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MESOSCALE MODELING OF ENERGETIC MATERIALS

Michael E Nixon and Martin J. Schmidt

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INTERIM REPORT

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14. ABSTRACT

The goal of the program is to incorporate deformation damage into material models for energetic materials and correlate the damage to changes in energetic behavior. Of primary interest is the effect on the energetic sensitivity of the material from internal damage occurring during a penetration event. Changes in the internal structure due to grain fracture and grain debonding from the matrix material may lead to both a change in the mechanical properties as well as the sensitivity to energetic behavior. This briefing represents interim progress towards these goals.

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Mesoscale Modeling of Energetic Materials

AFOSR Review

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Sponsor: Dr. David S. Stargel

July 25 2012

Background

- Collaborative effort within AFRL
  - Computational Mechanics Branch (RWWC)
  - High Explosives Research and Development Branch (RWME)
  - Damage Mechanisms Branch (RWMW)
- Goal: Predict survivability of energetic payload of high speed penetrating weapons
- Approach:
  - Use XCMT
    - Investigate internal structure of pristine and damaged materials
    - Generate representative computational meshes
  - Perform meso scale simulations of composite energetic materials used in AF penetrating weapons
  - Incorporate deformation damage into material models for energetic materials
  - Extract data from FEM simulations of RVE's to feed thermal-reactive prediction code

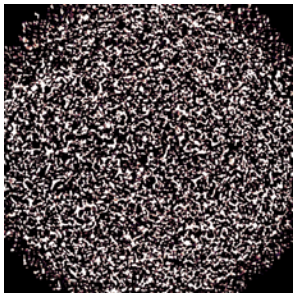
Status

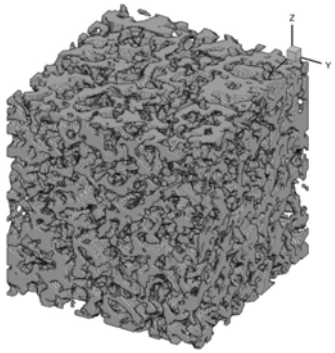
- Established capability to generate computational mechanical RVE from XCMT data
- Generated experimental data for the mechanical behavior of simple explosive
  - Pristine
  - Damaged
- Performed simulations on mechanical RVE's
  - From XCMT
  - Idealized
- Developed and performed initial thermal-reactive predictions (currently under development)

Aluminum Foam

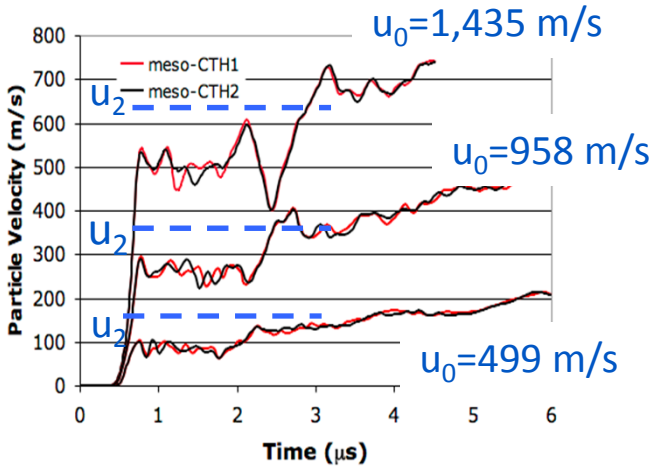
Photograph
(2.75 inch x 2 inch)

Slice from XCT-Scan

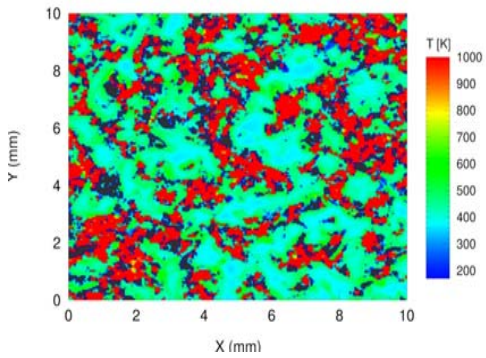




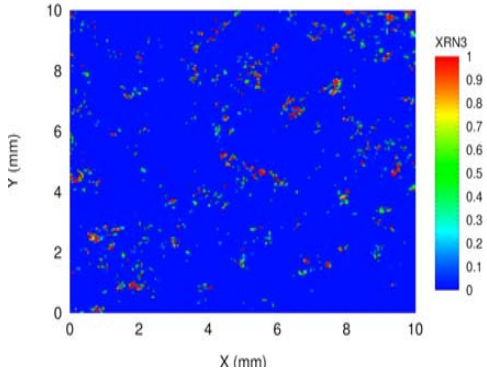
Representative Volume
(10 mm x 10 mm x 10mm)



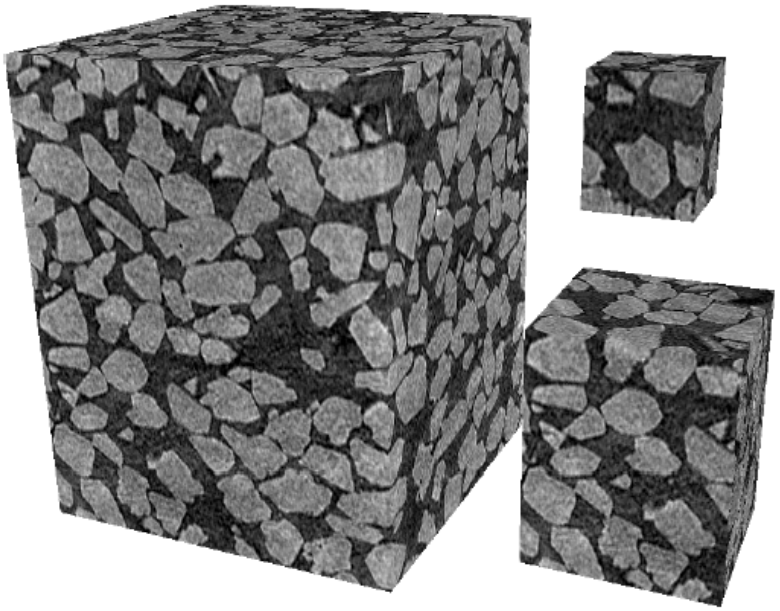
Temperature Distribution

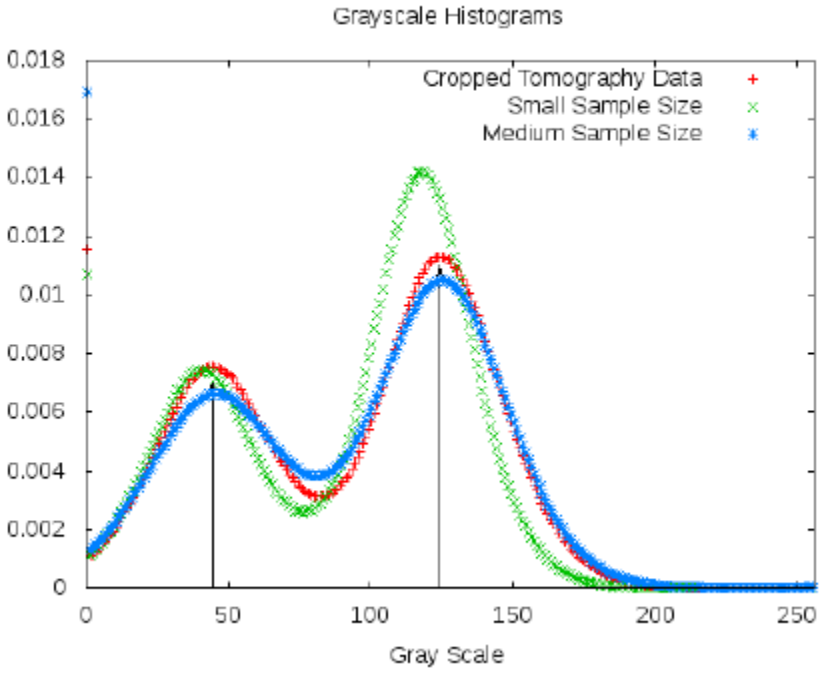


Extent of Reaction
0=unreacted and 1=reacted

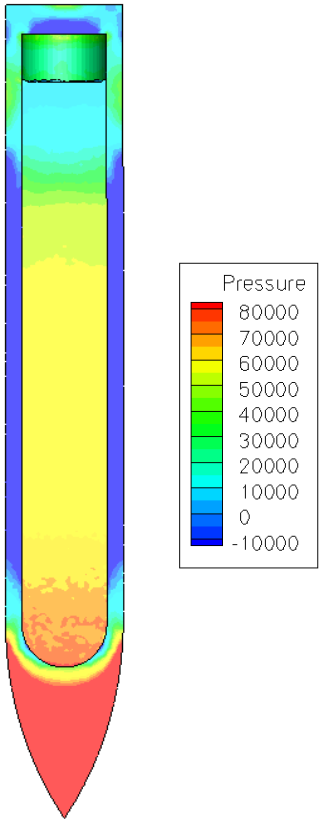


RVE Study

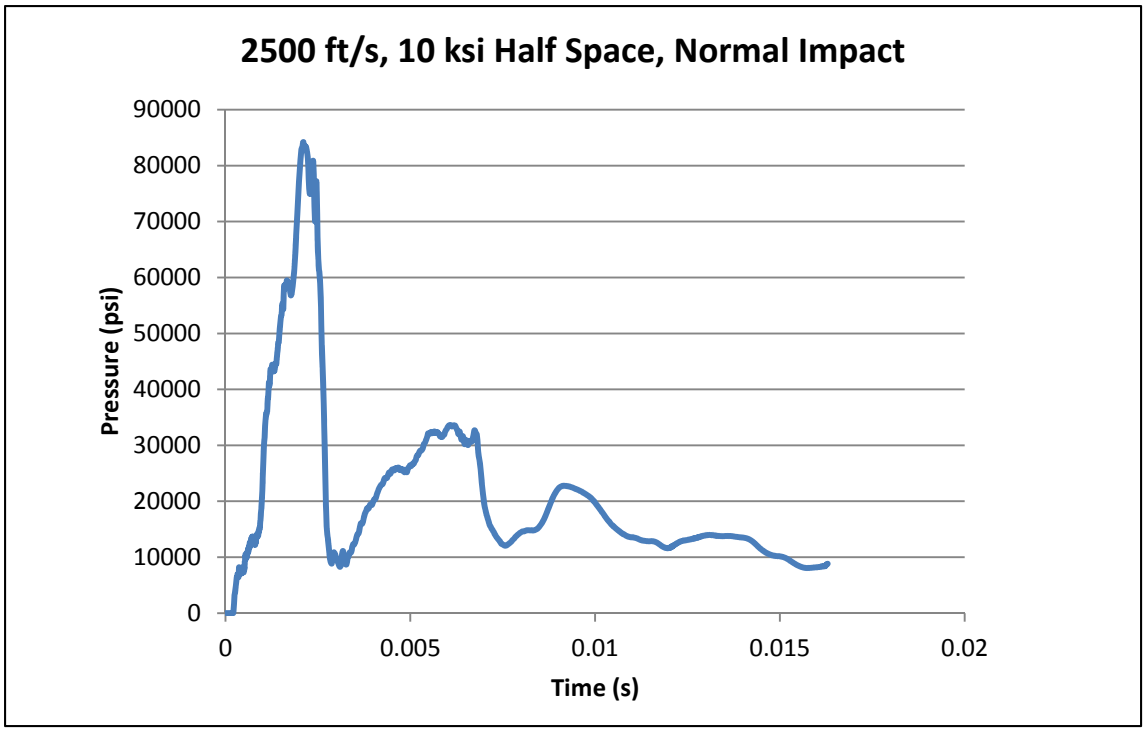




Pressure Loads from Systems Level Simulation

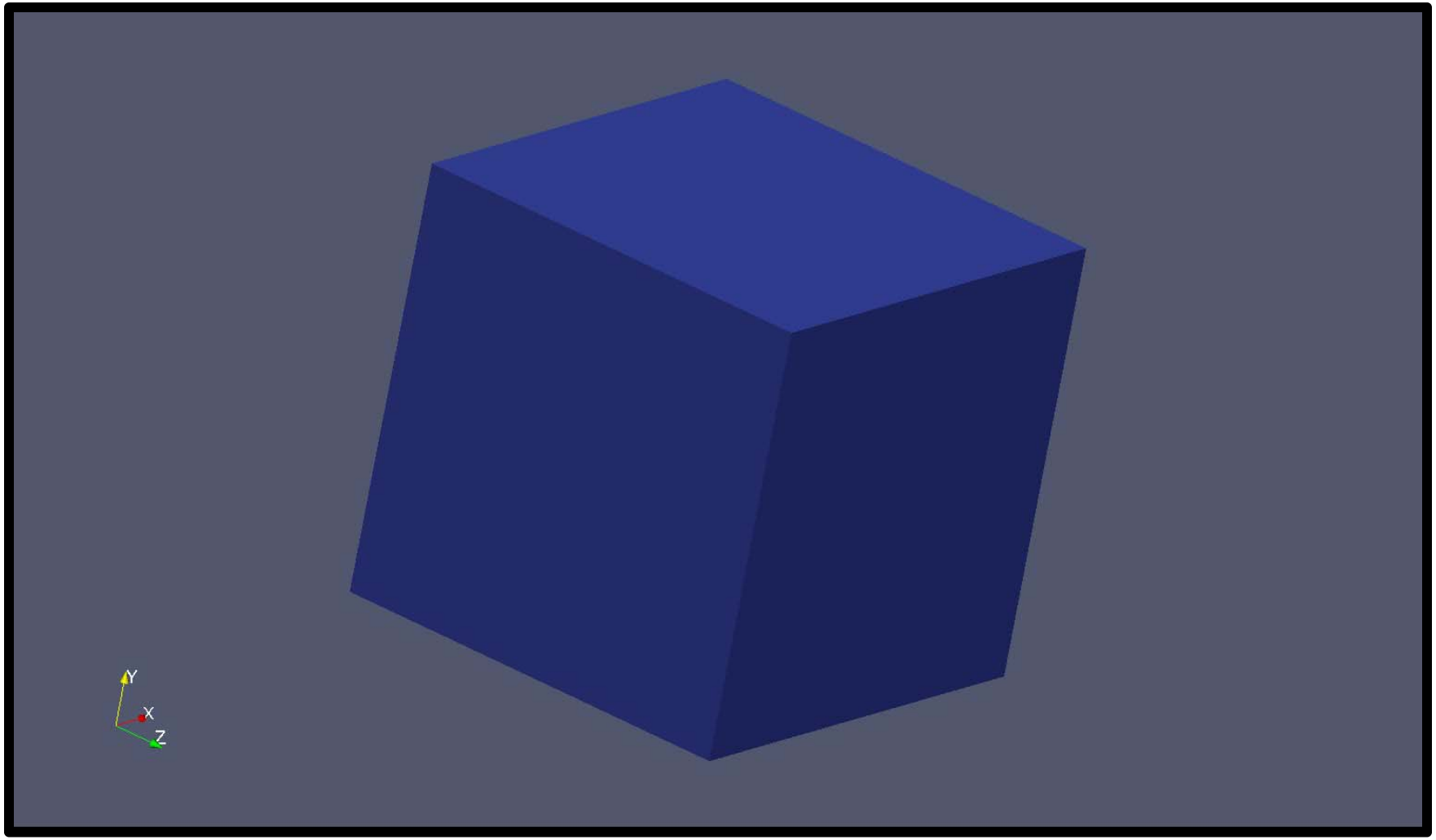


Pressure near the nose

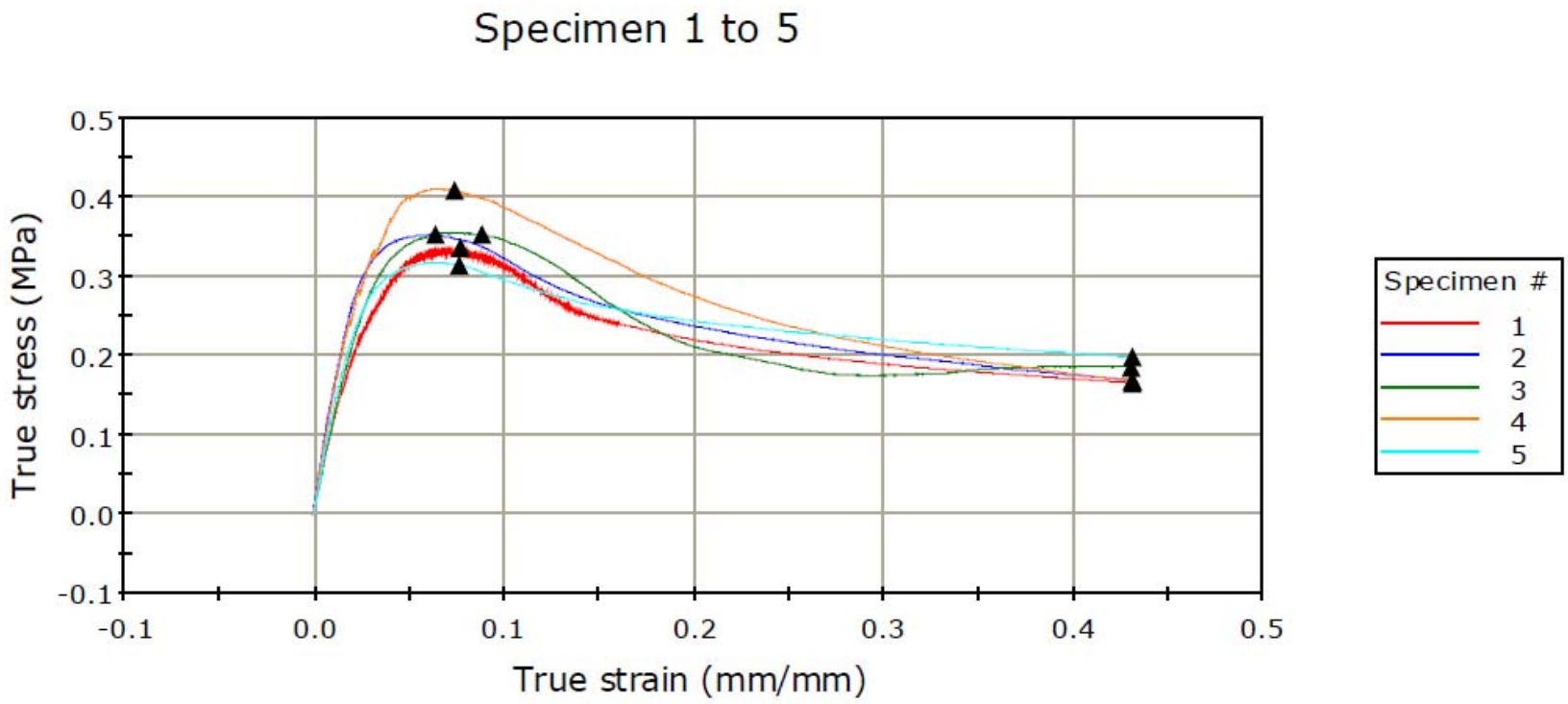


Contours of pressure shown at 0.002 s

RVE from XCMT

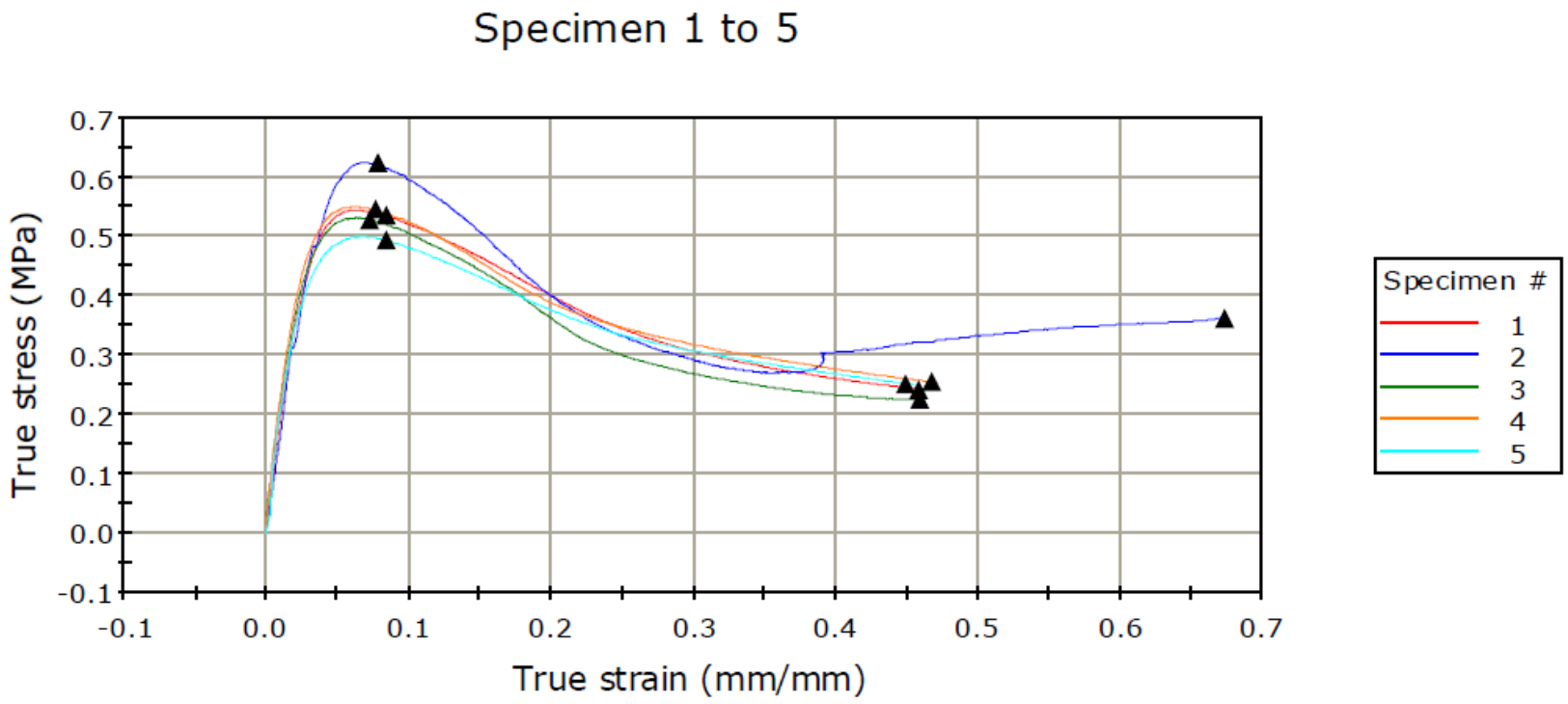


Characterization Data of Composite



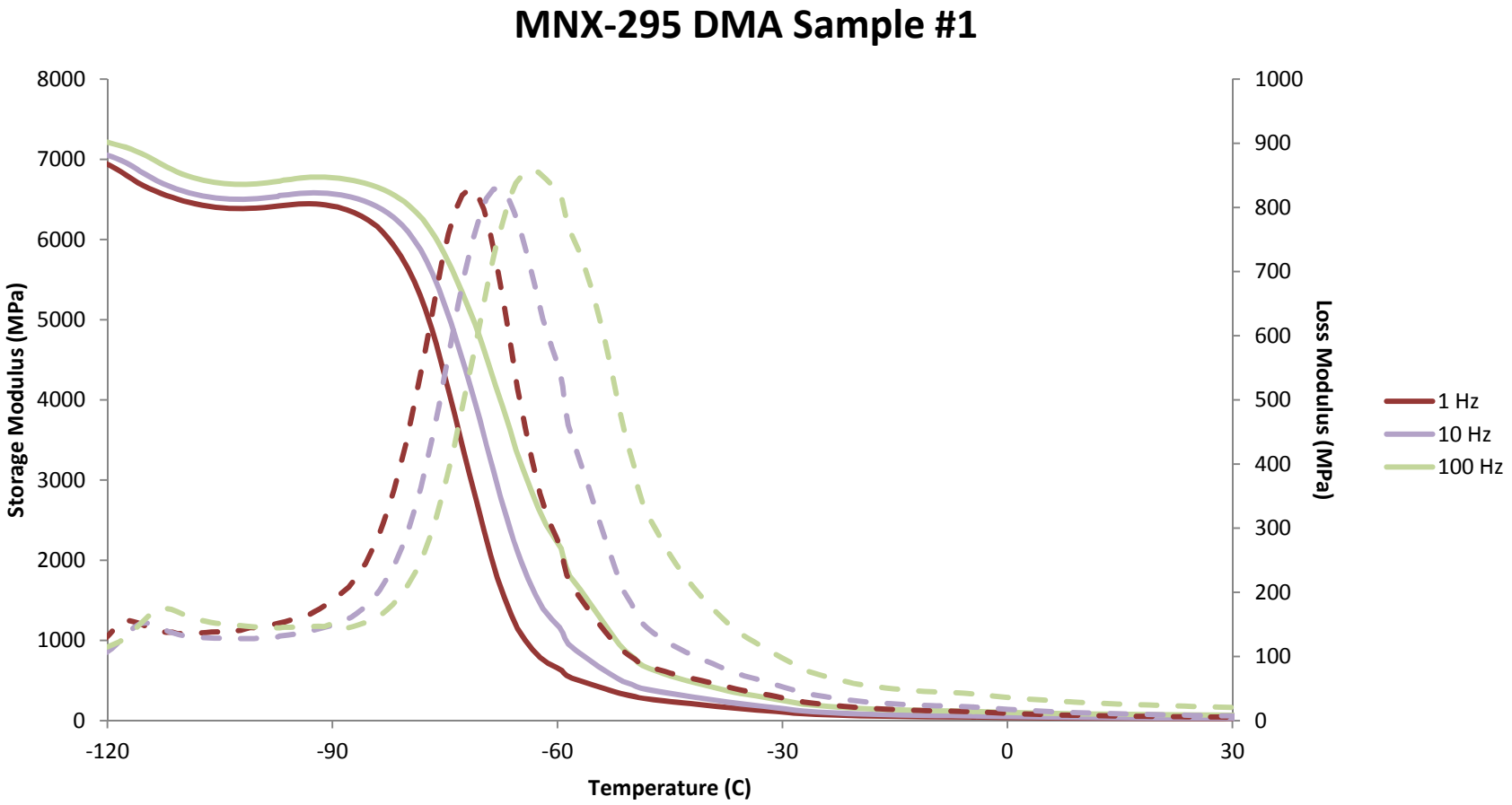
Compression Tests at 0.24mm/min

Characterization Data of Composite



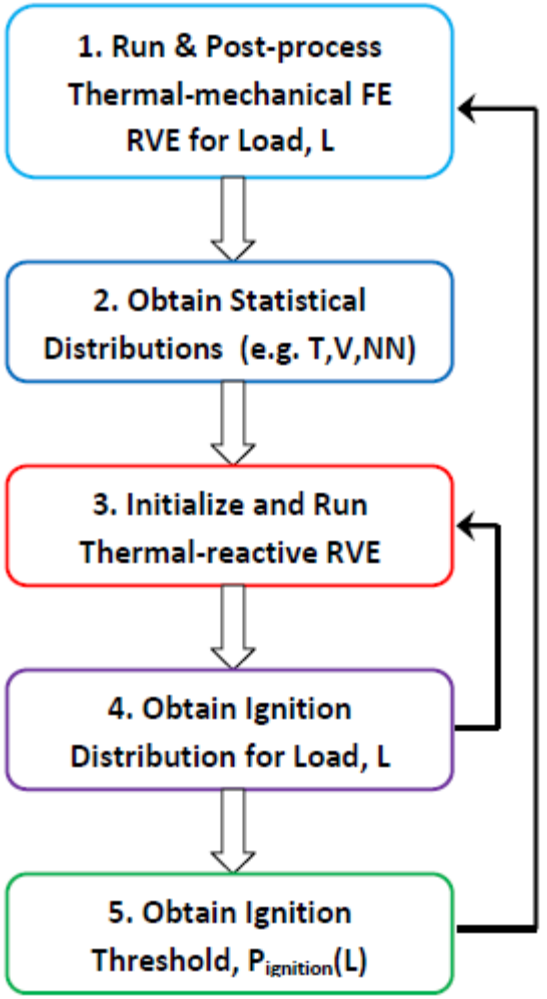
Compression Tests at 24 mm/min

Characterization Data of Composite



Thermal-reactive Model

- We can use nearest-neighbor distributions to help quantify explosive morphology.
- We may estimate statistical distributions of the heterogeneous temperature rise that results from mechanical loading.
- These distributions can be used to initialize a thermal-reactive representative volume element (RVE), which is called a “realization”.
- Many realizations can be initiated using the same statistics.
- Not all realizations will undergo complete chemical reaction, even with adiabatic RVE boundary conditions.
- We are interested in this uncertain “region”, or ignition threshold. It is our goal to understand and quantify this uncertainty.



Main Steps: Processing and Post-processing

Step #1: Run and post-process the finite element (FE) RVE

a. Specify a loading condition and run the FE simulation.

b. Post process the following for each crystal:

   i. centroids, X_i

   ii. size or volume, V_i

   iii. maximum temperature, $T_{max,i}$

   iv. average temperature, $T_{avg,i}$

Step #2: Obtain statistics (Gaussian mean μ and std. deviation σ)

a. Use the cutoff temperature, $T_{c,}$ to classify each $T_{max,i}$ as either a H.S. (hot spot) or a C.S. (cold spot).

b. For H.S. - $T_{max,i}$, $T_{avg,i}$, $V_{hs,i}$, and NN_{hs} (nearest neighbor) , find μ and σ.

c. For C.S. - $T_{avg,i}$, $V_{cs,i}$, and NN_{cs} , find μ and σ.

d. For H.S. – NN_{tmax} , find find μ and σ for 3 bins using all H.S. T_{max} values.

Main Steps: Processing and Post-processing

Step #3: Initialize and run a realization of a thermal-reactive RVE

a. For H.S., randomly initialize centroid values, $X_{hs,i}$ with $V_i=V_{hs}(\mu,\sigma)$.
b. For H.S., synthetically anneal $X_{hs,i}$ to fit desired NN_{hs} distribution.
c. For H.S., randomly assign hot spot $T_{max,i}$.
d. For H.S., anneal the 3 temperature nearest neighbor distributions using NN_{tmax} values.
e. For C.S., randomly initialize centroid values, $X_{cs,i}$ with $V_i=V_{cs}(\mu,\sigma)$.
f. For C.S., synthetically anneal $X_{cs,i}$ to fit desired NN_{cs} distribution.
g. Run the thermal-reactive RVE simulation.

Step #4: Obtain ignition distribution for a given load, L

a. Repeat Step #3 many times and record ignition results (either yes or no ignition).
b. Calculate the ignition probability based on multiple realizations for a single load, L.

Step #5: Obtain ignition threshold as a function of load, L

a. Repeat Steps #1-4.
b. Calculate the ignition threshold as $P_I(L)$ as a function of the load, L, where P_I is the probability of ignition that is obtained from the ignition probability in Step #4.

Synthetic Annealing

– Assume that the nearest neighbor, NN1, distribution is Gaussian

$$P[d_k||(d_i - \delta d/2) < d_k \leq (d_i + \delta d/2)] = a_{NN}\exp\left\{-\frac{1}{2}\left(\frac{d_i+\mu}{\sigma}\right)^2\right\}$$

- for i = 1, …. N_d, where N_d = number of bins to discretize NN1
- δd = width of the bins
- μ = mean distance
- σ = standard deviation of the distance
- a_{NN} = scaling parameter so that sum of d_i probabilities sum to unity

$$a_{NN} \cdot \sum_{i=1}^{N_d} P(d_i) = 1$$

Synthetic Annealing

- We let $P(d_i)_{syn}$ denote the synthetic probability obtained from the annealed configuration and $P(d_i)_{act}$ denote the actual or experimental distribution.
- The objective function to be minimized is

$$e_{NN} = \sqrt{\sum_{i=1}^{N_d} \left(P(d_i)_{syn} - P(d_i)_{act} \right)^2}$$

- Procedure:

  a) Randomly assign crystal centroids to locations

  b) A subset of the centroids are randomly perturbed in the x, y, and z directions.

Synthetic Annealing

– Procedure (cont.):

c) The objective function is evaluated again to give a new e_{NN}.

d) If the new value of e_{NN} is smaller than the previous value, then the new configuration is kept. If not, then the probability that the configuration will be kept is given by,

$$P = \exp\{-de_{NN}/T_v\}$$

T_v = virtual temperature (can be a function of number of attempts)

e) Steps b-d are repeated until either i) the maximum number of attempts has been reached, or ii) the number of temperature (T_v) decrements has been reached.

Example: Step #3

- The random centroid distribution is shown below.
- Hot spots (hs, red) and cold spots (cs, blue).

N_{hs} = 4 to 12 (varies linearly with load)

N_{total} = 30 crystals

$N_{cs} = N_{total} - N_{hs}$

Lx = Ly = Lz = 15 microns

$\mu_{(D,hs)} = \mu_{(D,cs)}$ = 2 microns

$\sigma_{(D,hs)} = \sigma_{(D,cs)}$ = 1 microns

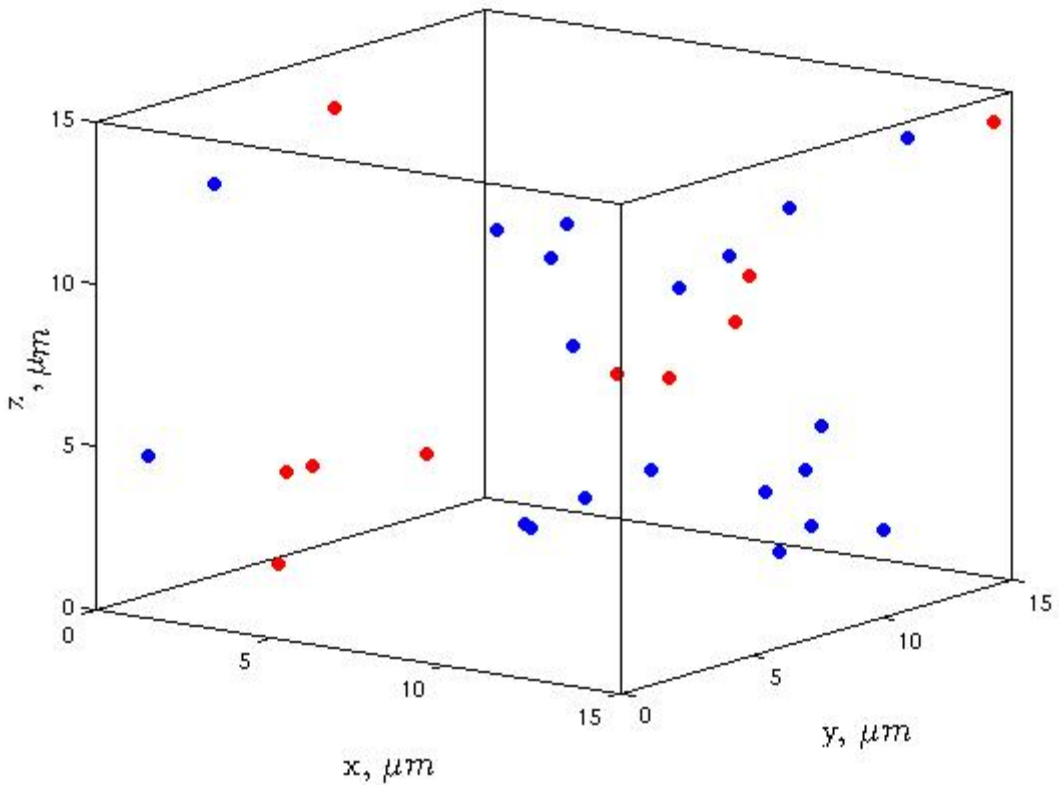
Min diameter = 0.5 micron (hs and cs)

$\mu_{(NN1,hs)} = (4.5 - N_{hs}/20)*1e\text{-}6$ microns

$\mu_{(NN1,cs)} = (3.0 - N_{cs}/20)*1e\text{-}6$ microns

$\sigma_{(NN1,hs)} = \sigma_{(NN1,cs)}$ = 1 microns

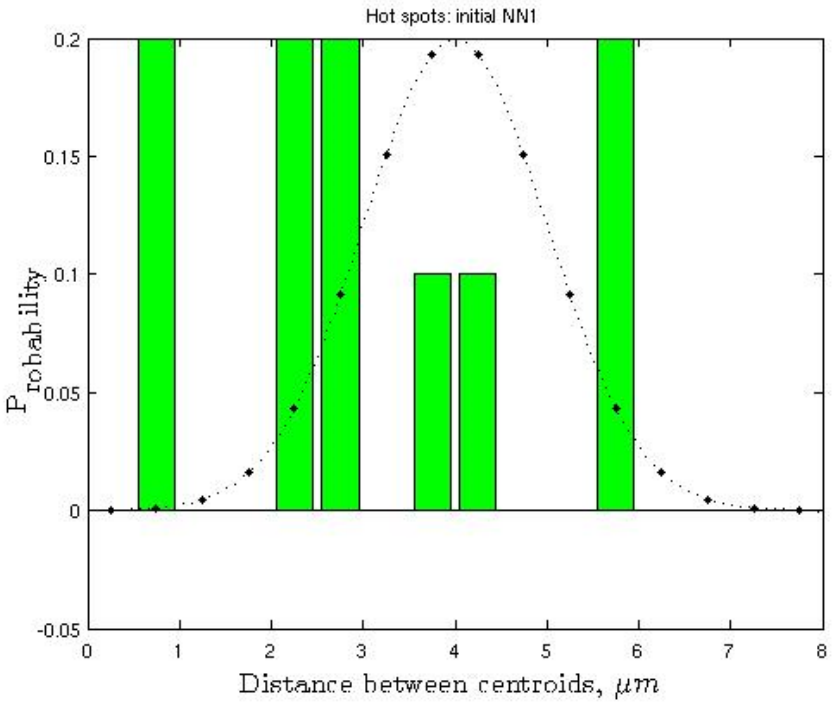
nx = ny = nz = 31

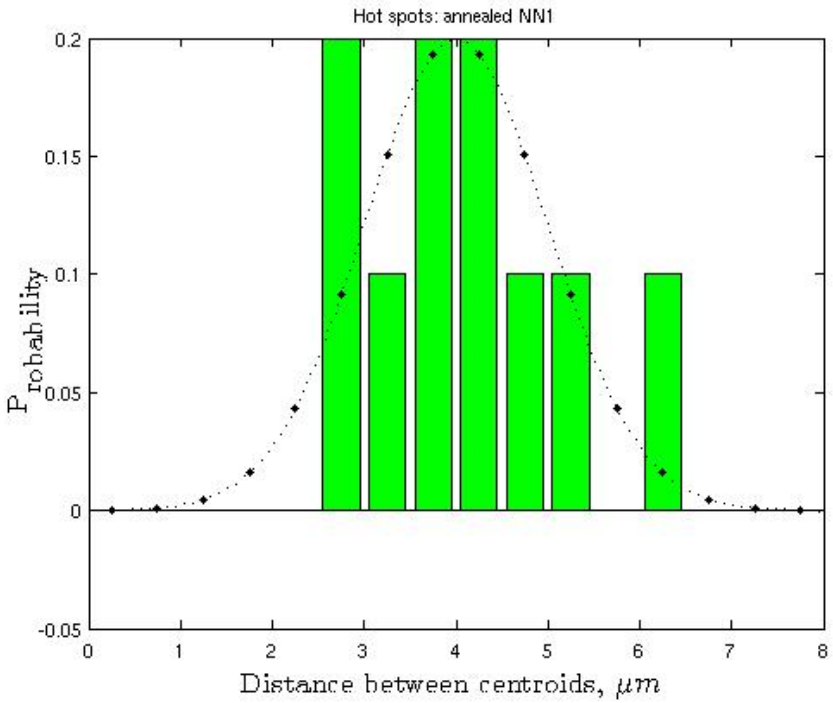


Example: Step #3

Hot spot centroid annealing – nearest neighbor distribution(NN1)

$N_{attempt}$ = 300, D_{move} = 2*dx, $T_{virtual}$ = 80, φ_{move} = 0.20



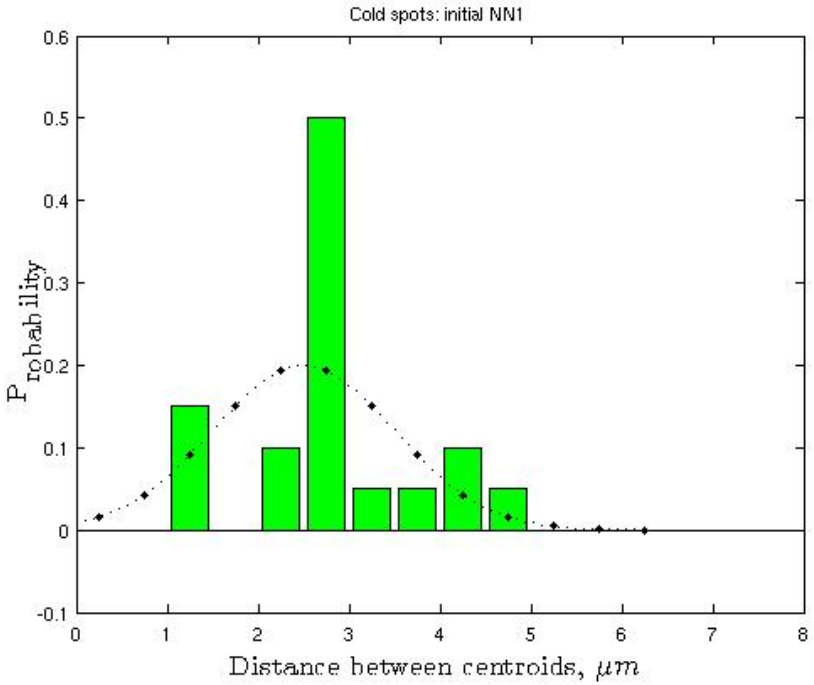


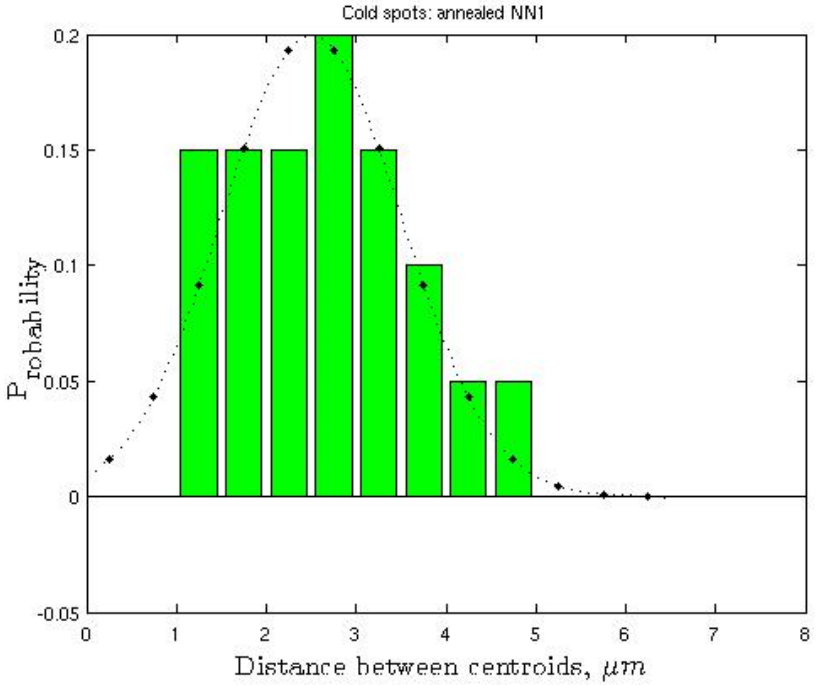
ENN1 (random) = 0.4151

ENN1 (annealed) = 0.1679

Example: Step #3

Non-hot spot centroid annealing – nearest neighbor distribution(NN1)





ENN1 (random) = 0.3837

ENN1 (annealed) = 0.0939

Example: Step #3

Demonstration assumptions for this example:

- All grains have the same volume.
- Initial temperature, within each grain, is equal to the bulk temperature of the RVE.
- The material properties Cp, rho, kc, and dHrxn are all constant.
- The hot spot maximum temperature distribution is constant.
- Loading is simulated by linearly varying the bulk temperature and the number of hot spots.
- There is no correlations between crystal temperature and the NN1 distribution.
- The RVE is adiabatic, and it has symmetric boundary conditions.

Example: Step #3

- (Right) Temperature contour on one face of the RVE cube at 300 microseconds.
- Periodic boundary conditions.

Run time = 300 microseconds

$\mu_{(T,hs)}$(avg) = $800\ K$

$\mu_{(T,bulk)}$(avg) = $522\ to\ 625\ K$

$\sigma_{(T,hs)}$(avg) = $100\ K$

$\sigma_{(T,cs)}$(avg) = $100\ K$

CFL = 0.6

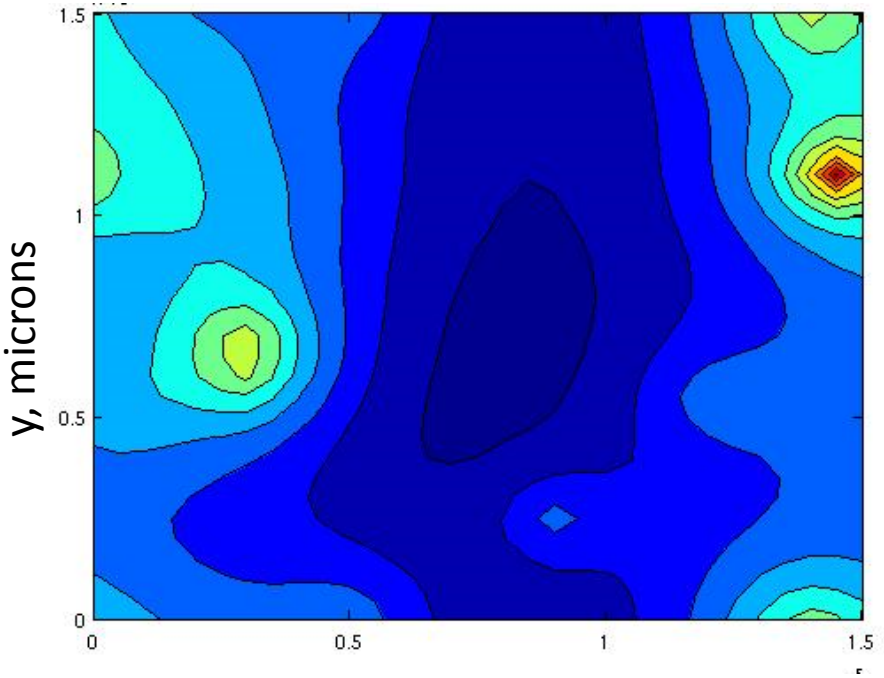
kc (conductivity) = 0.2 W/m*K

Cp = 1466 J/kg*K

Rho = 1180 kg/m^3

dHrxn (heat of reaction) = 2.0e9 J/m^3

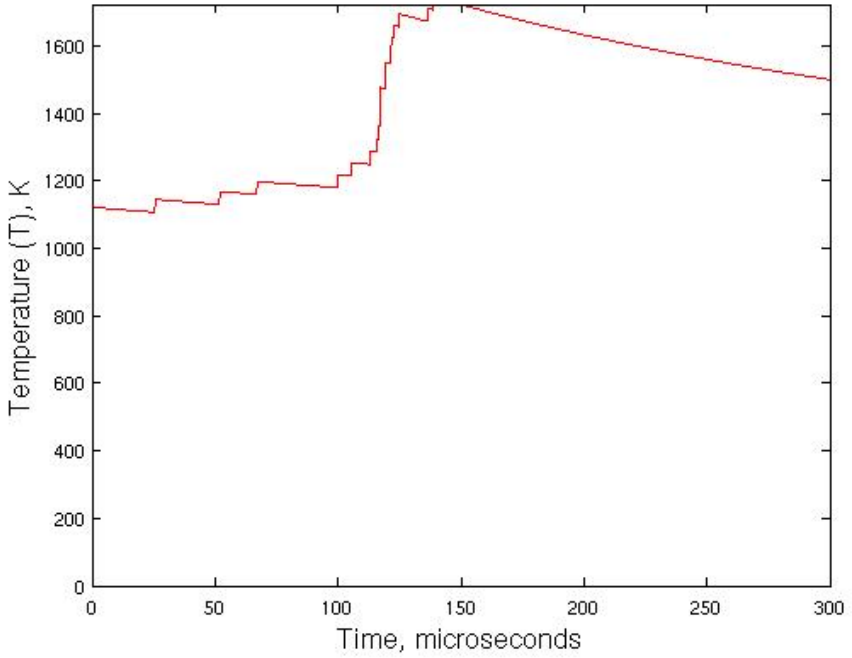
$T_{critical}$ = 700 K (crystal ignition criterion



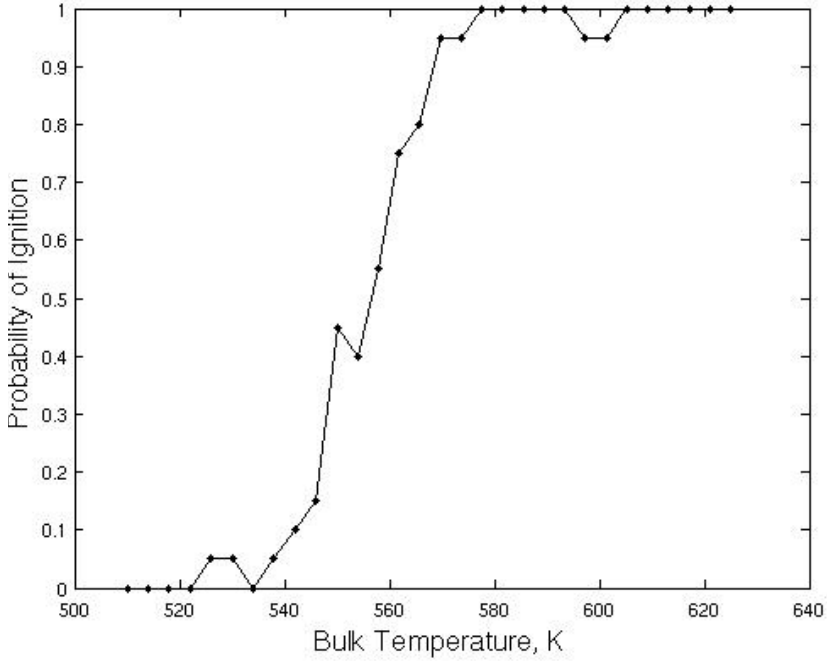
Example: Steps #4-5

- A single loading condition shows the average crystal temperature, not the bulk RVE temperature.
- 20 realizations for each loading condition.
- Threshold is approximately 530 to 580 K (50 degree range)

Average crystal temperature



Ignition threshold



Summary

- Can generate meshes from XCMT
- Have experimental data of mock and explosive composite
- Have carried out simulations on mechanical RVE's from XCMT and idealized
- Developed and demonstrated thermal ignition predictive approach

Future Work

- Develop approaches for extracting data from FEM to feed thermal ignition code
- Improve temperature computation approach in FEM
- Implement better thermal-reactive modeling
- Quantify the range of validity using experiments

Related Efforts

- SBIR's
  - Phase 2 PENETRATION SURVIVABLE ADVANCED ENERGETIC
  - Symmetrix
  - Streamline
  - Illinois RocStar
- STTR's
  - Phase I with Multiscale Design
  - Topic on NDE for low density gradient materials
- Los Alamos NL
- Should soon have a signed Project Agreement with Germany
- Udaykumar of University of Iowa

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