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Title: "Direct Numerical Simulations of Cemented Aggregates"

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Direct Numerical Simulations of Cemented Aggregates

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High Explosives (HE) are cemented aggregates that are endowed with constituents that exhibit complex behavior. In engineering applications these materials are treated as homogeneous, and having the behavior described by phenomenological models. In these macroscopic approaches, the material response is captured only in an average sense and important local phenomena are missing. To address the issues a Direct Numerical Simulation (DNS) approach using the Finite Element Method (FEM) is suggested. The HE microstructure is modeled here as randomly packed grains of different shapes and sizes and placed into a rate dependent matrix. The emphasis is focused on the micro-fractures occurring in the viscous matrix. For this reason, we have developed and included in the analysis a constitutive model capturing fracture process under complex loading scenarios. Our long term objective is to study the contribution of randomness in the microstructural arrangements and predict statistical distributions of the relevant damage/fracture mechanisms.

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Direct Numerical Simulations of Cemented Aggregates

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Funded by DOE/DoD Joint Munitions Program

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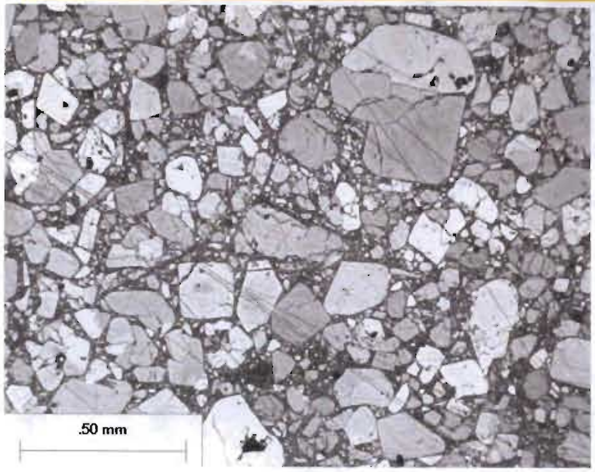
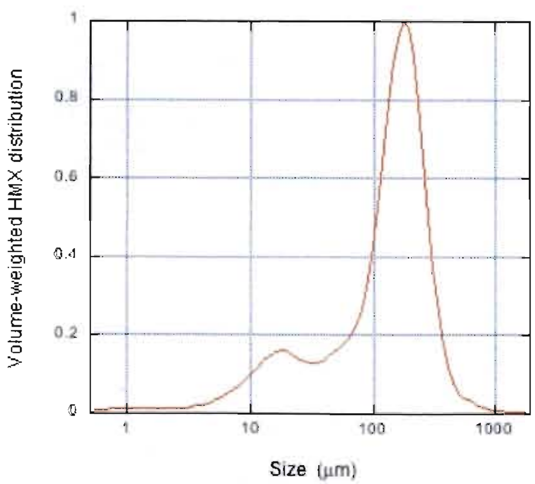
Direct Numerical Simulations for HE



Micrograph of PBX9501 (f_H=0.93)



HMX grains size distribution

- High explosives (HE) are highly dense cemented aggregates materials (f_H>0.9) having a micro-structure with constituents that are described by complex constitutive models (rate and temperature dependence, complex damage behavior, *etc*.).

- Modeling:
  - Homogeneous (Phenomenological) Models.
  - Heterogeneous Models (Two-Scale, DNS).

- Heterogeneous models are based on the Representative Volume Element (RVE) concept.

- DNS objective:
  - To understand the complex mechanical behavior at the RVE and sub-RVE scale.
  - For development of constitutive laws for HE materials used in engineering applications.

A Two-Dimensional Approach

- The heterogeneous material (PBX9501) is represented at the RVE level as a distribution of large (HMX) grains in a homogenized viscoelastic matrix.

$$\mathrm{div}\,\sigma = \rho\dot{v} \qquad \dot{\varepsilon} = \frac{1}{2}\left[\nabla v + (\nabla v)^T\right]$$

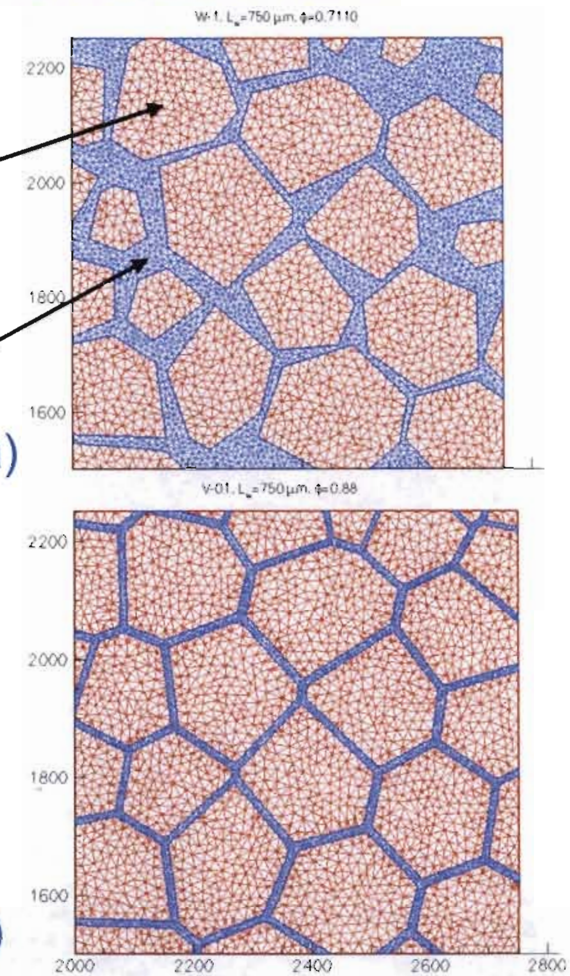
$$\overset{\circ}{\sigma} = C\left(\dot{\varepsilon} - \dot{\varepsilon}^p\right), \quad \dot{\varepsilon}^p = f(\sigma, \dot{\sigma}, ..)$$

$$\sigma(t) = \int_0^t K^*(t-\tau)\dot{\varepsilon}_V(\tau)\,d\tau + \int_0^t 2\mu^*(t-\tau)\dot{\varepsilon}_S(\tau)\,d\tau$$

(HMX)

(DB)

(a)



(b)

- The FEM explicit semidiscrete formulation

$$\begin{cases} \mathbf{M}\dot{\mathbf{v}} = \mathbf{F}^{\mathrm{ext}} - \mathbf{F}^{\mathrm{int}}(\sigma) \\ \dot{\mathbf{u}} = \mathbf{v} \end{cases}$$

- Two RVE models for HE:

  (a) Polygons, (b) Voronoi Cells

Homogenized Viscoelastic Matrix (DB)

- The small HMX particles and the binder are modeled as homogeneous viscoelastic matrix ("dirty binder" DB).

$$\sigma(t)=\int_0^t K^*(t-\tau)\dot{\varepsilon}_V(\tau)d\tau+\int_0^t 2\mu^*(t-\tau)\dot{\varepsilon}_S(\tau)d\tau$$

$$K^*(t)=K_0^*+\sum_{m=1}^{M}K_m^* e^{-t/\tau_m} \qquad \mu^*(t)=\mu_0^*+\sum_{m=1}^{M}\mu_m^* e^{-t/\tau_m}$$

$$K_m^*=\begin{cases}\dfrac{K_B K_{HMX}}{c_{HMX}K_B+c_B K_{HMX}}, & m=0\\[2ex] \dfrac{4c_{HMX}c_B\left(K_{HMX}-K\right)^2}{3\left(c_{HMX}K_B+c_B K_{HMX}\right)^2}\mu_0^m(t), & m\neq 0\end{cases} \qquad \mu_m^*=\begin{cases}0, & m=0\\[2ex] \left(1+2.5\dfrac{c_{HMX}}{1-fc_{HMX}}\right)\mu_0^m & m\neq 0\end{cases}$$

Failure criterion

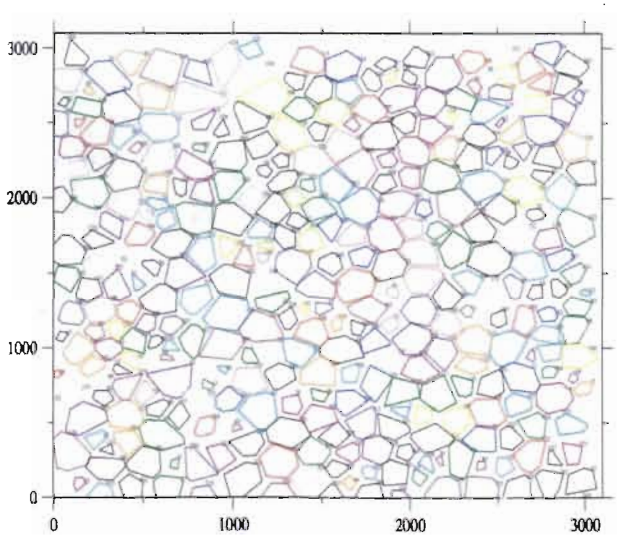
$$F(\varepsilon_1,\varepsilon_f)=1-\frac{\langle\varepsilon_1\rangle}{\varepsilon_f(x)}, \qquad \langle\varepsilon_1\rangle=\begin{cases}\varepsilon_1, & \varepsilon_1>0\\ 0, & \varepsilon_1<0\end{cases}$$

- At low rates the matrix DB is quasi-incompressible.
- At high rates the matrix DB becomes compressible.
- In the FEM special attention needs to be taken in evaluating the pressure term in the stress components.
- A damage model combined with a failure criterion can be introduced.

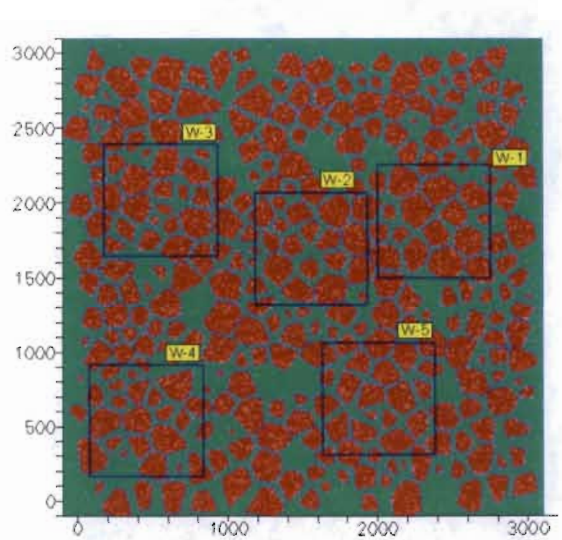
(B.E. Clements, E. M. Mas, J. Appl. Phys. 90,11, 2001)

2D-DNS RVE Models

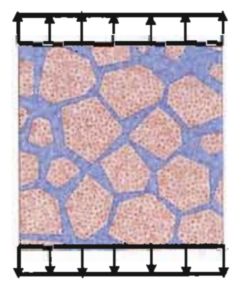
- Large domain filled with polygons (70%) simulating large HMX grains (a).
- Selection of five windows representing an RVE (b,c).
- Additional RVEs were build using the same windows position but a polygonal configuration resulted from a Voronoi discretization (88%) (d).
- The analyses were performed under plain strain condition using EPIC (explicit, lagrangian FEM code) with a user material subroutine and additional procedures for pressure calculation, explicit cracks formation and autocontact.



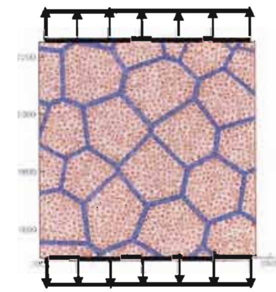
(a)



(b)



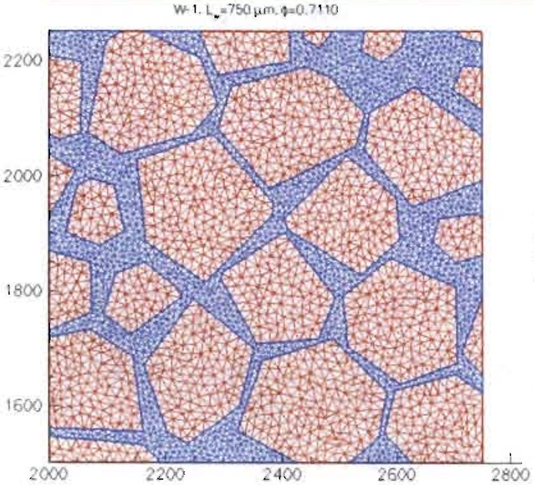
(c)

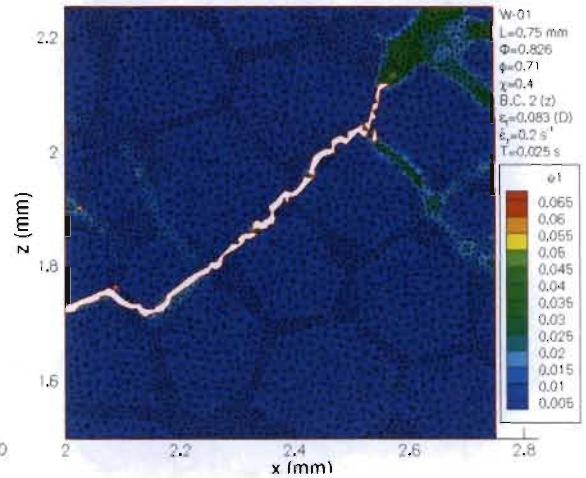


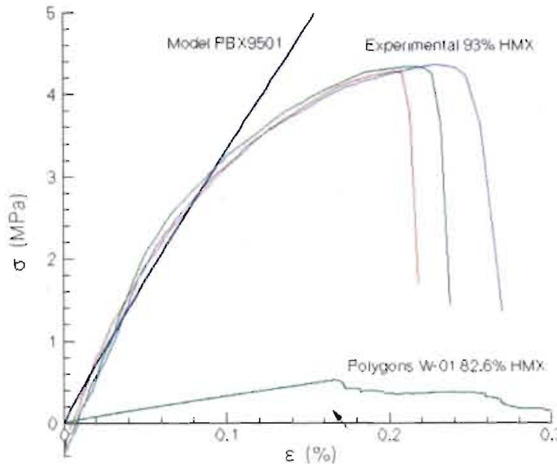
(d)

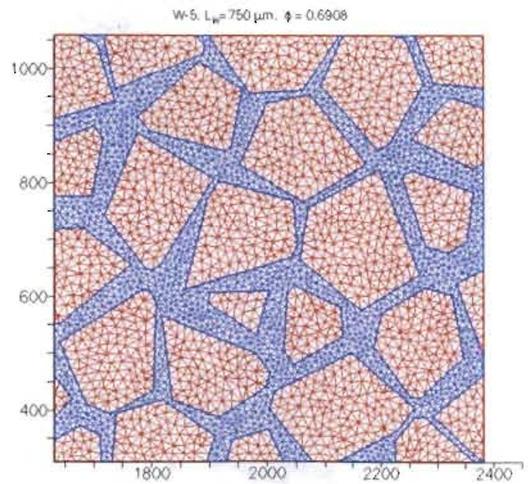
Velocity B.C.

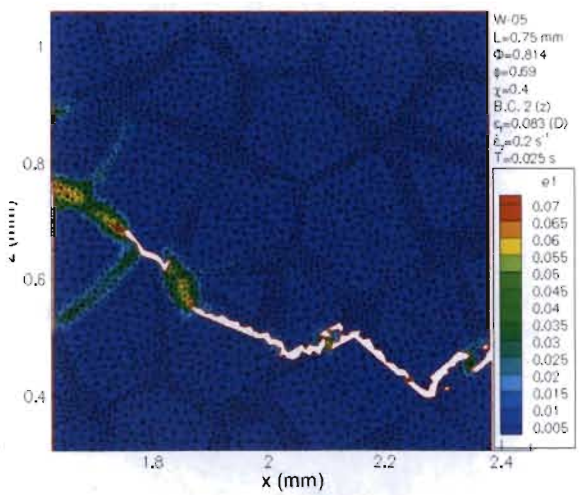
2D-DNS Results using Polygons

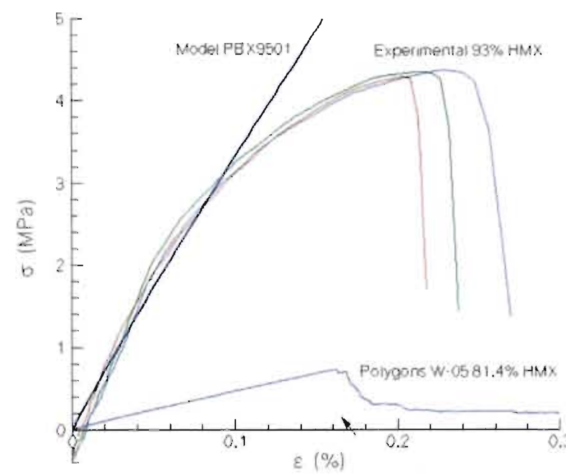












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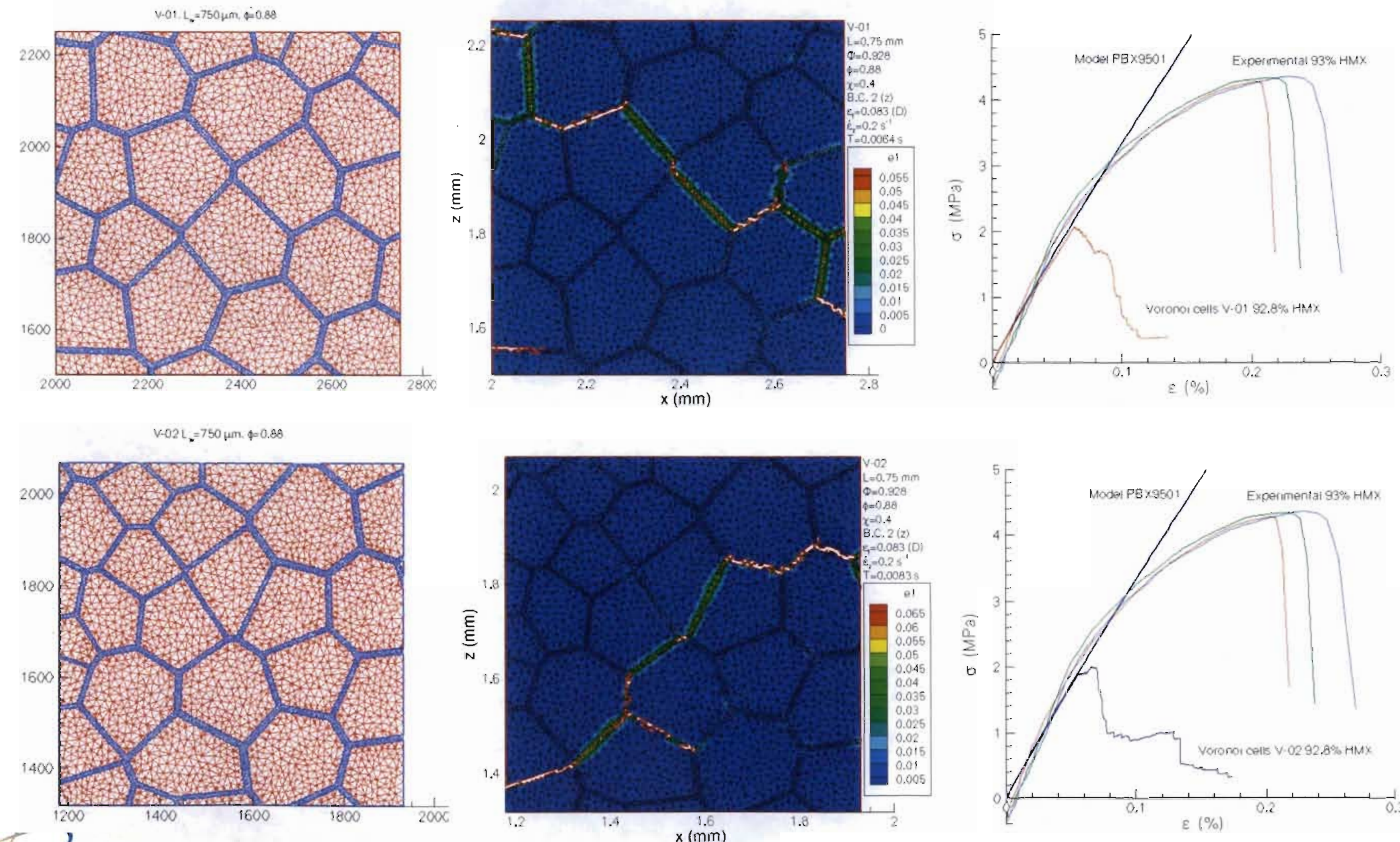
2D-DNS Results using Voronoi Cells



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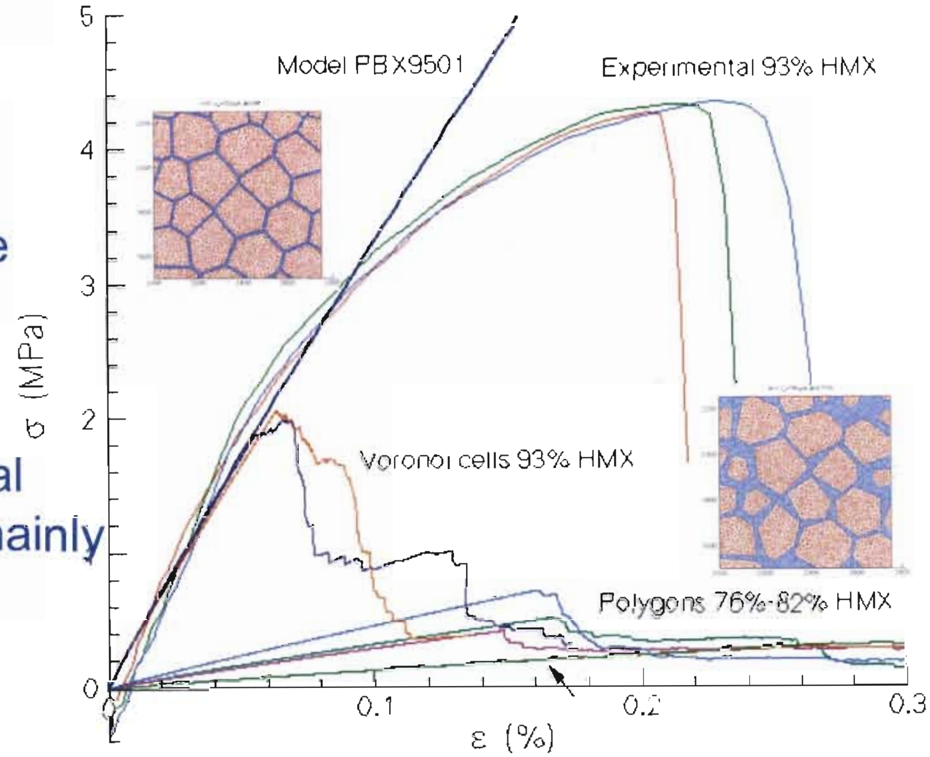
2D-DNS (PBX9501) Global Stress-Strain

- HMX fill fraction plays a very important role in obtaining correct the initial slope (undamaged) of the stress-strain curve.

- The Voronoi cells achieve the required fill fraction (93%) and predicts correctly the initial slope of the stress-strain curve which agree with experiments and the homogeneous model.

- The differences between the experimental data and the numerical simulations are mainly due to the absence of a damage model prior to the explicit cracks formations.



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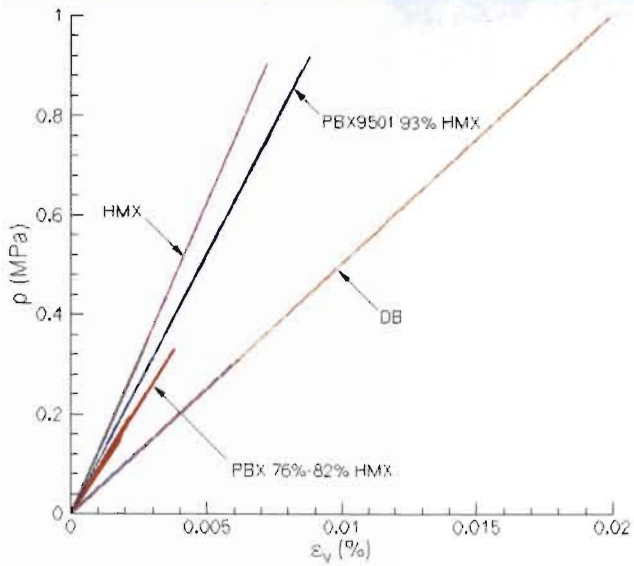
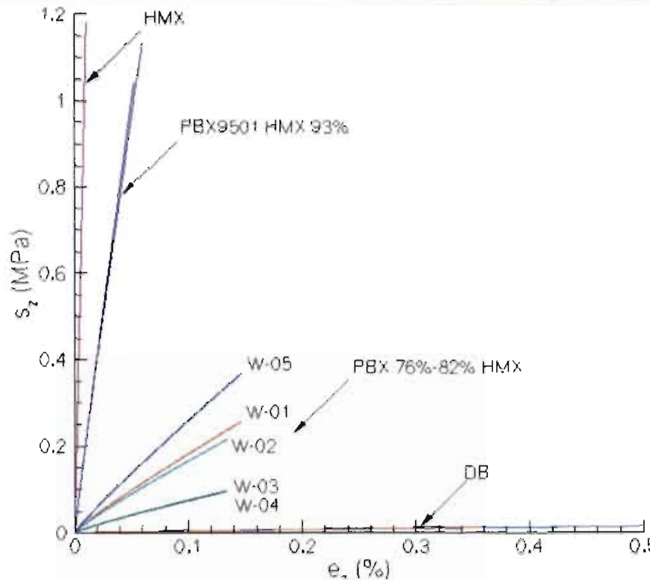
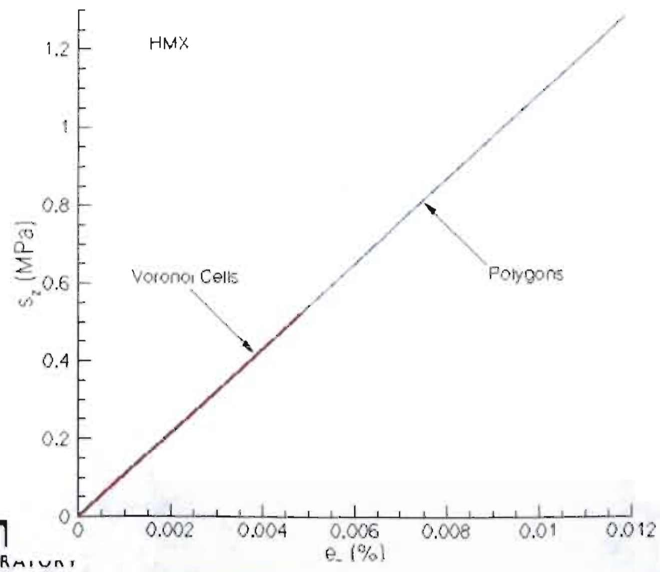
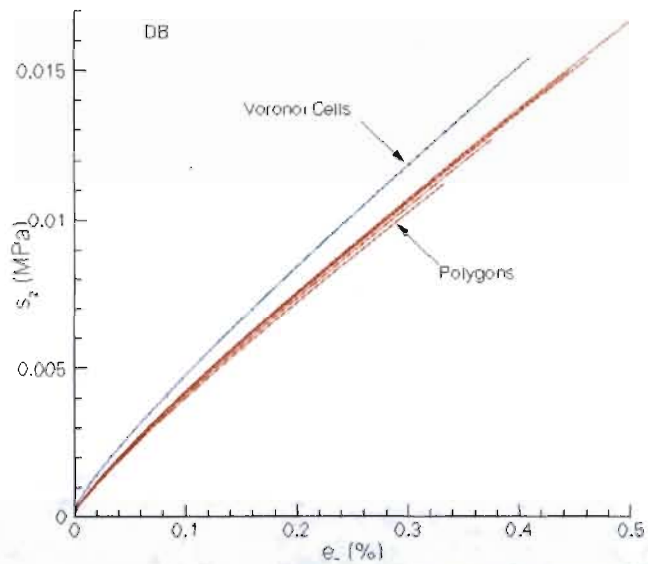
Pressure and Deviatoric Stress

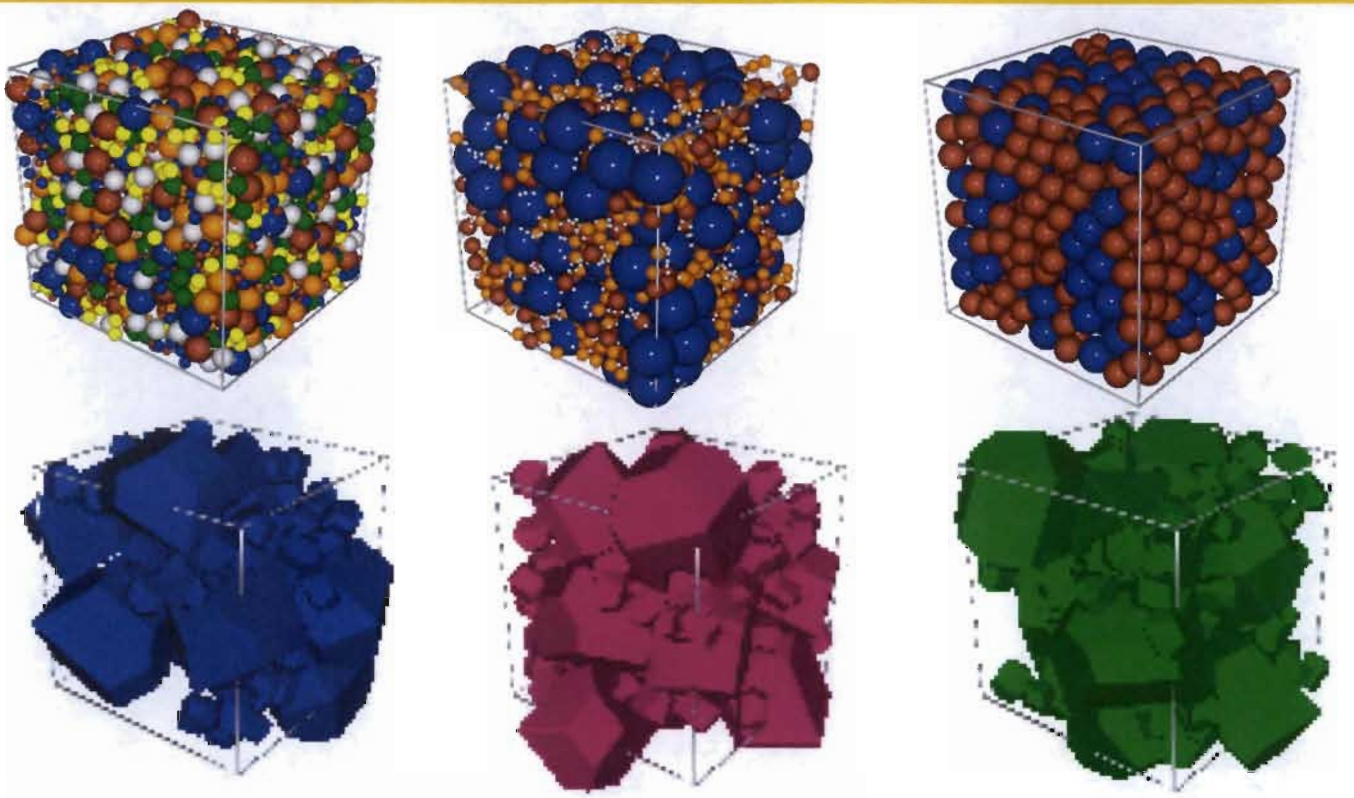








A Three-Dimensional Approach



$\phi_H \approx 0.66$

Different RVE using spheres and crystals*

$\phi_H \approx 0.73$

- DB model for the matrix can be used only up to f_{DB}=0.4 HMX volume fraction. For PBX9501 this requires f_H=0.88 in the crystals volume fraction.
- Difficult to obtain high HMX density from packing only.
- An alternative is to use a phenomenological model.

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*Packing code provided by Dr. Thomas Jackson (Univ. of Illinois at Urbana-Champaign)

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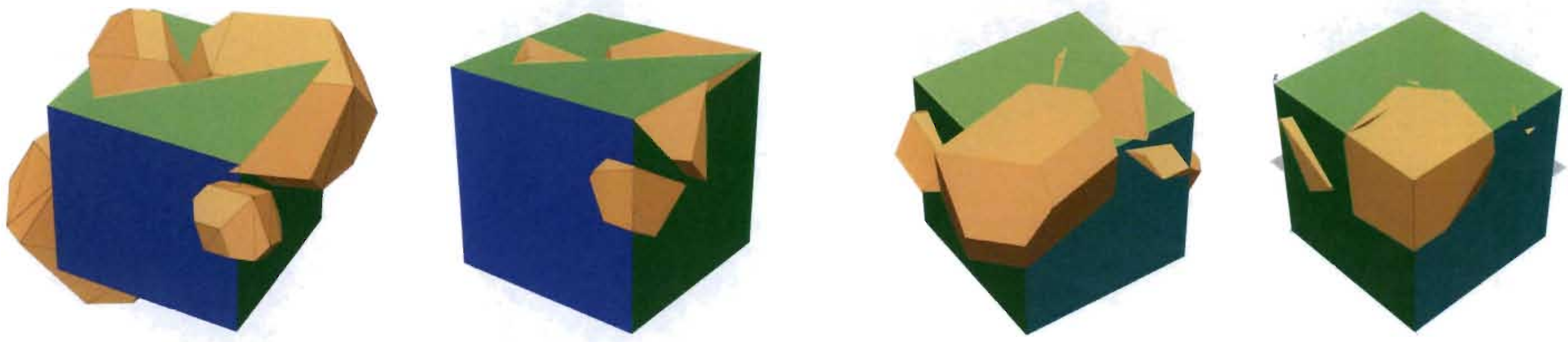
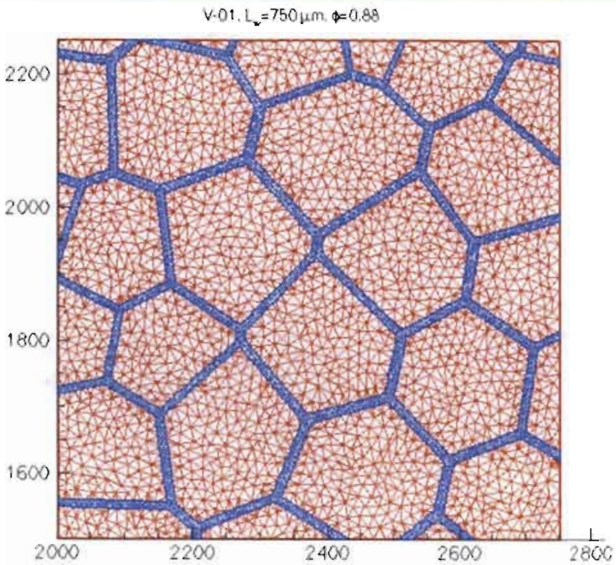
Grains-RVE Intersection

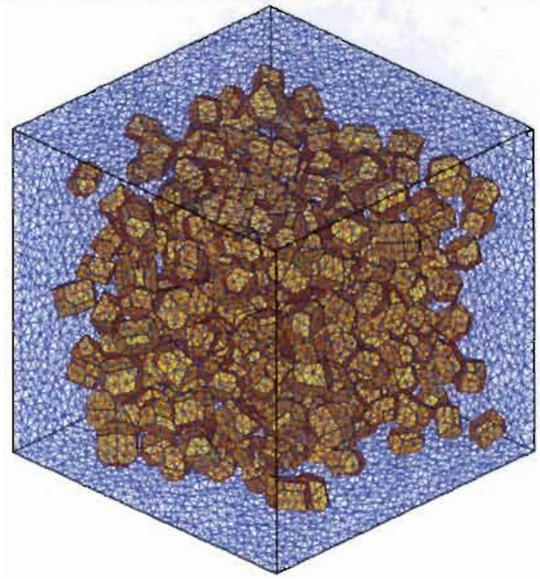


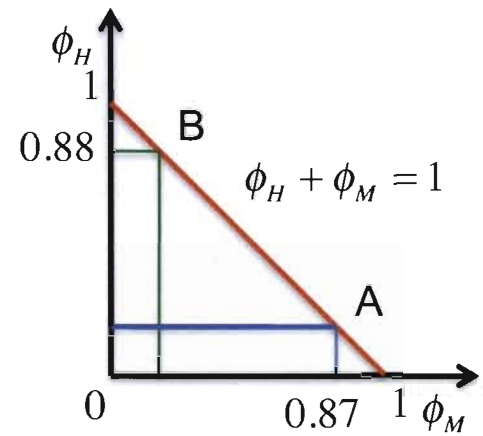
Grains intersecting RVE (a), (c). Resulted geometry after intersection (b), (d).

- For the FEM analysis only the grains inside the RVE (cube) are selected.
- The grains-RVE intersection is performed using a specific library.
- Grains are represented as a convex polyhedrons resulted from the intersection of all half-spaces corresponding to each face of the polyhedron.
- Resulted domain after the intersection is obtained as convex polyhedron reconstruction from the intersection points.
- Meshing is performed using tetrahedrons

Two DNS-RVE Models







$$\phi_{HMX} = \phi_H + (1-\phi_H)\phi_{DB}$$

(B) $\phi_H \approx 0.88$

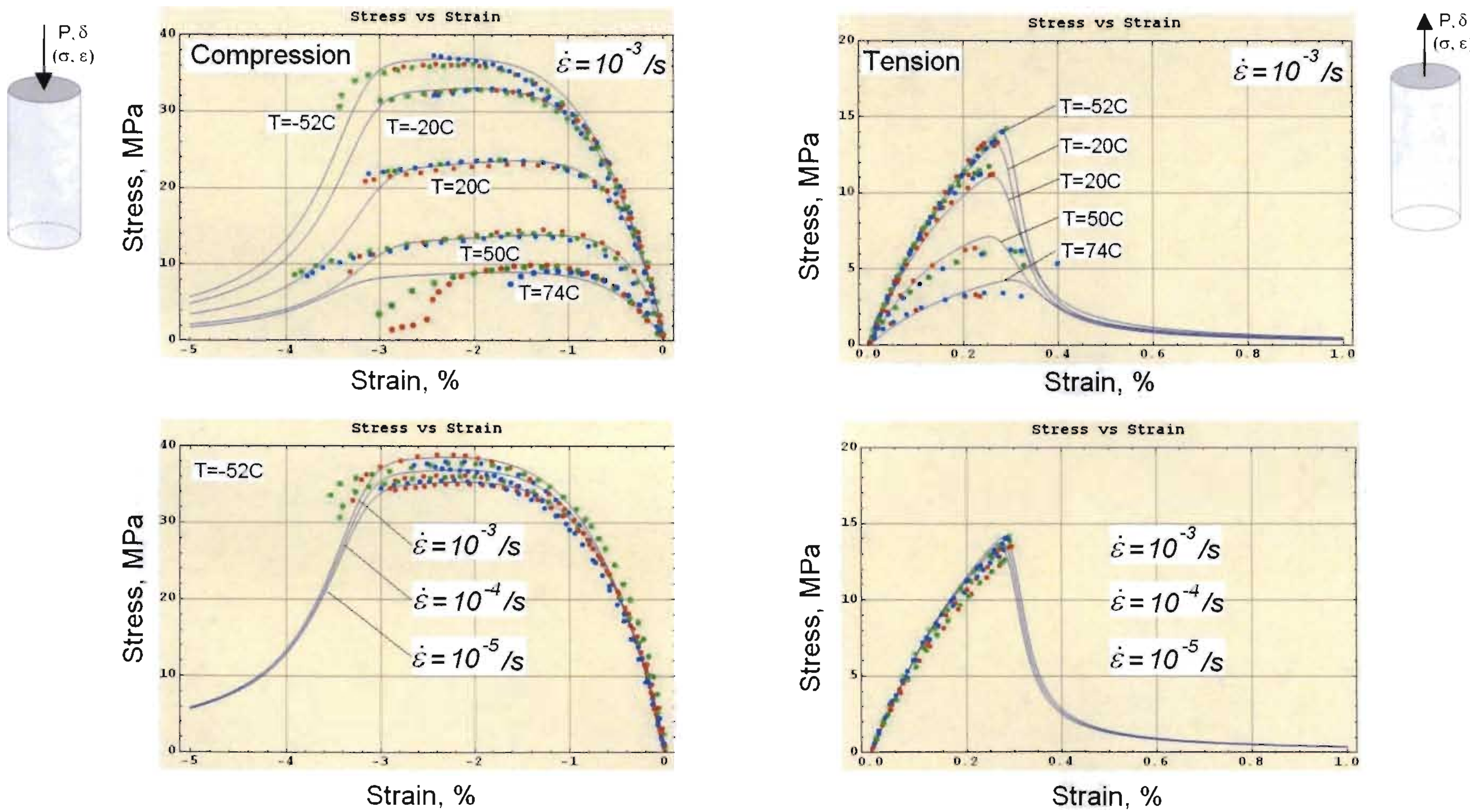
$$\phi^B_{HMX} = 0.88 + (1-0.88)\times 0.4 \approx 0.93$$

(A) $\phi_H \approx 0.13$

$$\phi^A_{HMX} = 0.13 + (1-0.13)\times 0.92 \approx 0.93$$

- The approach (B) can be extended to 3D Voronoi cells.
- In the case (A) one use a homogenized phenomenological model for the matrix.
- The two DNS-RVE (A) and (B) are complementary.
- DNS-(B) for local grain-binder interactions.
- DNS-(A) for global RVE response.

PBX9502: Model calibration



Experimental data (dots) by Darla Thompson

(Alek Zubelewicz: alek@lanl.gov)

FRAZ Fundamental Structure for HE materials
Elasticity with Embedded Fracture

Hyper-elasticity: $\sigma_{ij} = \partial F / \partial \varepsilon_{ij}^{e} = C_{ij\,kl}^{f}\, \varepsilon_{ij}^{e}$

Strain rate additivity: $\dot{\varepsilon}_{ij}^{t} = \dot{\varepsilon}_{ij}^{e} + \underline{\dot{\varepsilon}_{ij}^{s} + \dot{\varepsilon}_{ij}^{b}}$

Fracture tensors: $n_i n_j = \left(n_i n_j\right)_{(t,c)}^{\sigma}$

Elastic-fracture mechanism: $\eta = \eta_1 = \eta_2$

$\dot{\varepsilon}_{ij}^{e}$ – Elastic (reversible)

$\dot{\varepsilon}_{ij}^{s}$ – Mises-Schleicher plastic (load chains)

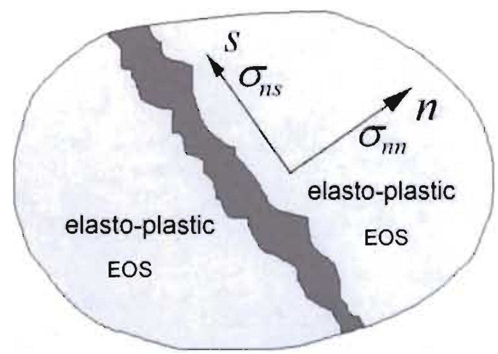
$\dot{\varepsilon}_{ij}^{b}$ – Inelastic strain in binder (outside load chains)

$$B(T,\rho)\ ,\ \ \mu(T,\dot{\varepsilon},\rho)$$

$$C_{ij\,kl}^{f} = C_{ij\,kl}^{f}\left[B, \mu, \eta_{t,c}, \left(n_i n_j\right)_{t,c}\right]$$

$(n_i)_{t,c}$ – Crack orientation

$\eta_{t,c}$ – Damage (0 to 1)



(Alek Zubelewicz: alek@lanl.gov)

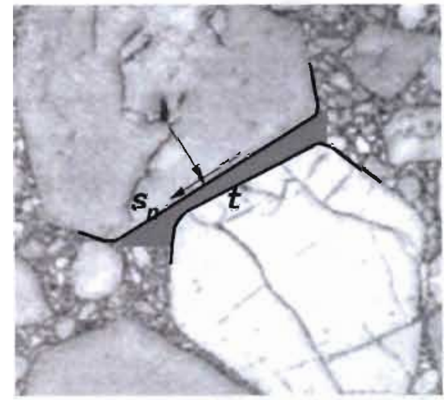
Visco-Plasticity: Deformation along Load Chains

Mises-Schleicher strain rates:

$$\dot{e}^t_{norm} = \frac{1}{2}\sqrt{\dot{\varepsilon}^t_{ij}\dot{\varepsilon}^t_{ij}}$$

Flow tensor: $$M^s_{ij} = \underbrace{\frac{\sqrt{3}\, S_{ij}}{\sqrt{J_2^\sigma}}}_{\text{shear}} + \underbrace{q\ \delta_{ij}}_{\text{dilatation}}$$

$$\dot{\varepsilon}^s_{ij} = \frac{1}{2} M^s_{ij}\, \dot{e}^s_{eq} \quad , \quad \dot{e}^s_{eq} = \Lambda_s \left(\frac{\sigma_{eq}}{\sigma_s}\right)^1 \quad , \quad \Lambda_s = \left(\dot{e}_s + \dot{e}^t_{norm}\right)^{\omega_s}$$

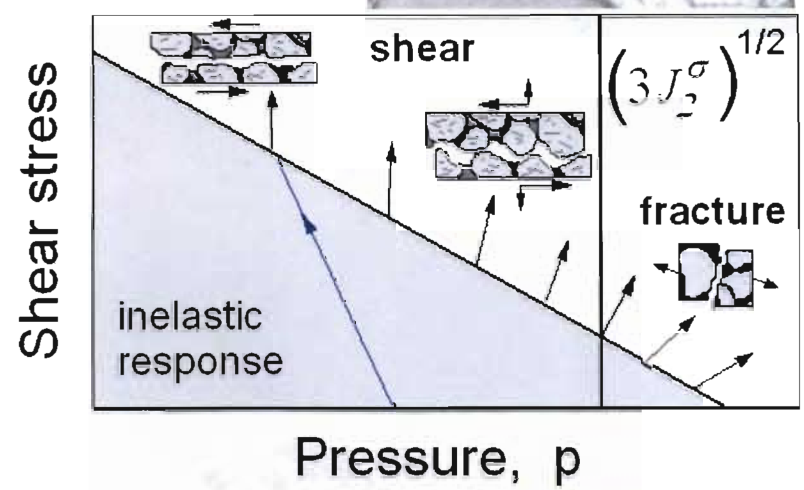


Invariance: $$\sigma_{ij}\ \dot{\varepsilon}^s_{ij} = \left(\frac{1}{2}\sigma_{ij}\ M^s_{ij}\right)\dot{e}^s_{eq} = \left(\sqrt{3J_2^\sigma} + \frac{3\,q\,p}{2}\right)\dot{e}^s_{eq}$$

Equivalent stress $$\sigma_{eq} = \frac{1}{2} M^s_{ij}\, s_{ij} = \sqrt{3J_2^\sigma} + \frac{3\,q\,p}{2}$$

Parameters: $\sigma_{tensile} / \sigma_{compressive}$

q - rate dependence
ω_s -
σ_s - strength



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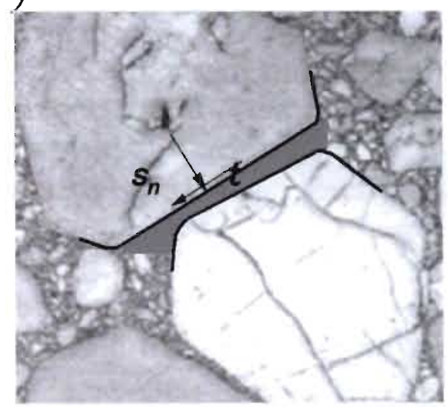
Von Mises Deformation in Binder outside Load Chains

Mises strain rates in inelastic binder:

Flow tensor:

$$M_{ij}^{b} = \underbrace{\frac{\sqrt{3}\,S_{ij}}{\sqrt{J_2^{\sigma}}}}_{\text{shear}} \quad \Rightarrow \quad \dot{\varepsilon}_{ij}^{b} = \frac{1}{2} M_{ij}^{b}\,\dot{e}_{eq}^{b} \quad , \quad \dot{e}_{eq}^{b} = \Lambda_s \left(\frac{\sigma_{eq}}{\sigma_b} \right)^{1} \quad , \quad \Lambda_b = \left(\dot{e}_b + \dot{e}_{norm}^{t} \right)^{\omega_b}$$



Measure invariance:

$$\sigma_{ij}\,\dot{\varepsilon}_{ij}^{b} = \left(\frac{1}{2} \sigma_{ij}\, M_{ij}^{b} \right) \dot{e}_{eq}^{b} = \sqrt{3J_2^{\sigma}}\;\dot{e}_{eq}^{s}$$

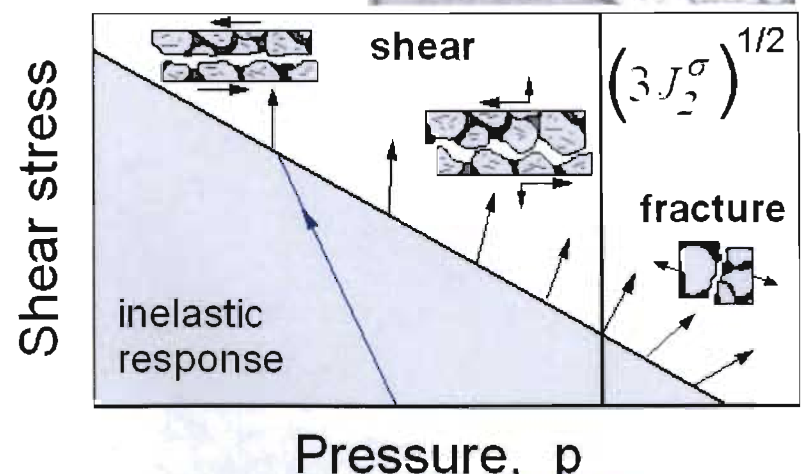
Equivalent stress

$$\sigma_{eq} = \frac{1}{2} M_{ij}^{b}\,\sigma_{ij} = \sqrt{3J_2^{\sigma}}$$

Parameters:

ω_b - rate dependence

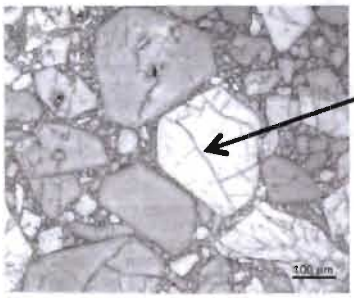
σ_b - strength



(Alek Zubelewicz: alek@lanl.gov)

Complete Set of 9 Parameters/Variables

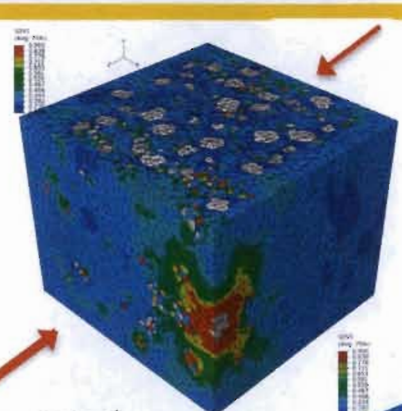
Set of 9 parameters/variables	
Elastic constants	$B(T) \quad \mu(T, \dot{e}^{t}_{norm})$
Internal friction Strengths	q $\sigma_s(T) \quad \sigma_b(T)$
Strain rate dependence: Load chains Binder	 ω_s ω_b
Manufacturing and stress induced damage: Tensile Compressive	$\eta_t(T, e^{s}_{eq}, \varepsilon^{t}_{nn}, \dot{e}^{t}_{norm})$ $\eta_c(T, e^{s}_{eq}, \varepsilon^{s}_{kk}, \dot{e}^{t}_{norm})$

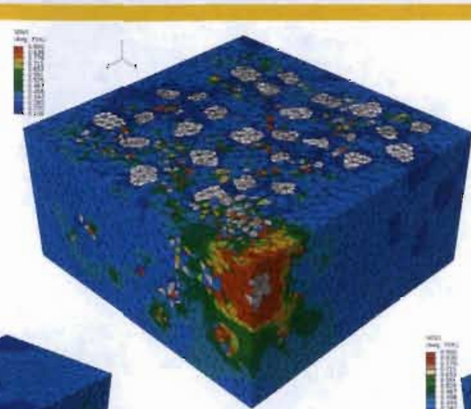


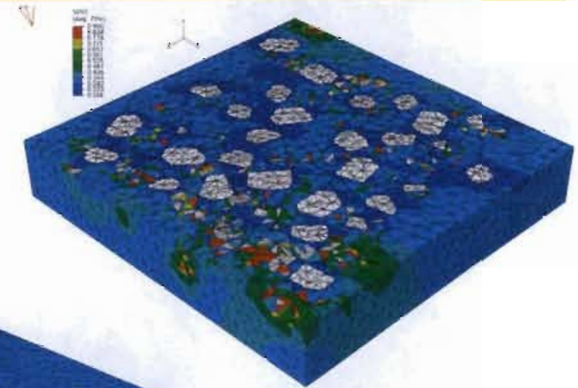
Pre-existing cracks

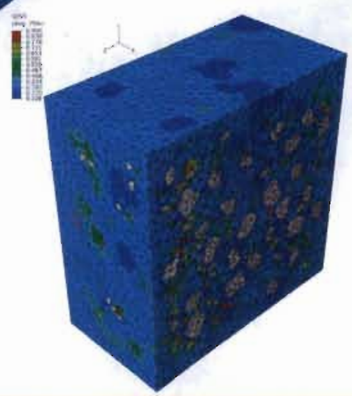
(Alek Zubelewicz: alek@lanl.gov)

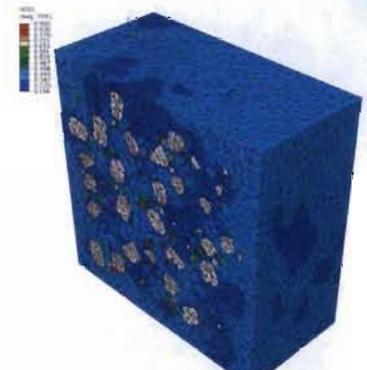
3D-DNS-(A) Results







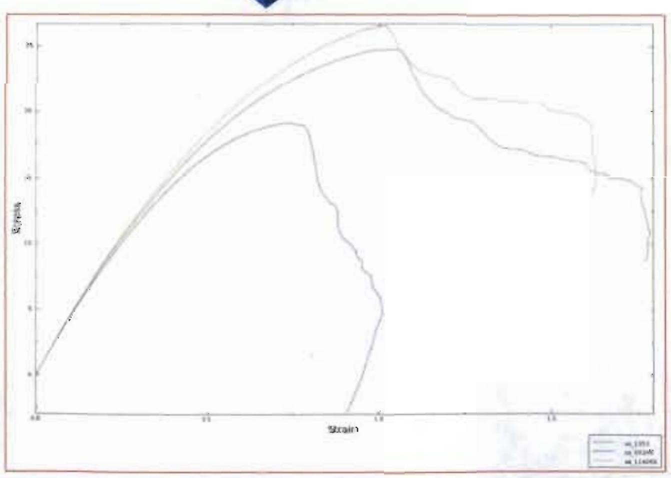




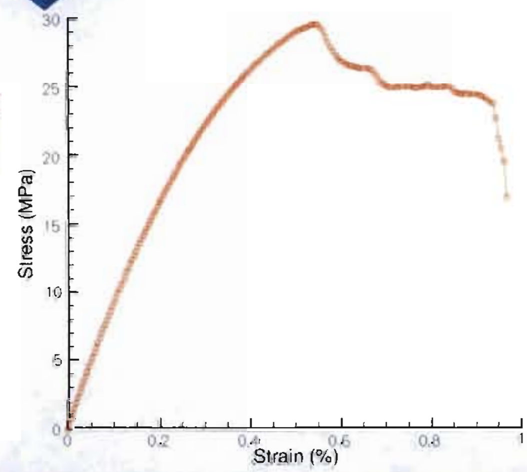
$\dot{\varepsilon}_z = \text{const.}$

Compressive damage plot

Local (element) stress-strain in the z-direction



Global (RVE) stress-strain in the z-direction



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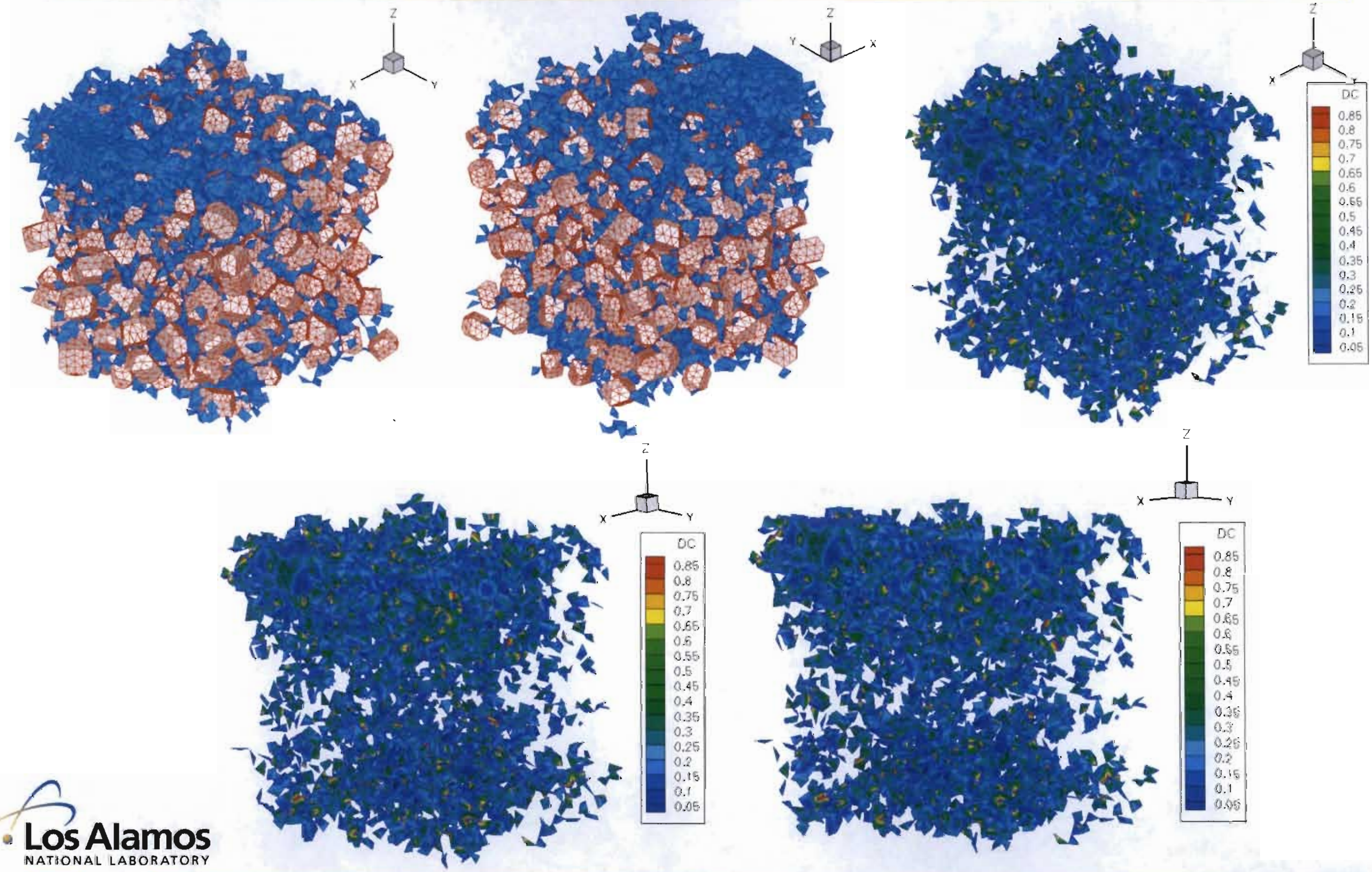
3D-DNS-(A) Failed Elements Distribution



Conclusions

- Direct Numerical Simulation (DNS) can be used to determine the averaged response of HE materials capturing at the same time local deformation at the RVE level.
- DNS can be used to calibrate the parameters used in phenomenological models.
- Including damage (material) and failure (structural) in the DNS simulations one can obtain information about failure mechanism at the homogeneous level.
- The use of homogenized models should be considered only within their limits of applicability.
- In the FEM analysis of quasi-incompressible materials, using low order elements, the pressure term in the stress evaluation needs a special treatment.
- The two approaches presented for the case of high volume fraction depend on the availability of constitutive laws.