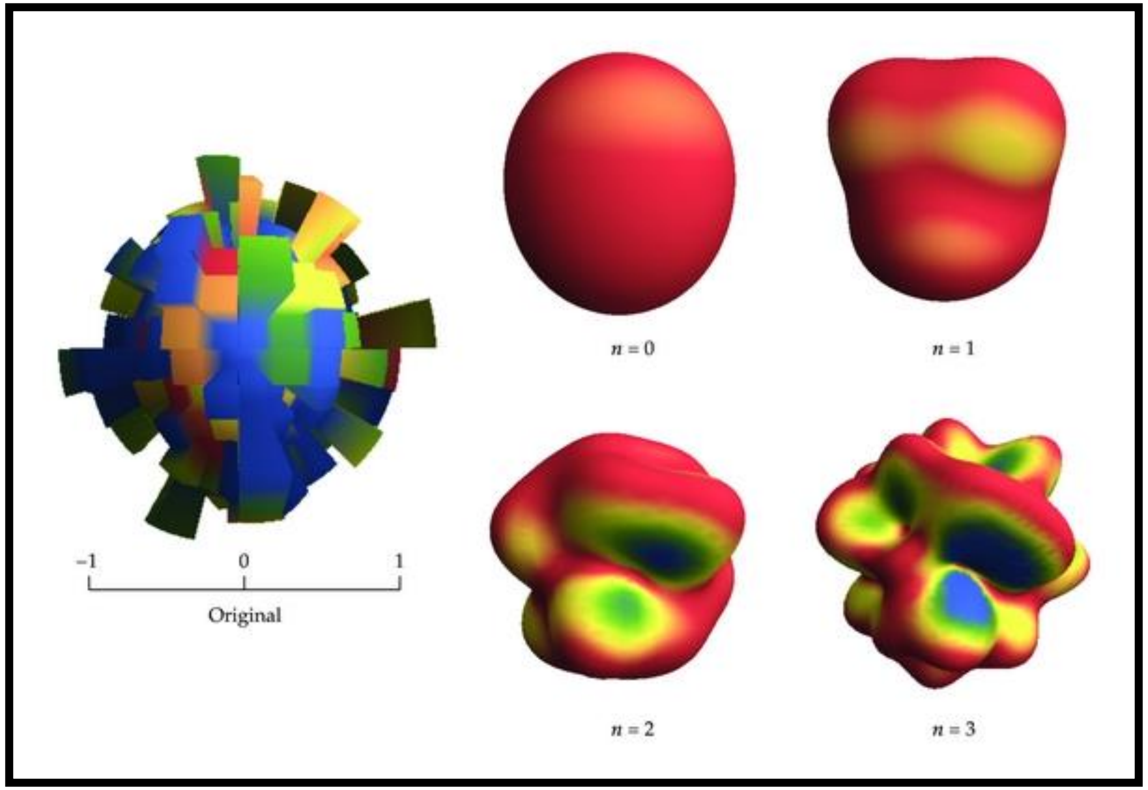
- Determine contact vectors from geometric approximations
- Apply granular model Discrete Element Method from particle size distribution
- Compare fabric tensors before & after compression

Fabric Tensor Definition

- Tensor approximation of directional dataset



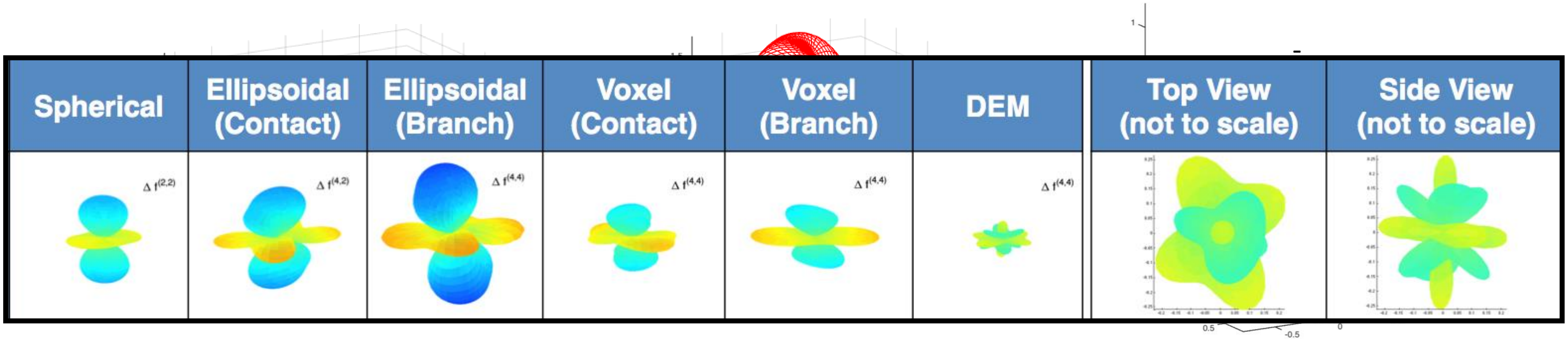
(adapted from Subhash *et al.*, 1991)



(Leng *et al.*, 2012)

Fabric Tensor Comparison

- Consider differences in fabric tensors during cathode compression

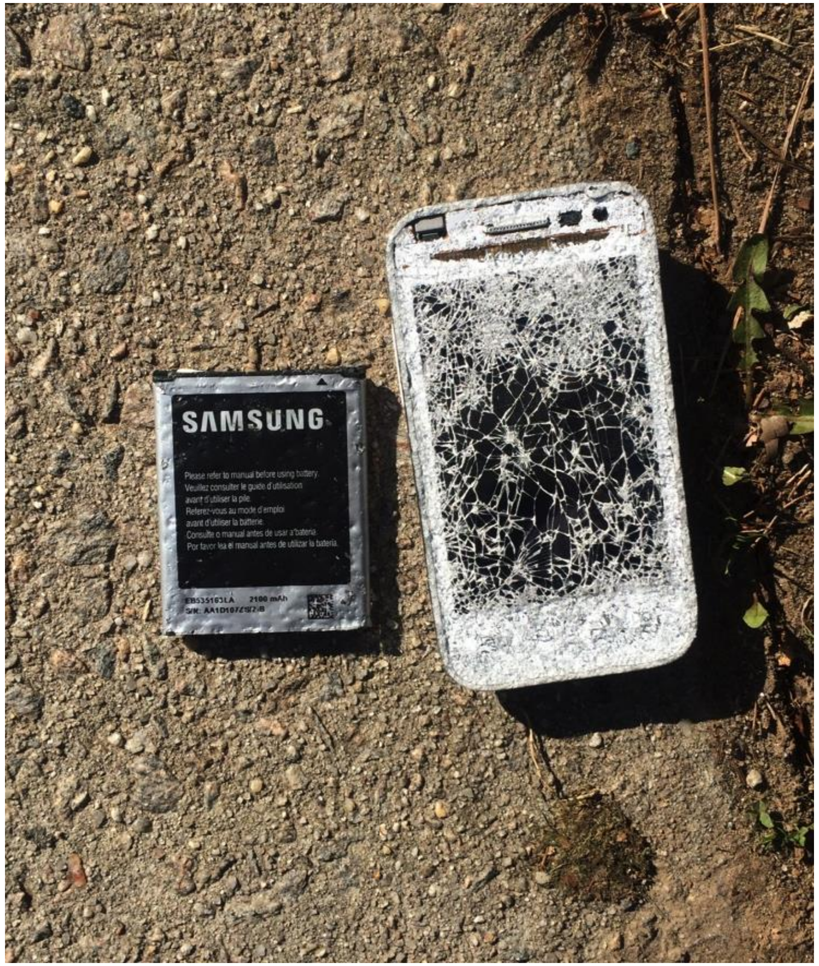


2000 bar | 0 bar | 2000 bar – 0 bar

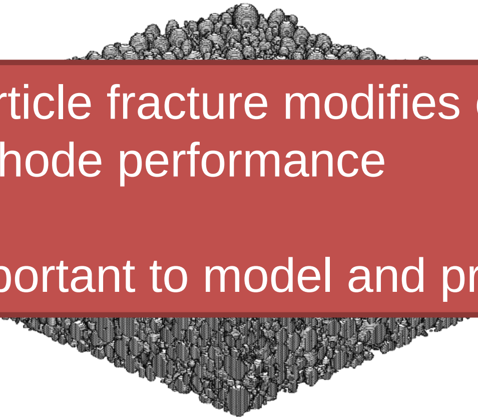
- Fabric tensors capture contact evolution consistently
- DEM does not match well, missing particle fracture

Key: Yellow-red : positive
Green-blue : negative

Motivation



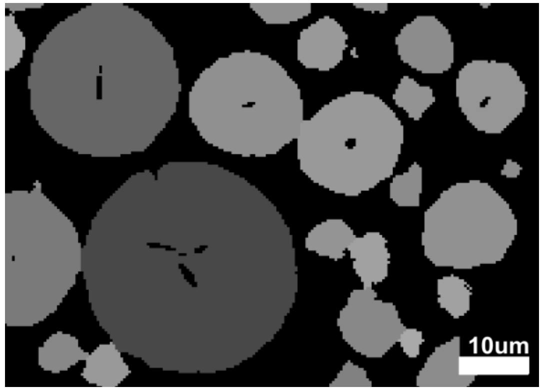
Electrode Compaction in Manufacturing



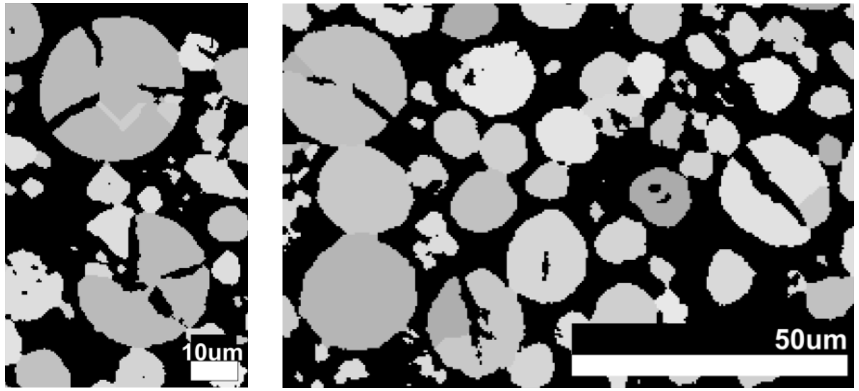
Particle fracture modifies contact pathways & linked to deterioration of cathode performance

Important to model and predict particle fracture!

Before Compaction

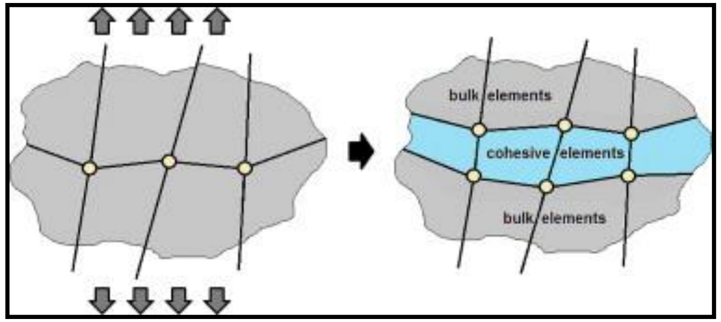


After Compaction @ 2000 bar ≈ 29ksi



X-Ray Tomographic Imagery (Laboratory for Nanoelectronics, ETH Zürich)

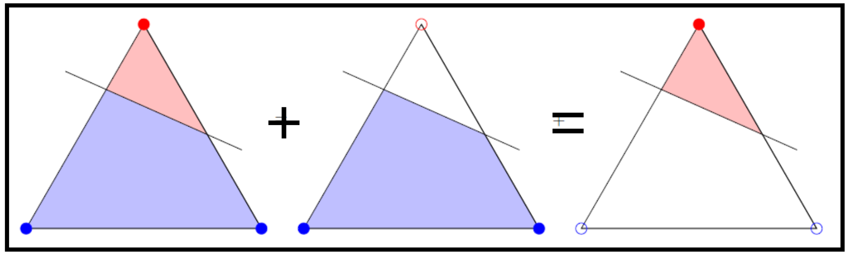
Existing Fracture Model: Cohesive



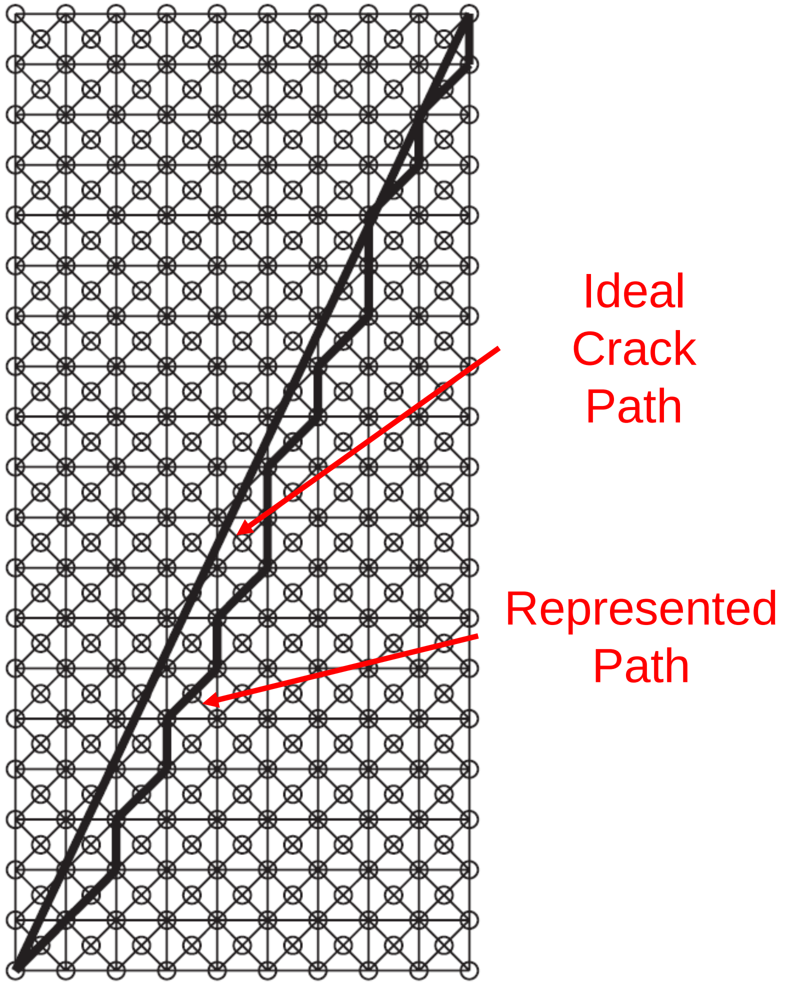
(Khoei *et al.*, 2012)

With a structured triangular mesh, this linear crack path will be approximated by a path 8% longer, no matter the refinement.

- Same-length cracks dissipate more energy
- Same-energy cracks are shorter and may deviate from ideal path
- Can be addressed with XFEM, but difficult 3-D implementation



XFEM Crack Representation, cut through element



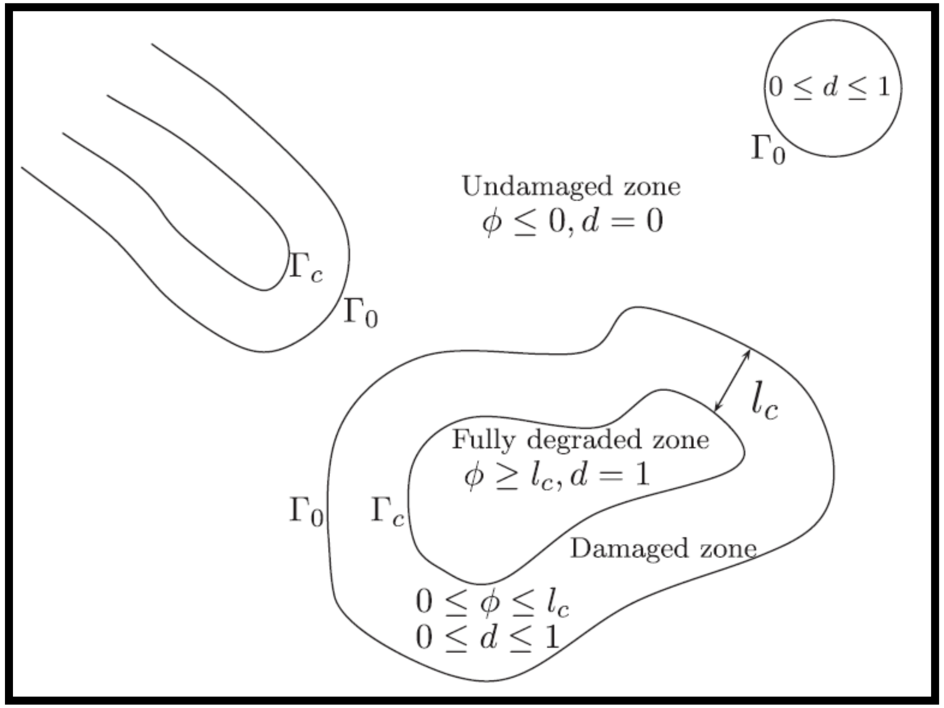
(Papoulia *et al.*, 2006)

Thick Level-Set Method

Thick-Level Set Method:

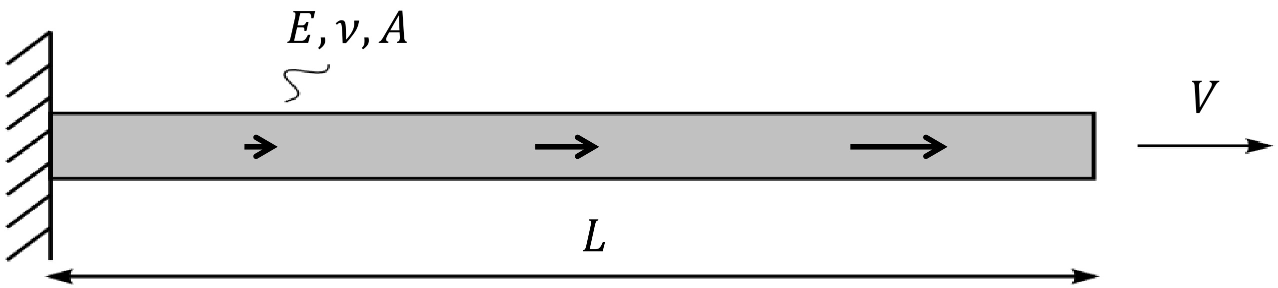
- Non-local damage model
- Incorporates characteristic length (l_c) to limit gradient
- Level-set-based crack identification
- Damage evolution via averaged quantities
- Damage zones updated individually

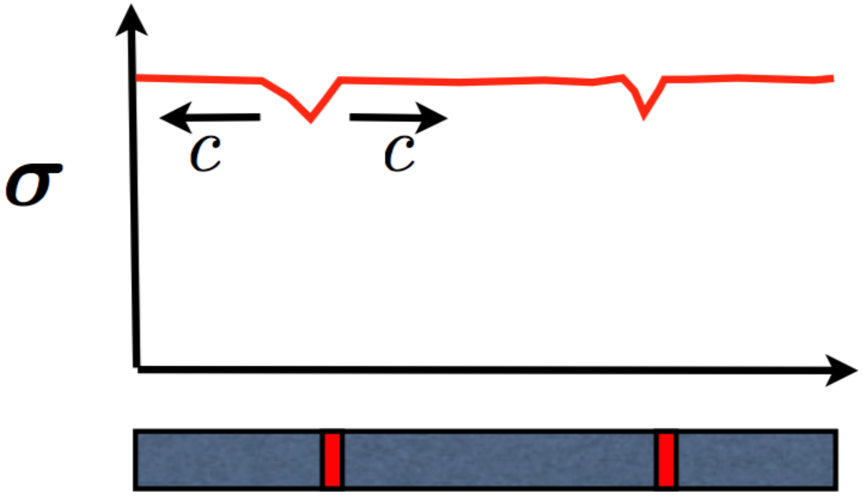
- Addresses weaknesses of other models:
  - Mesh independent / arbitrary crack geometry
  - Natural crack branching and coalescence
  - Mesh convergent / avoids spurious damage localization
  - Straightforward crack surface identification
  - No global solve needed



TLS Damage Zones and Iso-surfaces
(Moës et al, 2011)

1-D Fragmentation Problem





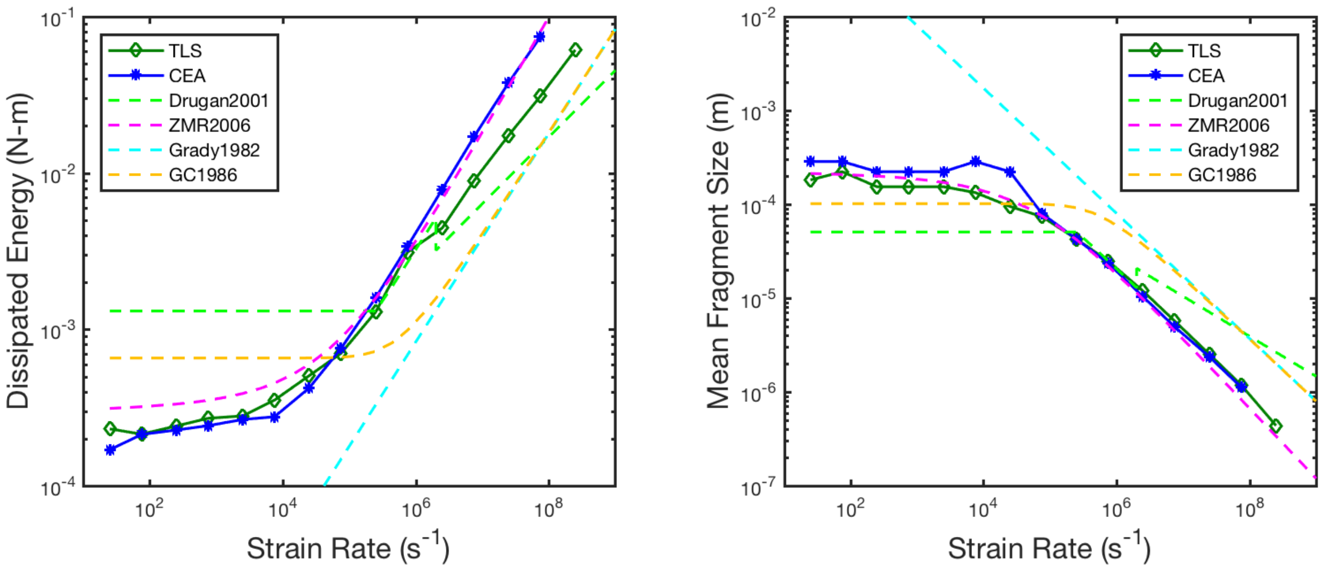
- Fracture of brittle one-dimensional domain
- Constant strain-rate loading
- Small-strain elastodynamics
- Characterized by many, highly-interactive cracks

Rate-dependent result of competition between loading & unloading waves:

- Slow loading = unloading dominates, few fragments
- Fast loading = loading dominates, many fragments

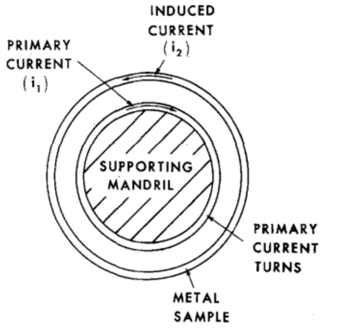
1-D Fragmentation Problem

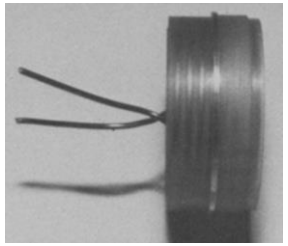
Dense alumina AD993 (aluminum oxide, Al_2O_3)



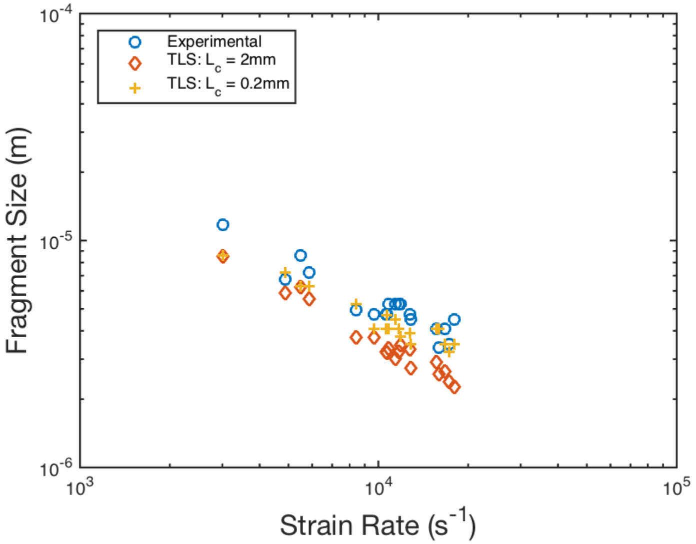
- Match analytical & experimental predictions well
- Performs well to compared to experimental tests

Uranium-6%-Niobium "U6N"



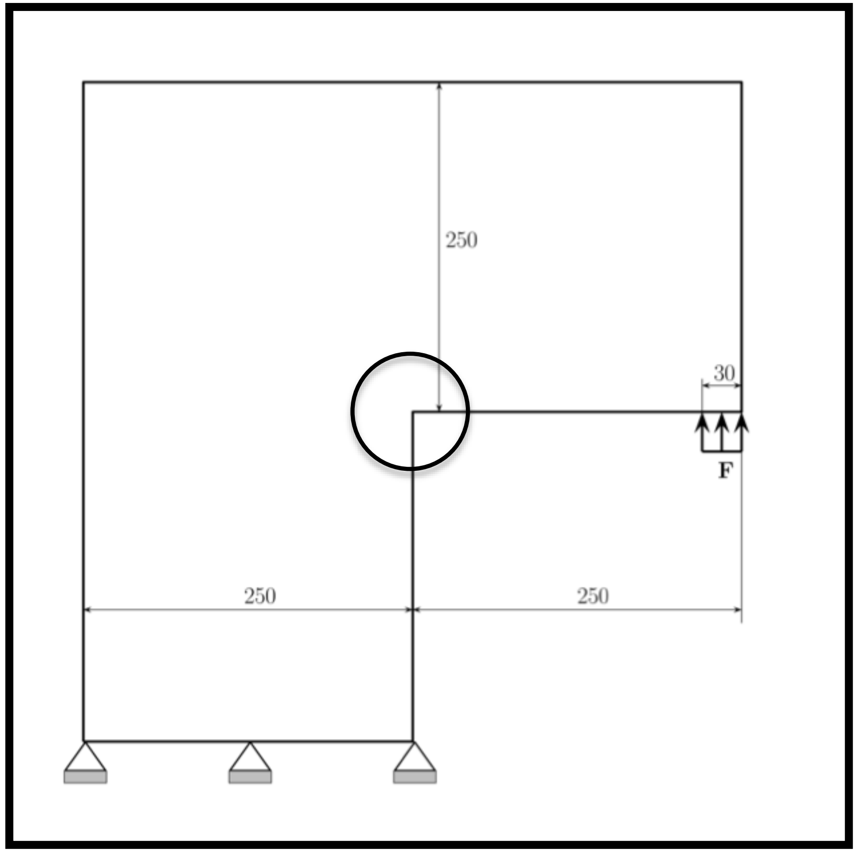


(Grady, 1983)

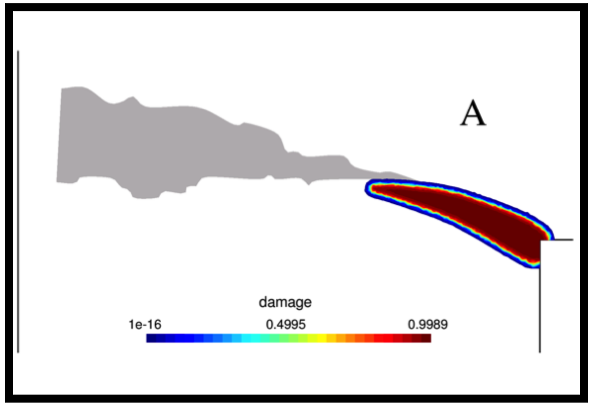


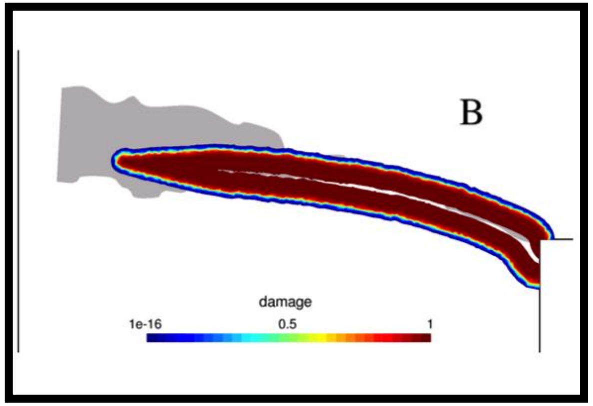
2-D Fracture Problems

Cracking of L-shaped panel – 2D Quasistatic



L-Bracket Loading
(Bernard et al, 2012)



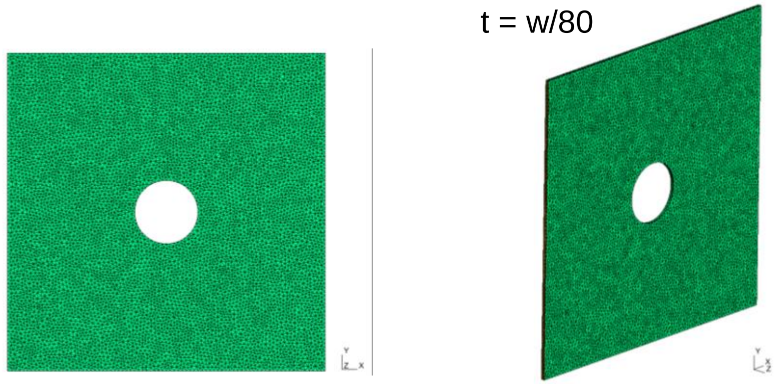


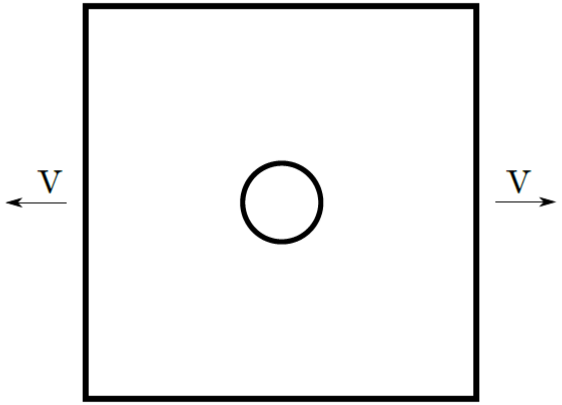
Damage in L-Bracket vs. Experimental (grey)
(Bernard et al, 2012)

3-D Plate Tension

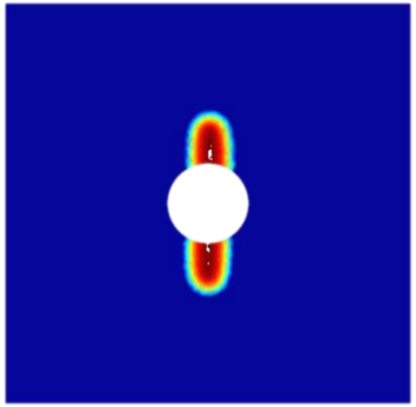
- Three-dimensional plate with hole
- Testing in tension, constant velocity

- Stress concentrations develop at top & bottom of hole

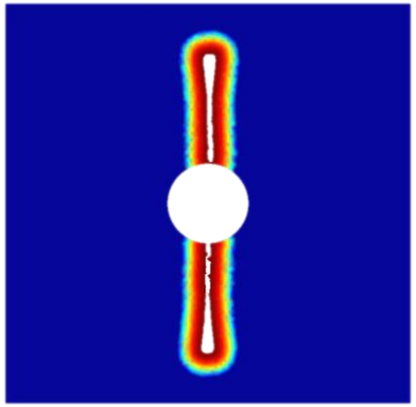




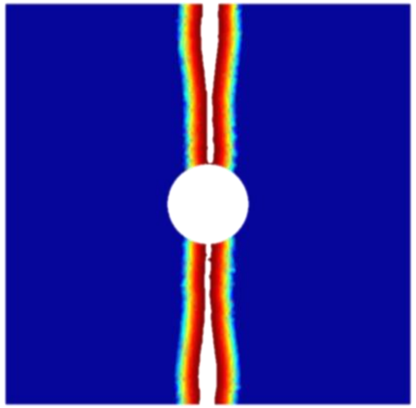
Loading Diagram



T = 0.44μs



T = 0.55μs



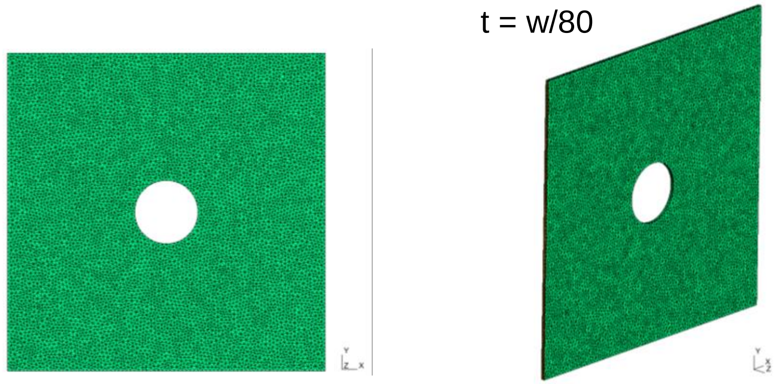
T = 0.66μs

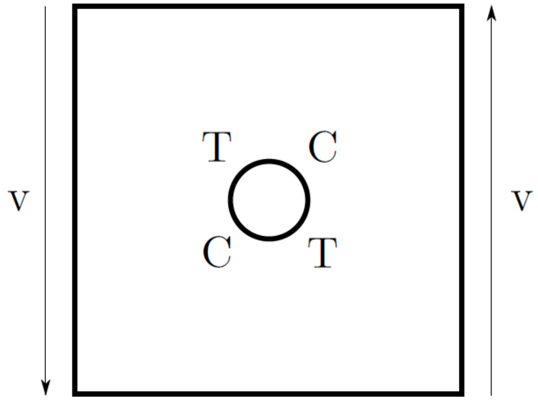
- Cracks develop outward to edges, as expected

3-D Plate Shear

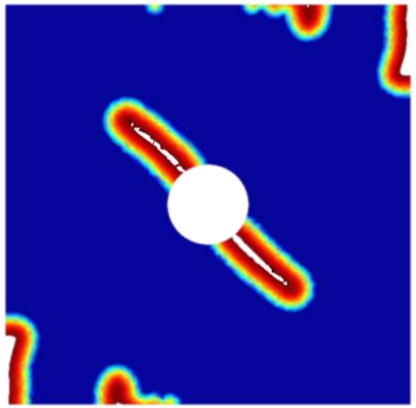
- Three-dimensional plate with hole
- Testing in shear, constant velocity

- Stress concentrations develop at top-left & bottom-right of hole

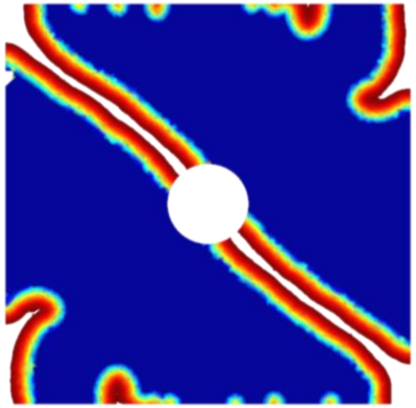




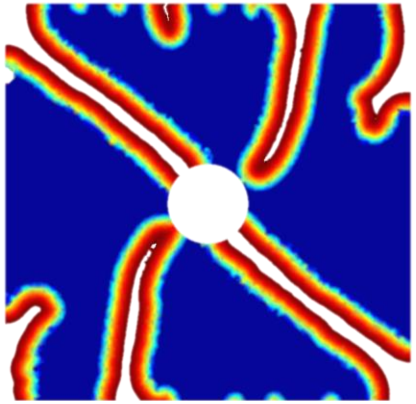
Loading Diagram



T = 0.33μs



T = 0.66μs



T = 0.99μs

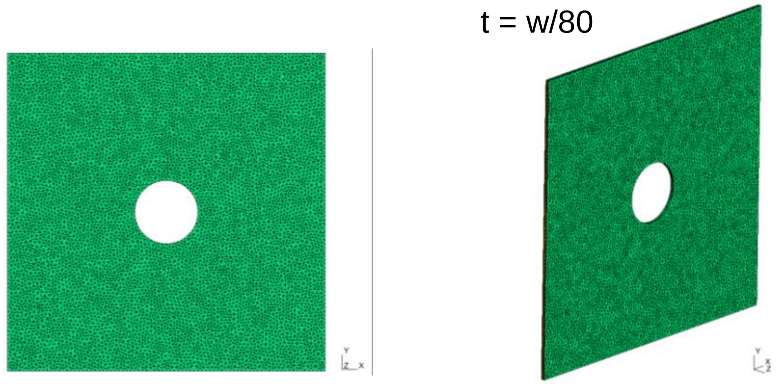
- Cracks develop outward to corners, as expected
- Due to high load rate, subsequent cracks develop from edges toward center

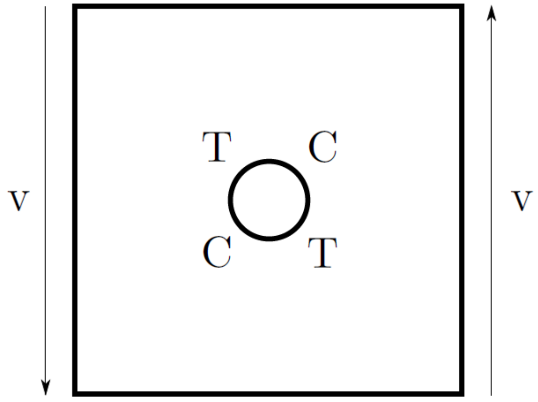
3-D Plate Shear

- Three-dimensional plate with hole
- Testing in shear, constant velocity

- Stress concentrations develop at top-left & bottom-right of hole

t = w/80





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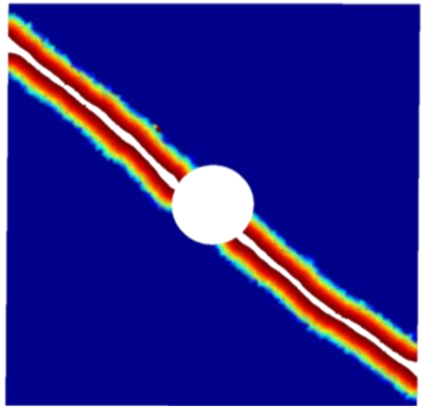
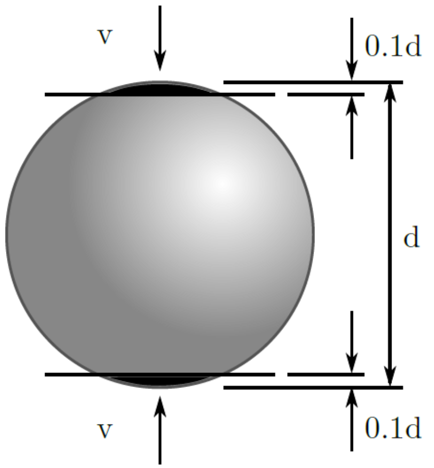


Slower Loading
v = 0.4 mm/ms
$Y_c = 6 \cdot 10^{-5}$ GPa

Shear Wall Failure
(air-worldwide.com)

3-D Sphere Compression

- Spherical geometry (one octant only, by symmetry)
- Compressive impact loading (loading surface in blue)



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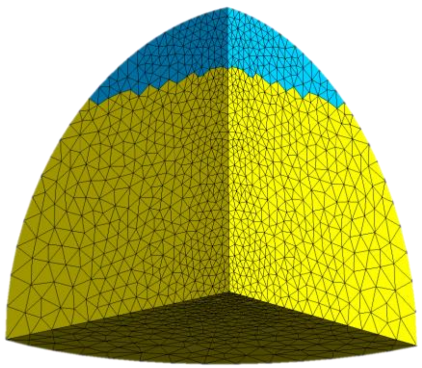
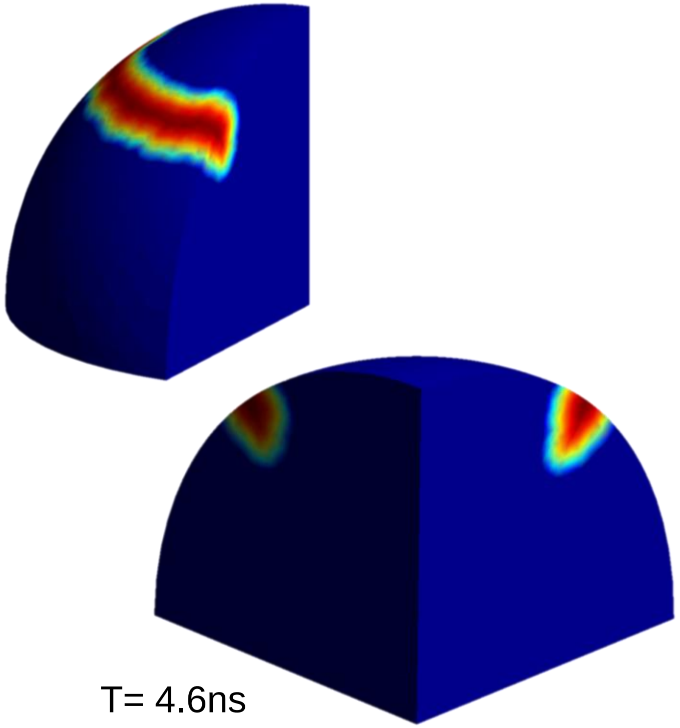
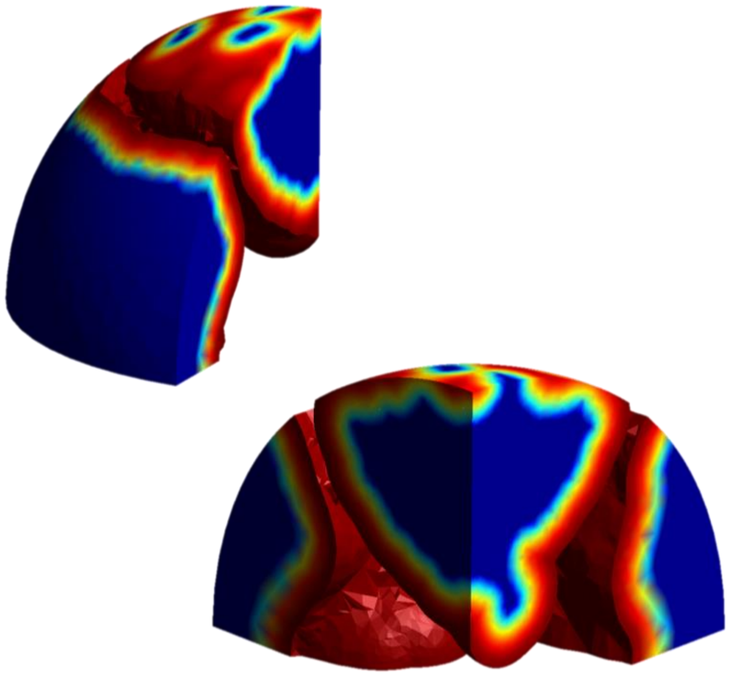




T= 4.6ns



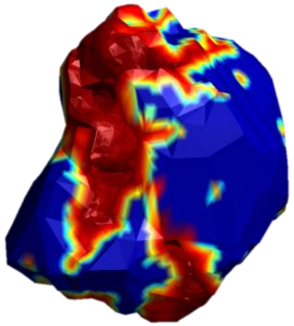
T = 6.1ns

- Damage field indicates formation of conical crack developing from load surface
- Matches experimental observations

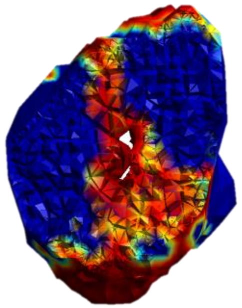
3-D Particle Compression

Sample particle simulation damage fields:

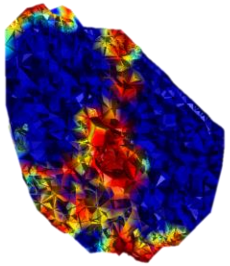
- Particle 4383, Icosahedral-0 Orientation



Exterior

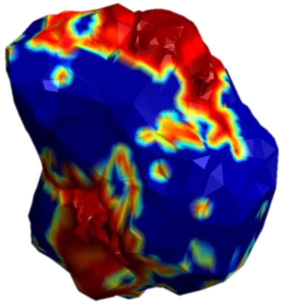


Cut-away 1

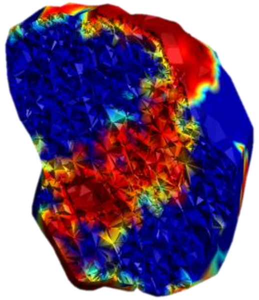


Cut-away 2

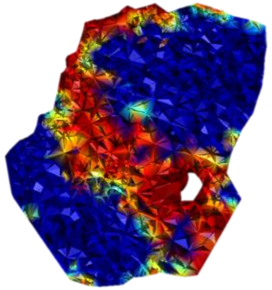
- Particle 4383, Icosahedral-2 Orientation



Exterior



Cut-away 1



Cut-away 2

Engineering Significance & Extensions

Significance:

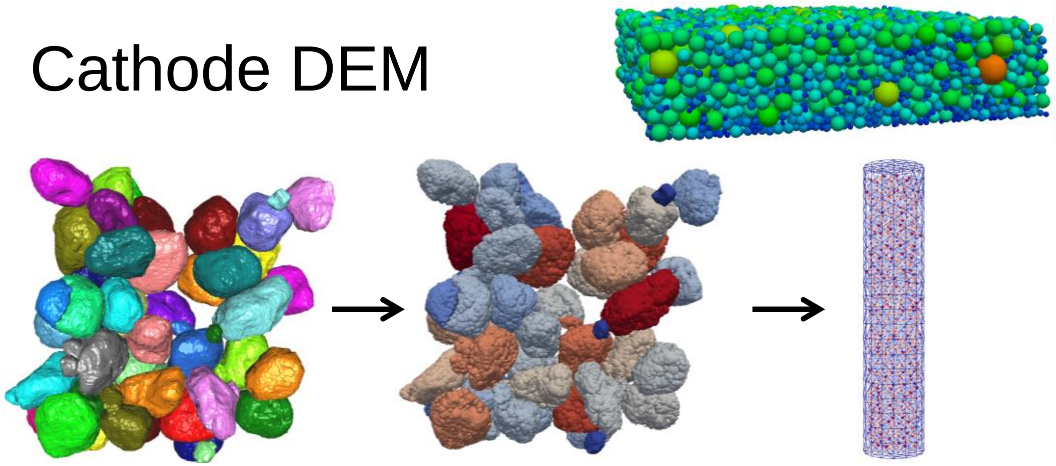
- Fabric tensor analysis can identify transport pathways
- Battery designers can use TLS to effectively analyze particle failure due to manufacturing, operational, and exceptional loadings.
- TLS model can efficiently model fracture in many diverse fields of application

Extensions:

- Use FTs to develop continuum-scale cathode models
- Use TLS to predict particle fracture to inform DEM model

Parallel & High-Performance Computing

Cathode DEM

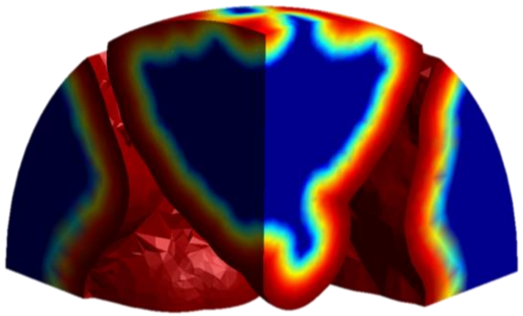


Calculations made tractable by running on ORNL cluster and supercomputer

TLS 1-D Fragmentation

Distributed parameter & mesh studies on Duke cluster, 128 simultaneous

TLS 3-D Fracture



Hastened simulation via parallel solve, necessary for simulating many particles

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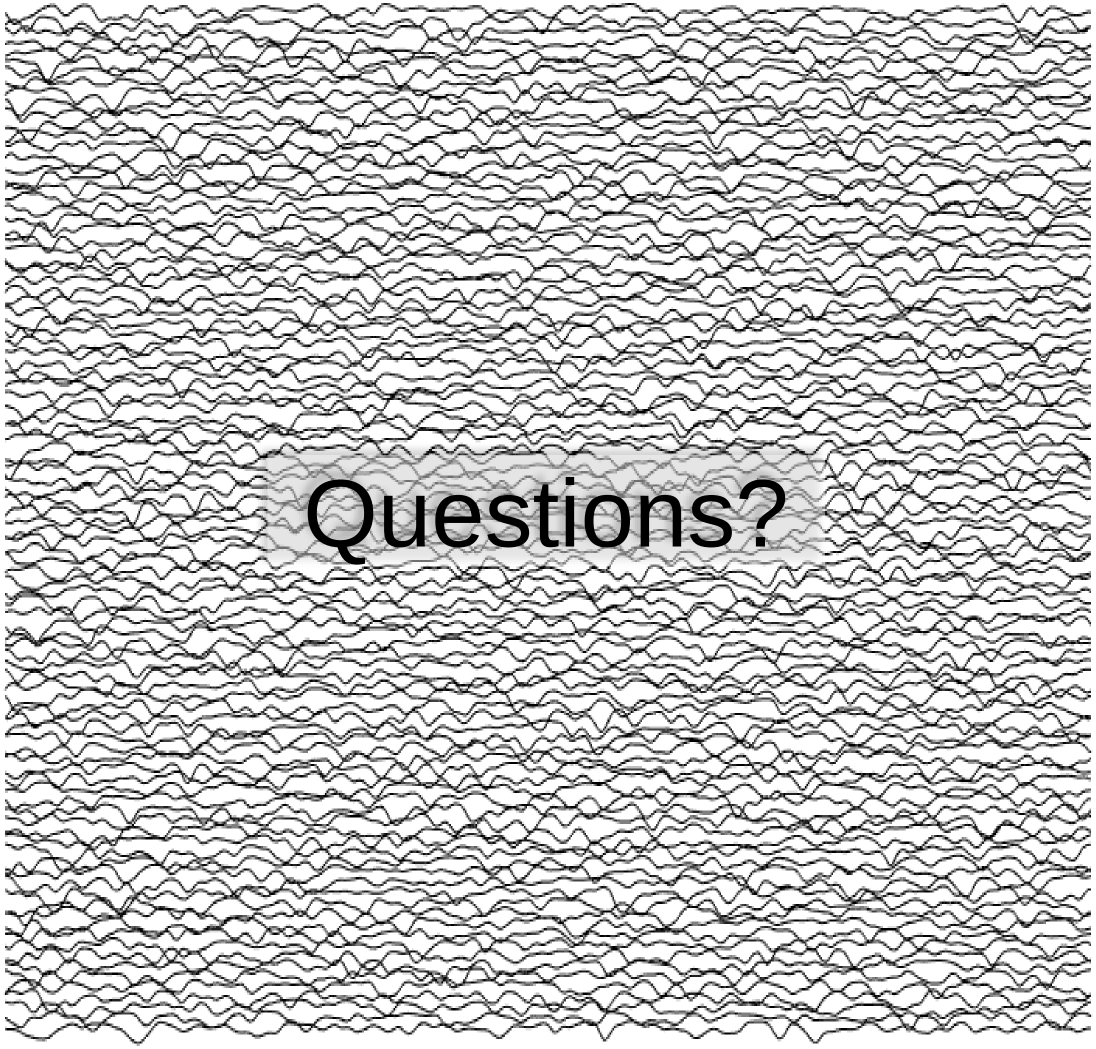

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