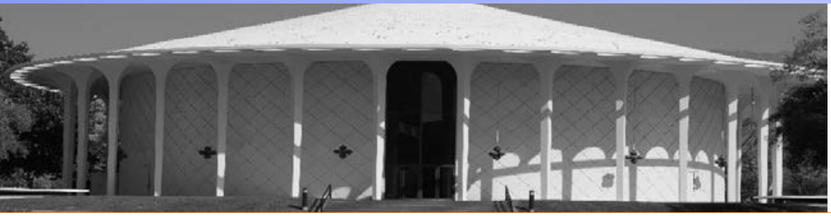


The Anomalous Elastic and Yield Behavior of Fused Silica Glass: A Variational and Multiscale Perspective

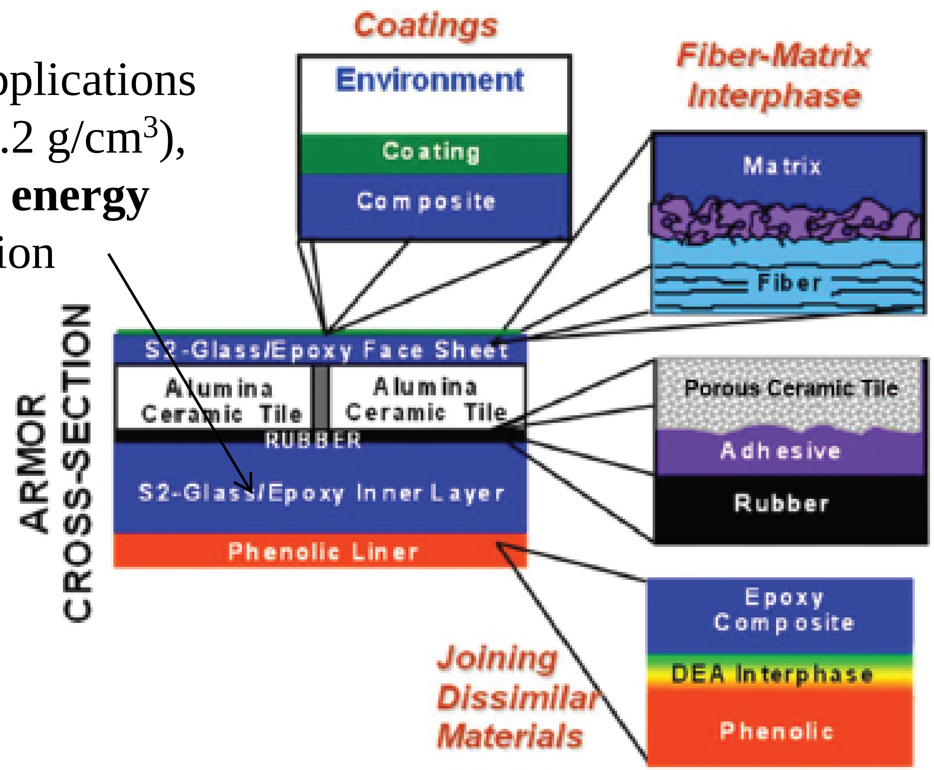
Michael Ortiz
California Institute of Technology

MEAM Seminar
School of Engineering and Applied Sciences
University of Pennsylvania

February 27, 2018

Glass as protection material

- Glass is attractive in many applications because of its **low density** (2.2 g/cm^3), **high strength** (5-6 GPa) and **energy dissipation** due to densification

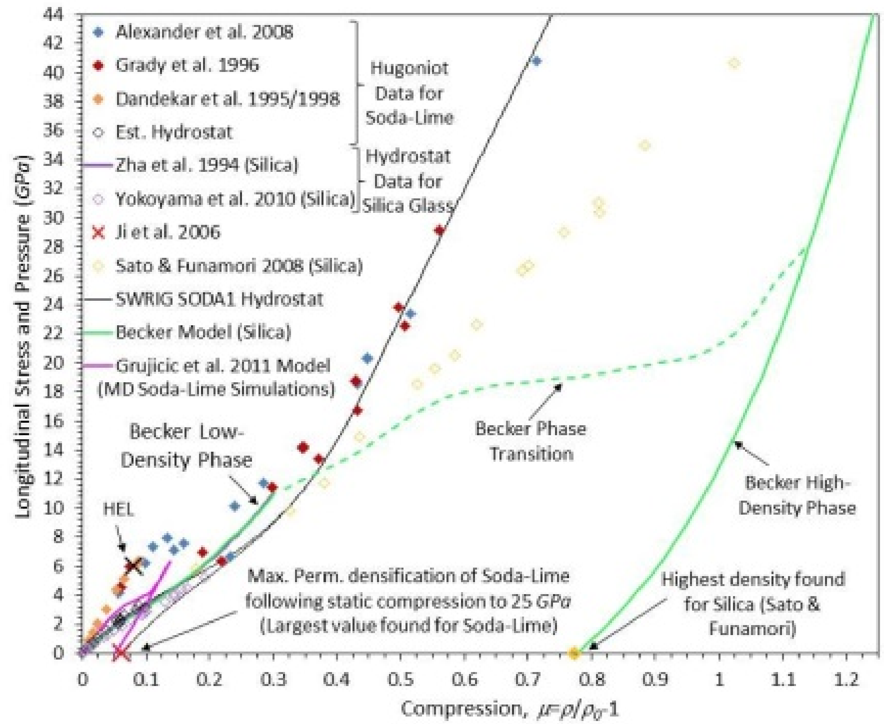


Cross section of armor tile typically used in armored vehicles showing complexity of armor architecture.

J.W. McCauley, in: *Opportunities in Protection Materials Science and Technology for Future Army Applications*, US National Research Council, 2011.

Fused silica glass: Densification

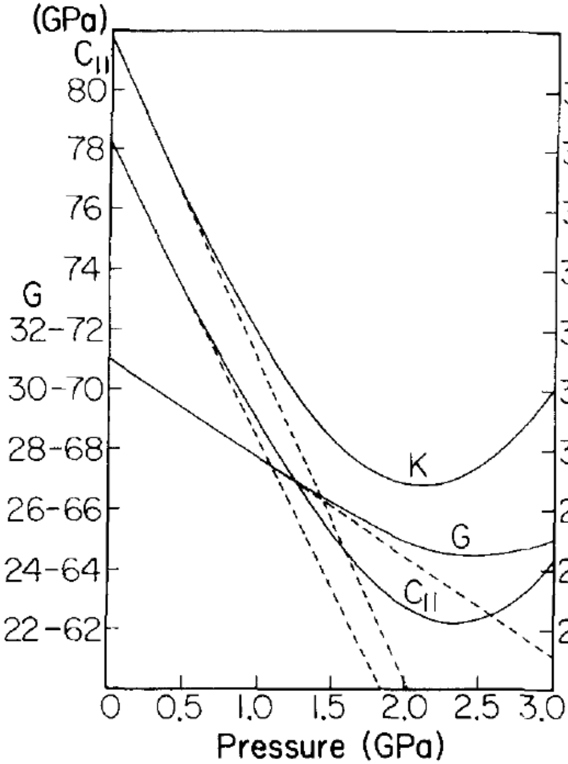
- The equation of state of glass in compression exhibits a **densification** phase transition at a pressure of 20 Gpa
- For a glass starting in its low-density phase, upon the attainment of the transition pressure the glass begins to undergo a **permanent reduction in volume**
- Reductions of up to 77% at pressures of 55 GPa have been reported
- The transformation is **irreversible**, and unloading takes place along a densified equation of state resulting in permanent volumetric deformation



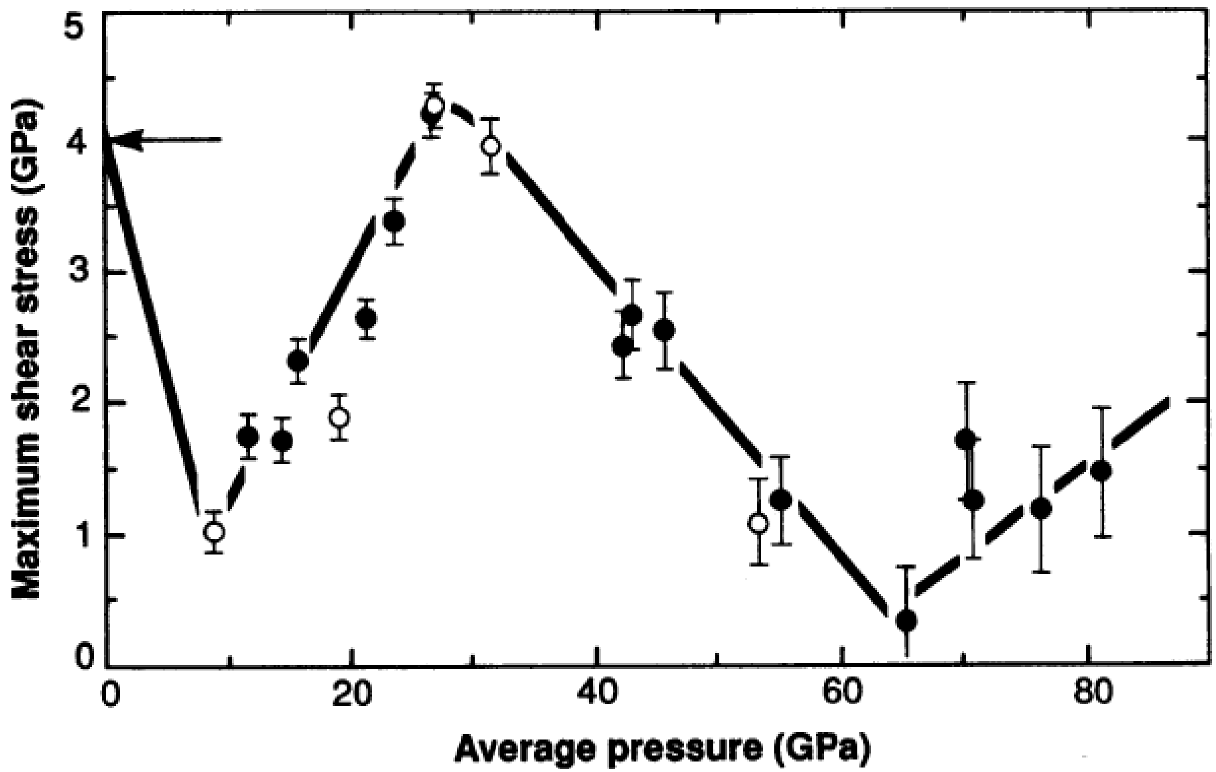
Compilation of equation-of-state data for glass (soda lime and fused silica)[1].

[1]R. Becker, *ARL Ballistics Protection Technology Workshop*, 2010.

Fused silica glass: Pressure-shear



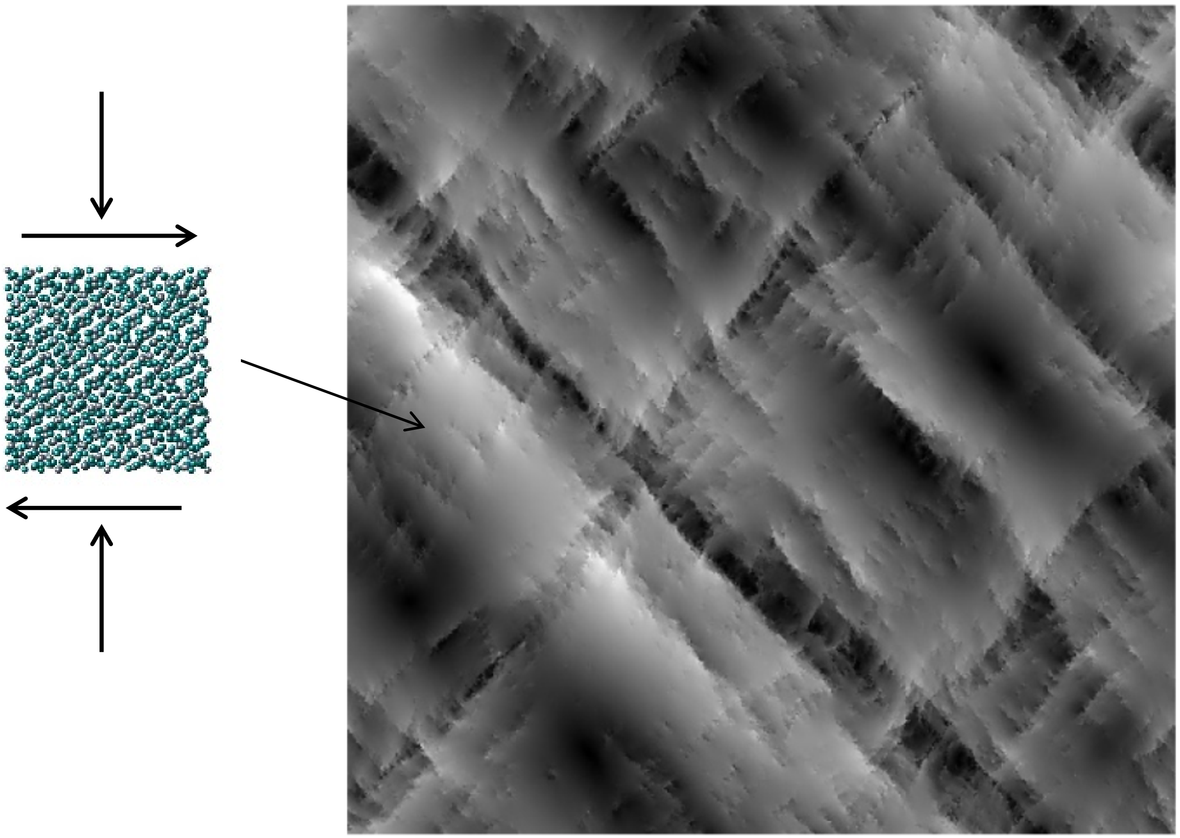
Measured elastic moduli showing *anomalous* dependence on pressure[1]



Measured shear yield stress vs. pressure showing *non-convex* dependence on pressure[2]

[1]K. Kondo, *J. Appl. Phys.*, **52**(4):2826-2831, 1981.
[2]C. Meade and R. Jeanloz, *Science*, **241**(4869):1072-1074, 1988.

Fused silica glass: Pressure-shear



Molecular Dynamics (MD) simulation of amorphous solid showing patterning of deformation field[1]

[1]C.E. Maloney and M.O. Robbins, *J. Phys.: Cond. Matter*, 20(24):244128, 2008.

Multiscale modeling approach

Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

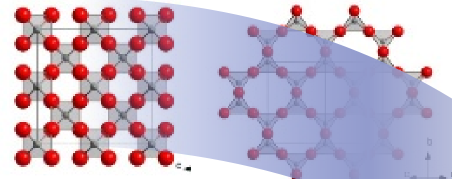
Mesoscopic modeling:

- Critical-state plasticity

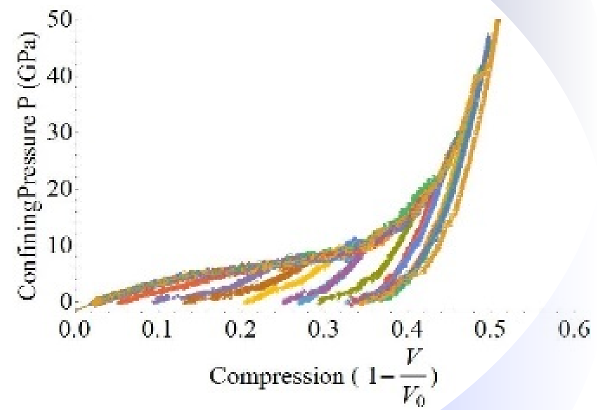
Macroscopic modeling:

- Relaxation

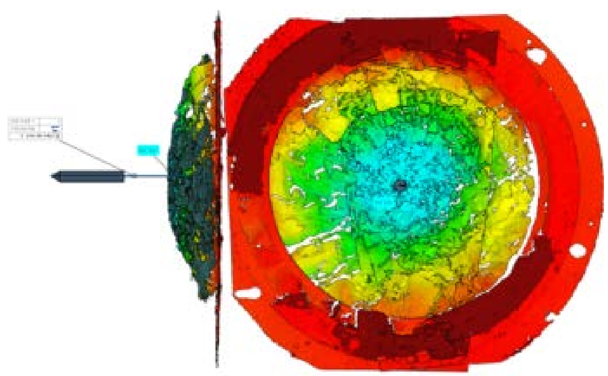
Continuum Models



Data Mining



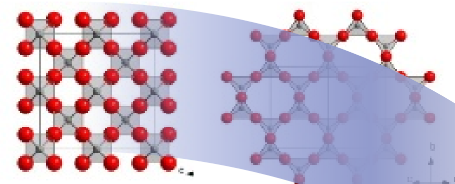
Applications



(OTM ballistic simulation of brittle target , Courtesy B. Li)

Michael Ortiz
UPEN 2018

Multiscale modeling approach



Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

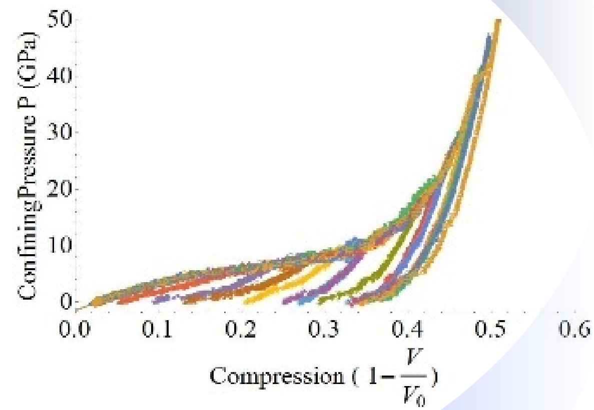
Mesoscopic modeling:

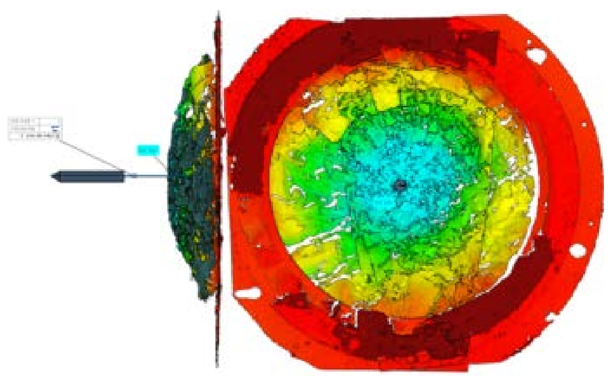
- Critical-state plasticity

Macroscopic modeling:

- Relaxation

Continuum Models





(OTM ballistic simulation of brittle target , Courtesy B. Li)

Applications

Computational model – MD

Molecular Dynamics Calculations:

- Calculations performed using **Sandia National Laboratories** (SNL) **L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator **LAMMPS** *(Plimpton S, J Comp Phys, 117(1995):1-19).*

Long-Range Coulombic Interactions:

- Summation is performed in K-space using **Ewald summation**

Short-Range Interactions:

- **BKS** Interatomic potential[1]

$$E(r_{ij}) = A\exp(-r_{ij}/\rho) - C/r_{ij}^{6} + D/r_{ij}^{12}$$

Other computational details:

- Stresses computed through virial theorem
- Strain rate ~ $1\text{x}10^{7}$ 1/s
- NVE ensemble: temperatures computed from kinetic energy
- NVT ensemble: Thermostating

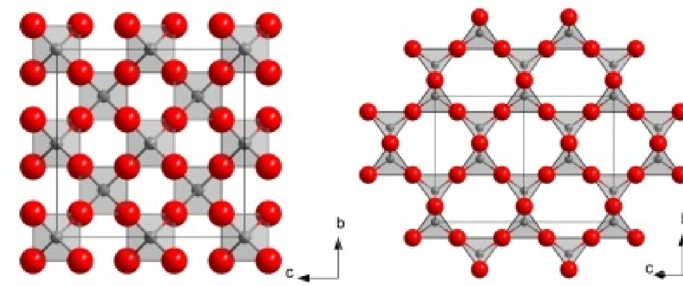
[1]Malavasi, G., Menziani, M. C., Pedone, A., Segre, U., 2006. *Journal of Non-Crystalline Solids* **352** (3), 285-296.

RVE setup – Quenching

Starting structure: β-cristobalite

β-cristobalite: Polymorph characterized by **corner-bonded SiO_4 tetrahedra**

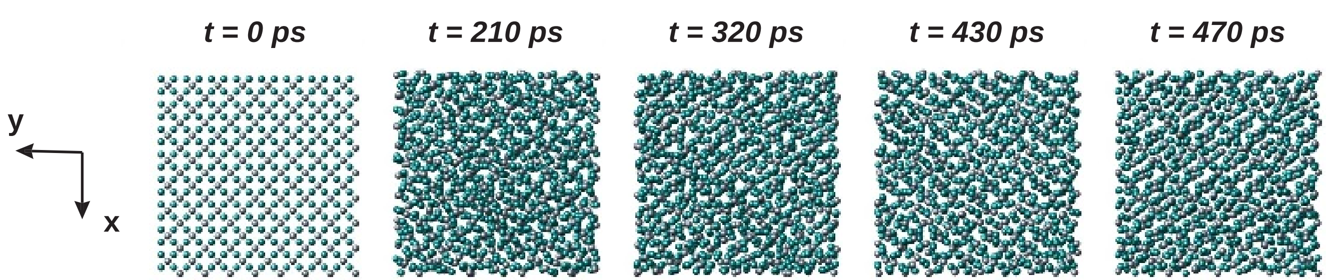
Amorphous structure of fused silica: Obtained through the **fast quenching** of a melt



Ideal structure of β-cristobalite (adapted from https://en.wikipedia.org/wiki/Cristobalite)

Steps taken during **quenching** process[1]:

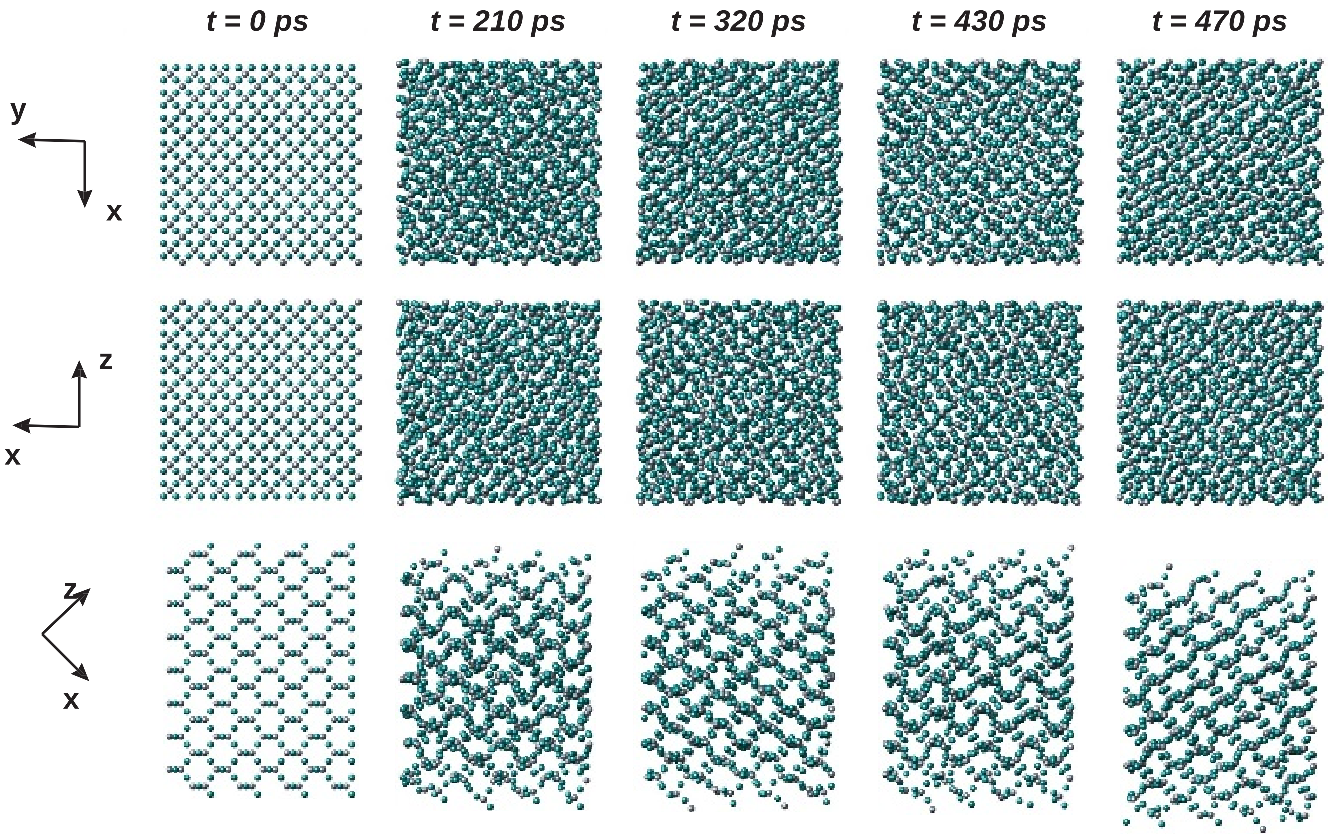
- Uniform temperature decrease from 5000 K to 300 K, decreasing the temperature with steps of 500 K
- Total cooling time: 470 ps



[1]Malavasi, G., Menziani, M. C., Pedone, A., Segre, U., 2006. *Journal of Non-Crystalline Solids* **352** (3), 285-296.

RVE setup – Quenching

Rapid cooling of a β-cristobalite melt: Generation of an **amorphous** structure



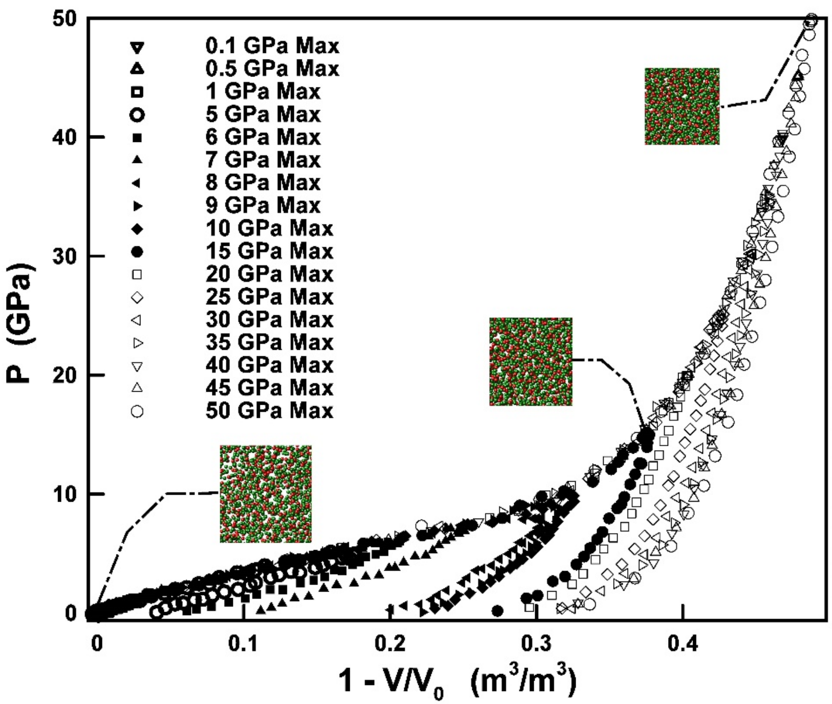
Quenching procedure for the generation of amorphous silica.T=5000K at t=0ps and T=300K at t=470ps.

Michael Ortiz
UPEN 2018

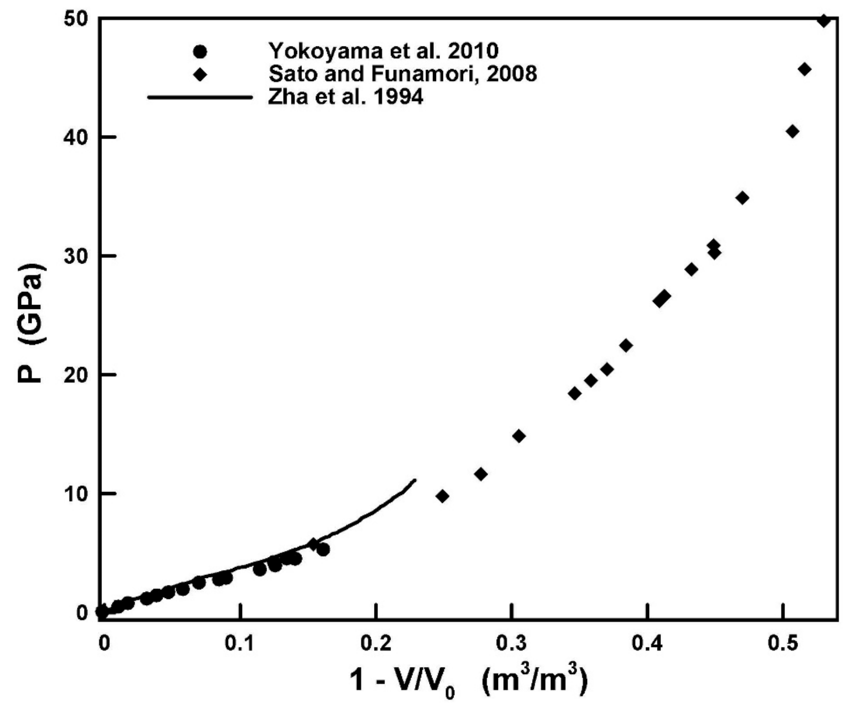
Volumetric compression

Hydrostatic compression/ decompression of amorphous silica:

- Molecular dynamics results exhibit irreversible densification at 14-20 GPa



MD calculations



Experimental[1,2,3]

[1]Yokoyama, A., Matsui, M., Higo, Y., Kono, Y., Irifune, T., Funakoshi, K., 2010. *Journal of Applied Physics* **107** (12).

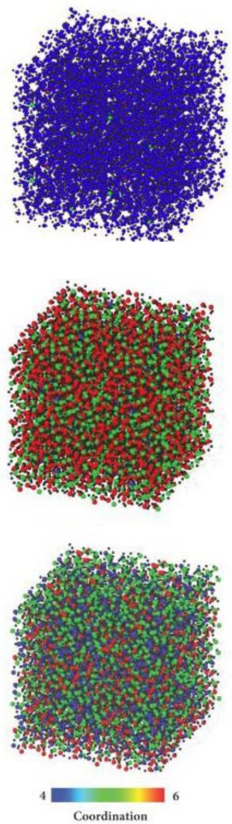
[2]Sato, T., Funamori, N., Dec 2008. *Phys. Rev. Lett.* **101**, 255502.

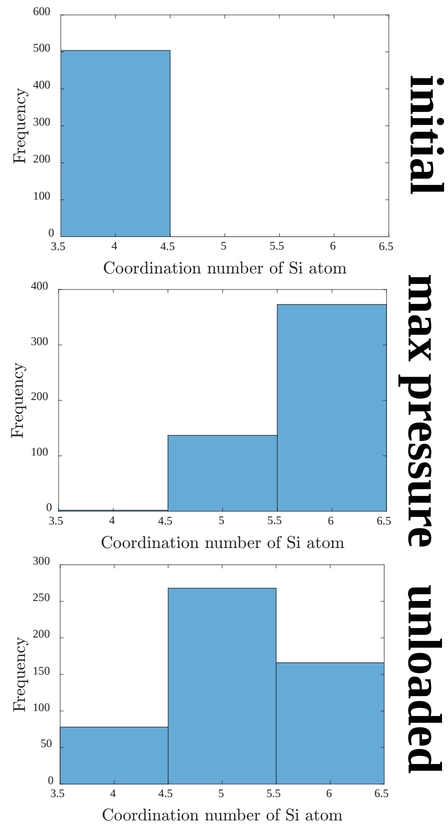
[3]Zha, C. S., Hemley, R. J., Mao, H. K., 1994. *High-Pressure Science and Technology* - 1993, Pts 1 and 2, 93-96.

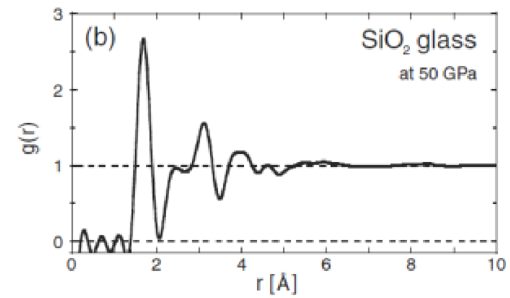
Molecular basis of densification

Hydrostatic compression/ decompression of amorphous silica:

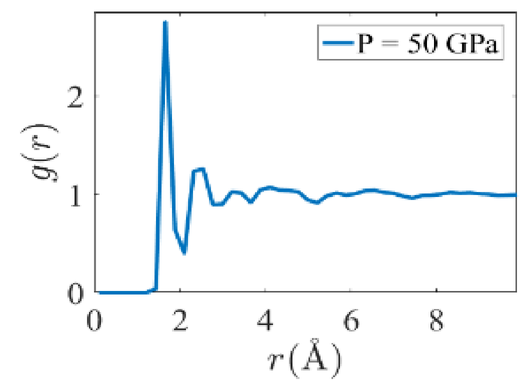
- Irreversible 4-fold to 6-fold coordination transition
- Intermediate 5-fold coordinated dense silica polymorph[1]







(Sato and Funamori, 2010)

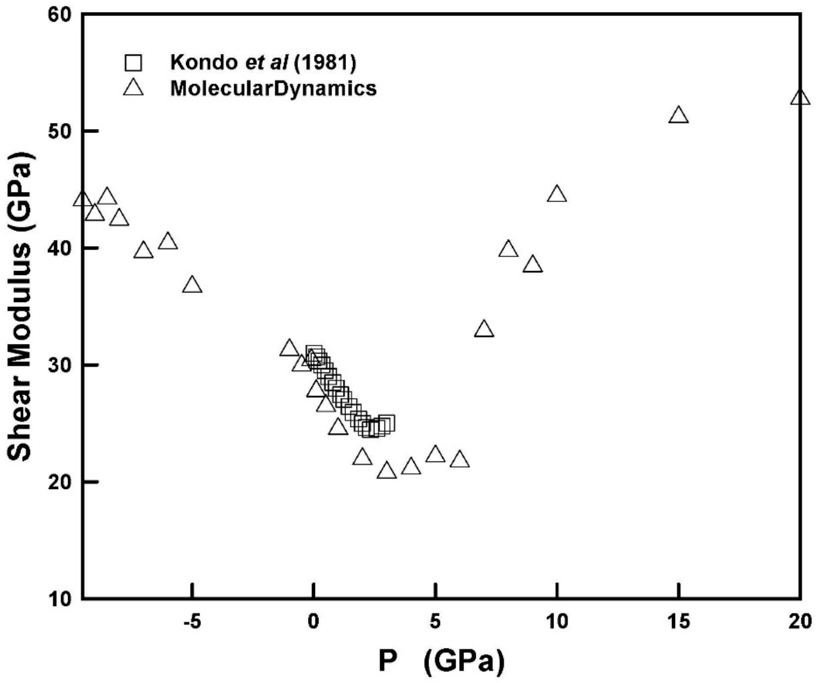


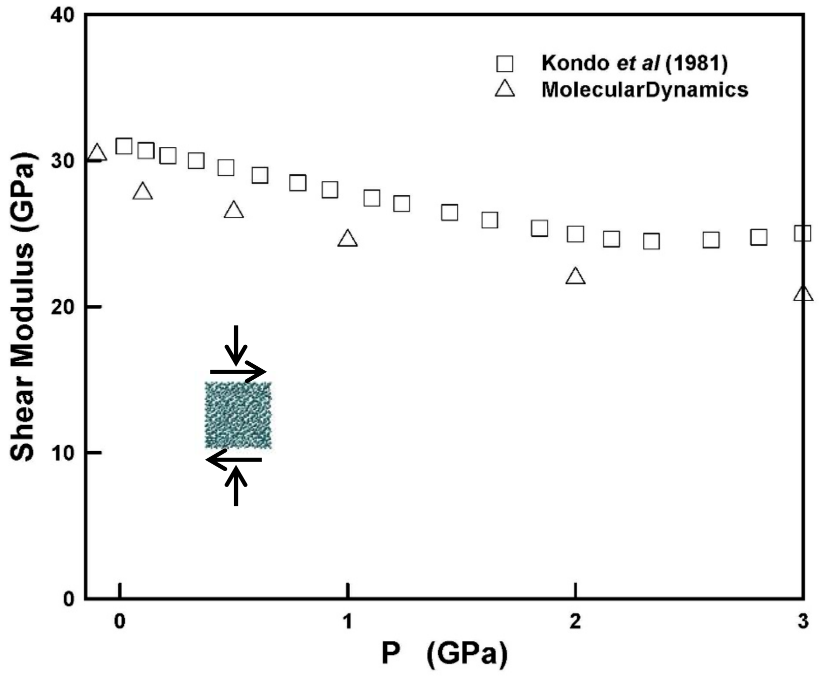
[1]Luo, S. N., Tschaune, O., Asimow, P. D., Ahrens, T. J., 2004. American Mineralogist 89, 455461.

Shear modulus *vs.* pressure

Shear modulus of amorphous silica at constant pressure:

- Shear modulus decreases (increases) at low (high) pressure
- Anomalous shear modulus shows agreement with experiment





Initial shear modulus *versus* pressure

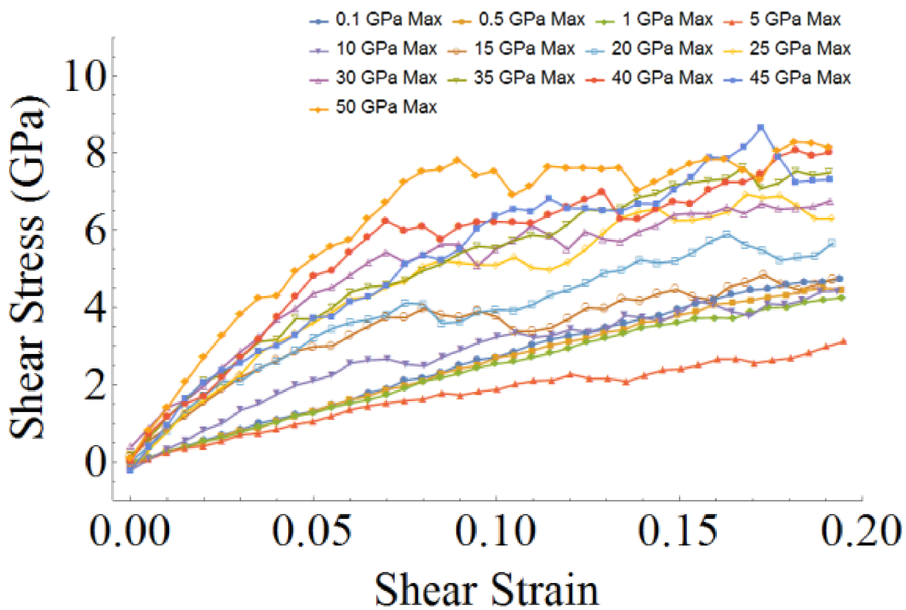
Anomalous pressure dependence of shear modulus!

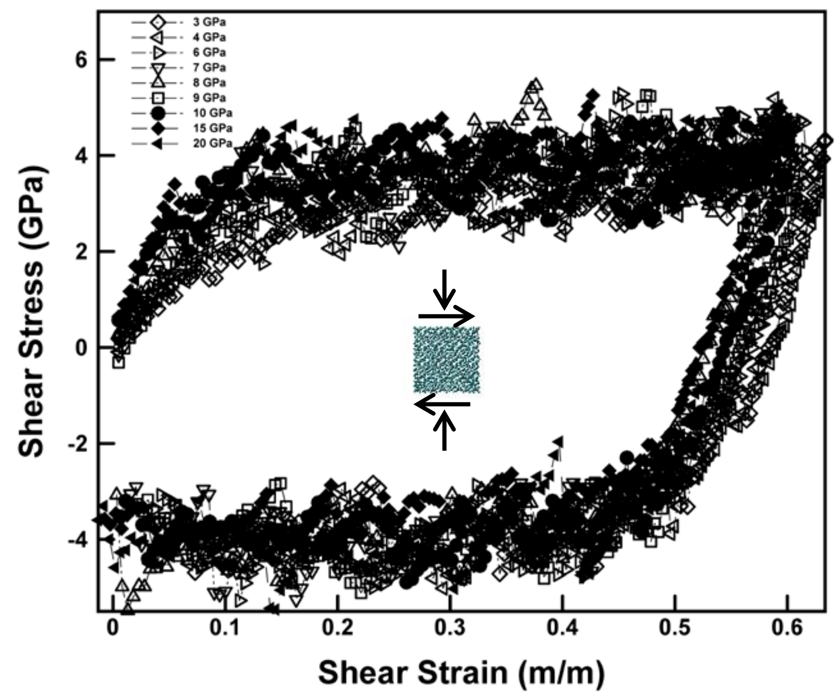
(shear modulus initially decreases with increasing pressure)

Pressure-shear coupling

Simple shear of amorphous silica at constant hydrostatic pressure:

- Hydrostatic compression is performed followed by simple shear
- The pressure-dependent shear response is computed





Shear deformation is irreversible upon unloading!

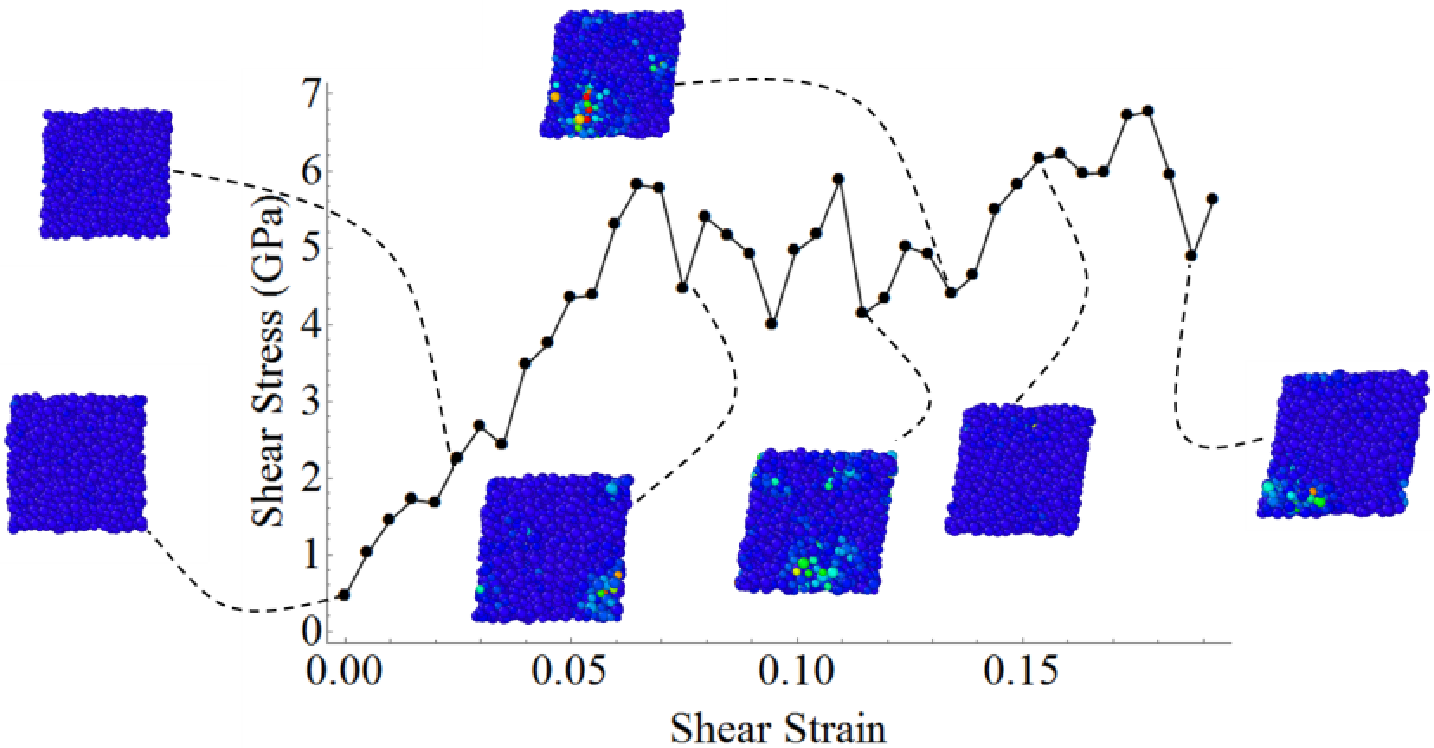
(permanent or plastic shear deformation, pressure-dependent plasticity)

Michael Ortiz
UPEN 2018

Molecular basis of glass plasticity

Shear Transformation Zones:

- Local microstructural rearrangements accommodate shear deformation
- Colored regions indicate large deviation from affine deformation from the previous step



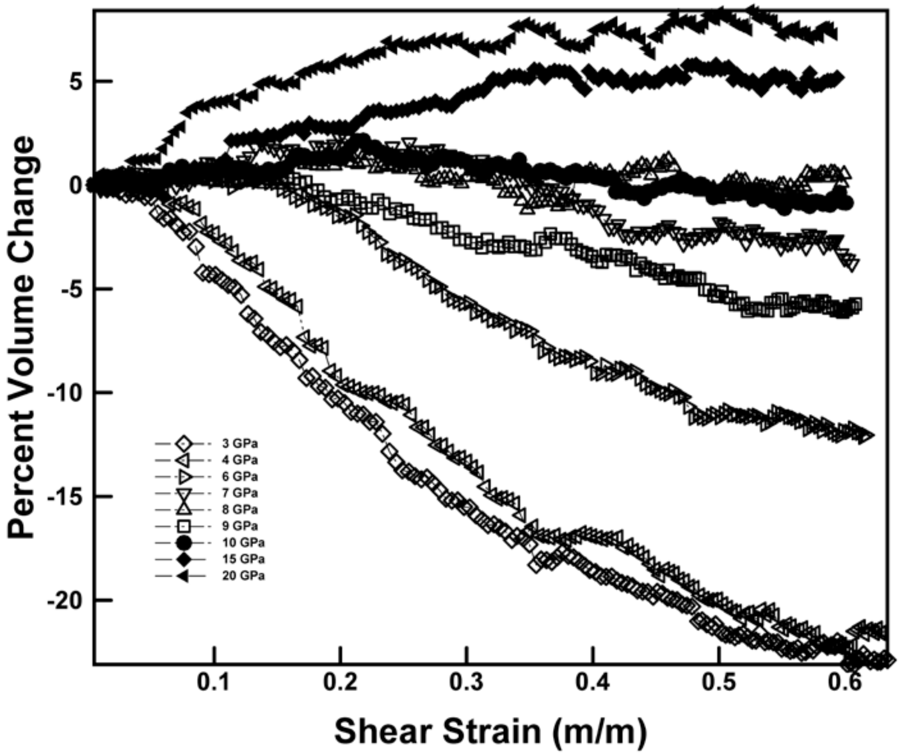
Local avalanches controlled by free-volume kinetics!

(shear deformation proceeds inhomogeneously through local bursts)

Volume evolution

Volume vs. shear and degree of pre-consolidation:

- Volume attains constant value after sufficient shear deformation (critical state)
- Volume decreases (increases) in under- (over-) consolidated samples



Evidence of critical state behavior!

(in analogy to granular media)

Multiscale modeling approach

Atomistic modeling of fused silica:

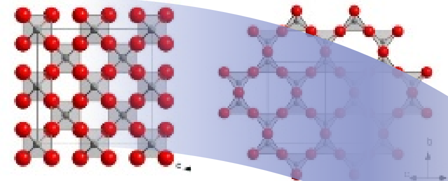
- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

Mesoscopic modeling:

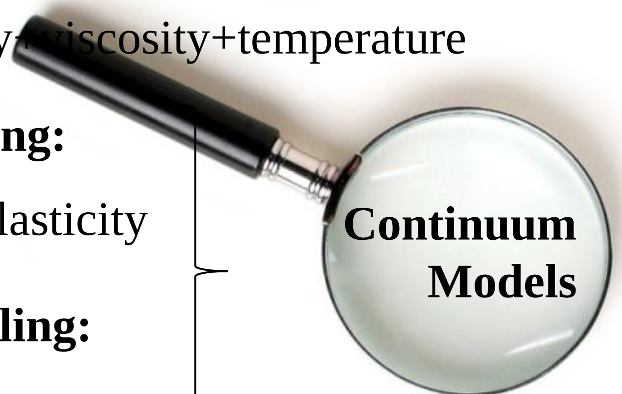
- Critical-state plasticity

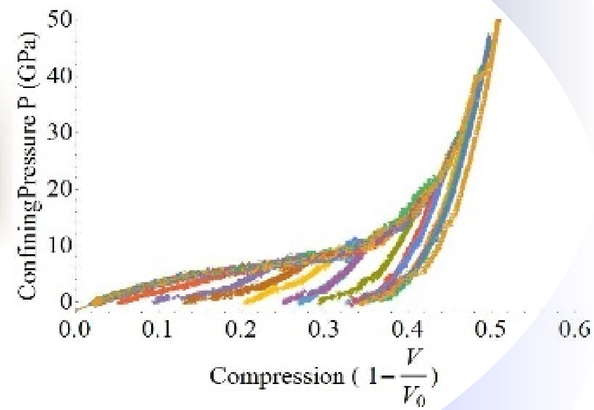
Macroscopic modeling:

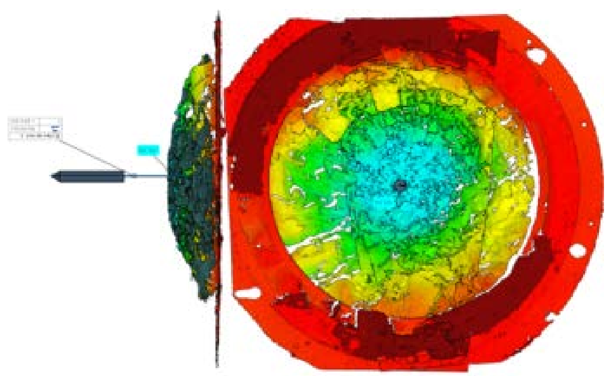
- Relaxation



Data Mining







(OTM ballistic simulation of brittle target , Courtesy B. Li)

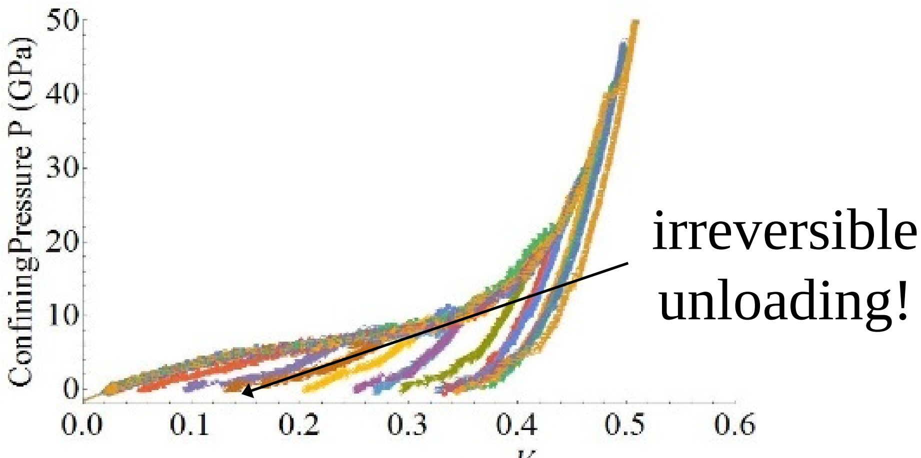
Applications

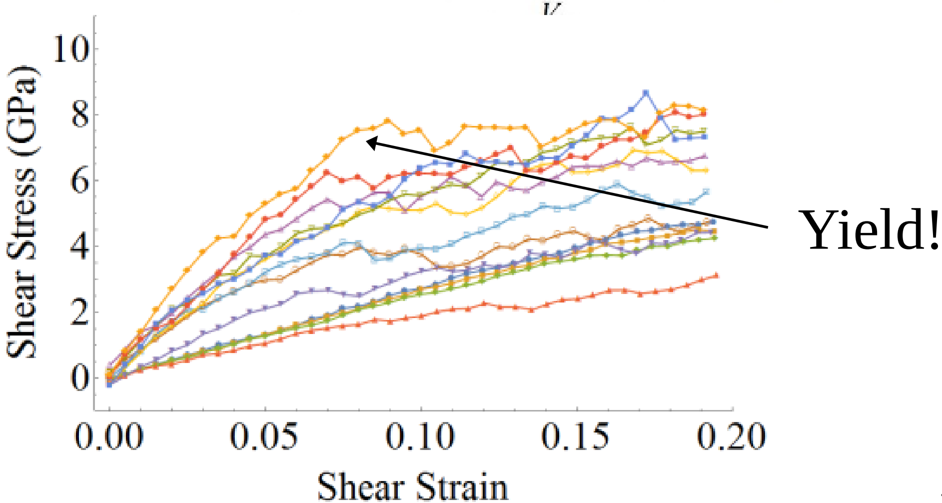
Michael Ortiz
UPEN 2018

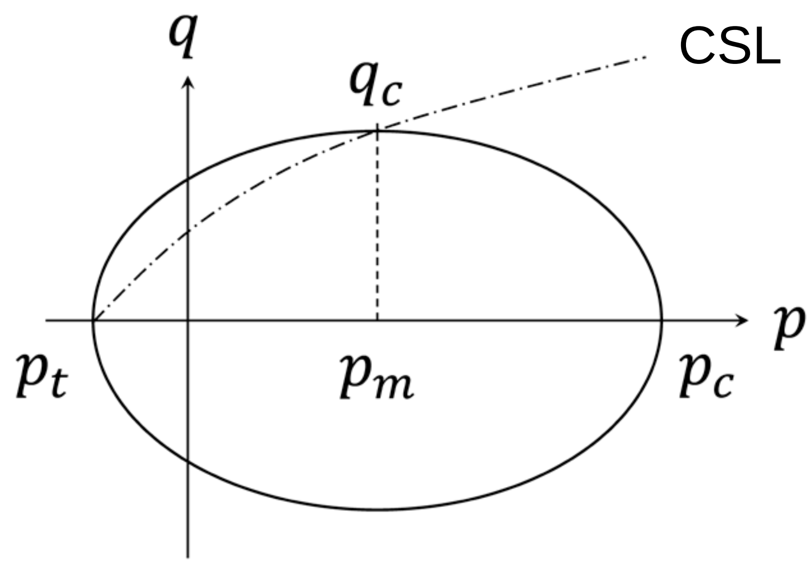
Critical-state plasticity model

Modeling approach:

- Critical-state theory of plasticity (Cam-Clay)







Assumed yield locus in pressure (p) Mises shear stress (q) plane and critical-state line (CSL)

Michael Ortiz
UPEN 2018

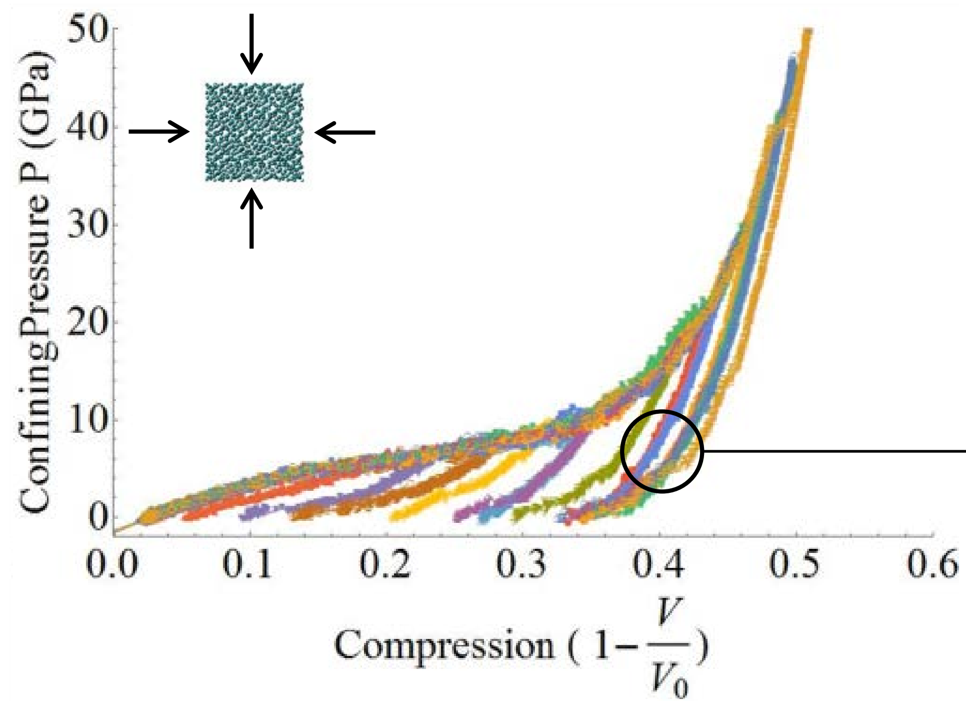
W. Schill, S. Heyden, S. Conti and M. Ortiz, *JMPS*, **113** (2018) 105-125.

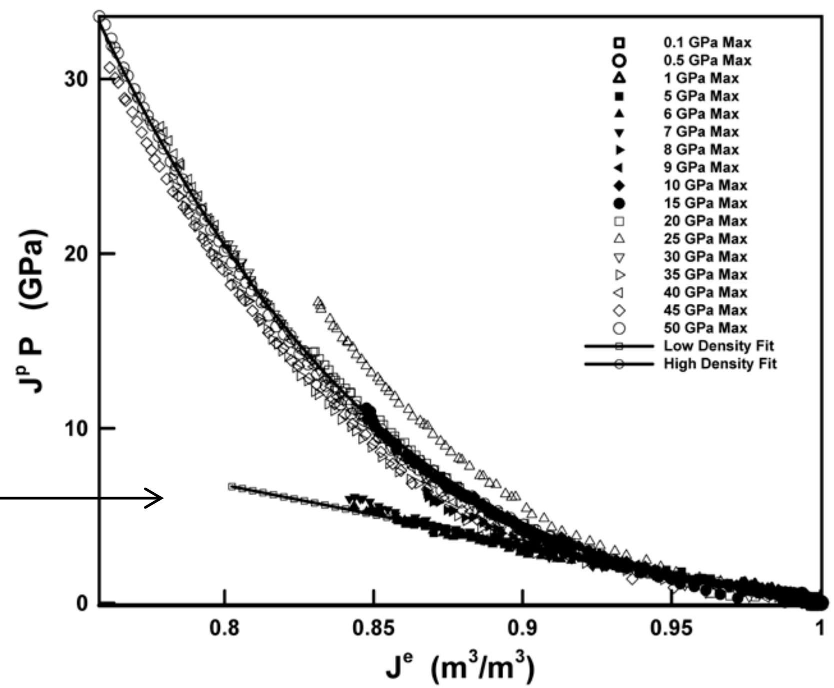
Elastic pressure-shear response

Neo-Hookean elastic response fitted to:

- Volumetric compression data (elastic unloading)
- Pressure-shear data (elastic regime)

$$W^e(\mathbf{C}^e) = \frac{\mu(J^e)}{2}\left(J^{e-2/3}\mathrm{tr}(\mathbf{C}^e) - 3\right) + f(J^e)$$



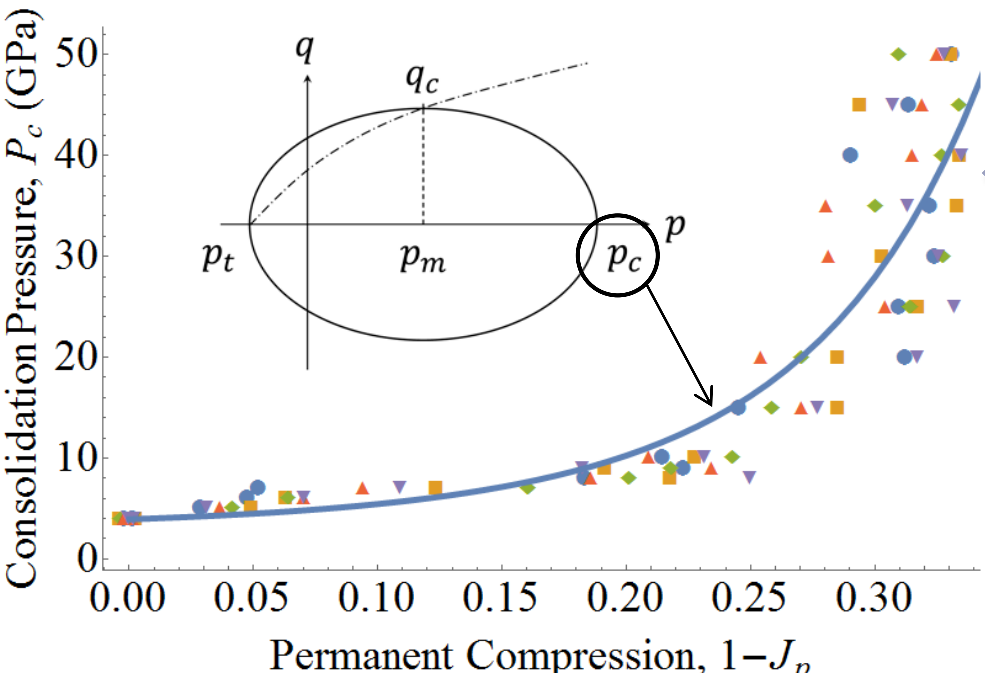


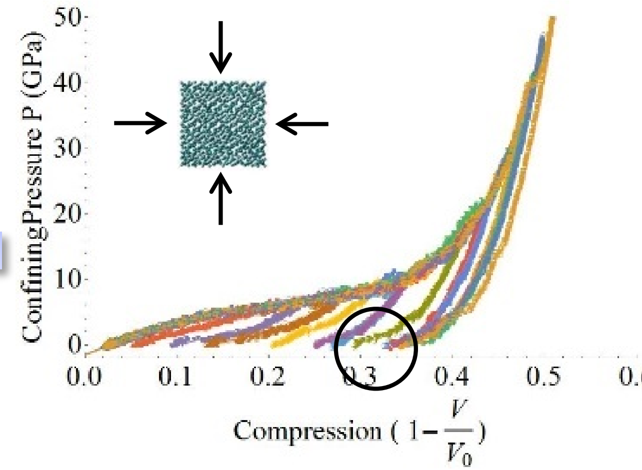
W. Schill, S. Heyden, S. Conti and M. Ortiz, *JMPS*, **113** (2018) 105-125.

Critical-state plasticity model

Densification:

- Pressure-volume response of fuse silica interpreted as consolidation curve in critical state plasticity





$$p_c = -\frac{K_b}{k_b}\left[(J_p)^{-k_b} - 1\right] + \Gamma$$

Table 1: Hardening Rule Parameters

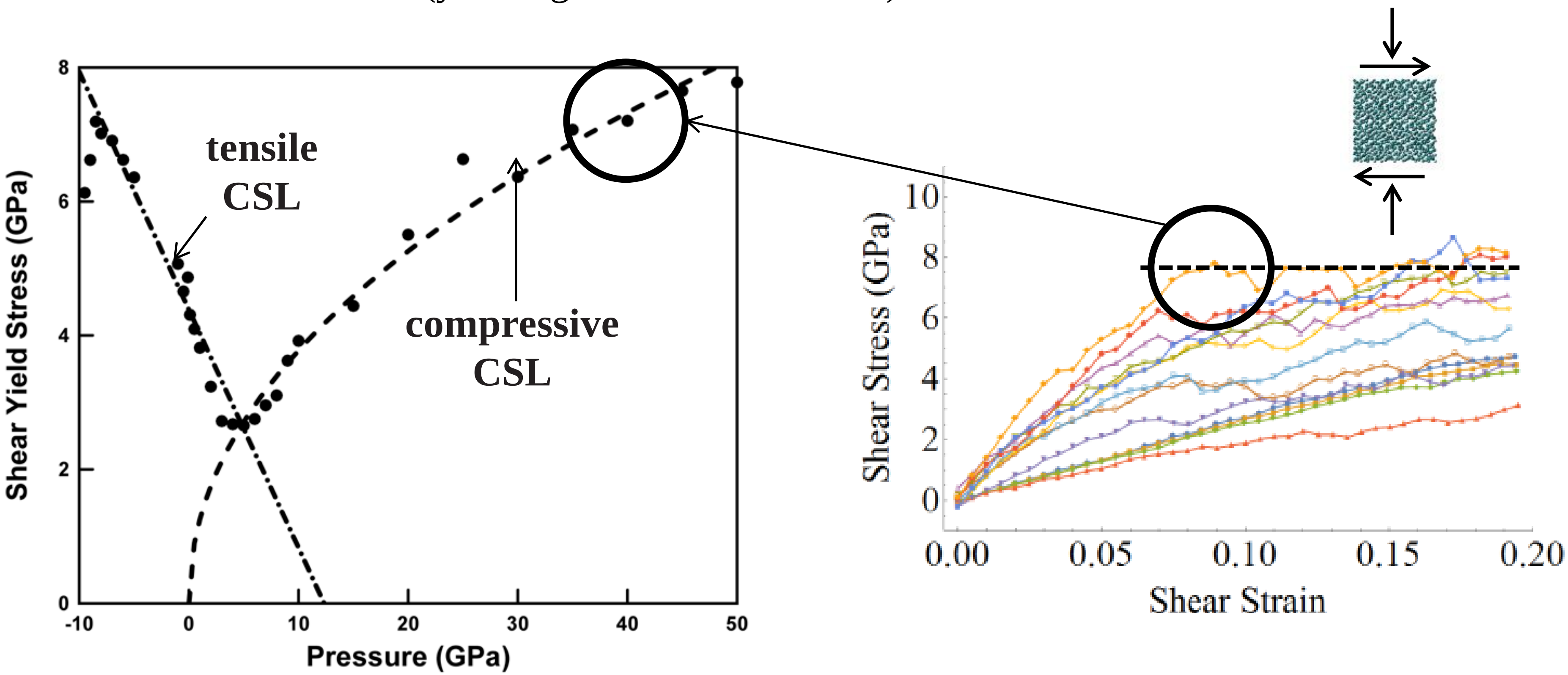
K_B	k_b	Γ
8.48613 GPa	9.2689	3.02934 GPa

W. Schill, S. Heyden, S. Conti and M. Ortiz, *JMPS*, **113** (2018) 105-125.

Critical-state plasticity model

Pressure-shear plasticity:

- Critical states (yielding at constant volume) define Critical State Line



Anomalous pressure dependence of shear yield stress!
Non-convex Critical-State Line!

Michael Ortiz
UPEN 2018

Anomalous plasticity of fused silica

Effect of a Coordination Change on the Strength of Amorphous SiO_2

CHARLES MEADE AND RAYMOND JEANLOZ

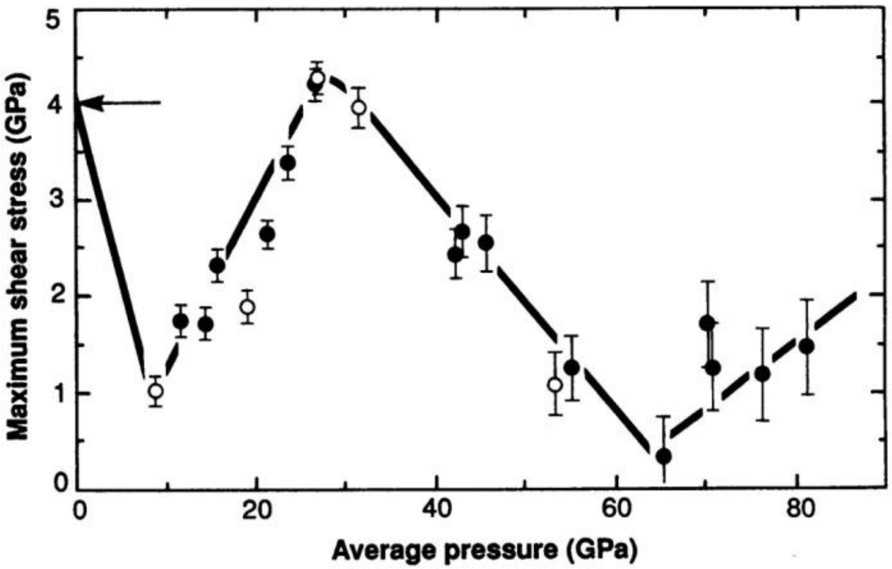
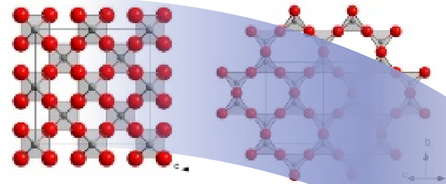


Fig. 1. Maximum shear stress in silica glass at room temperature and average pressures ($\bar{P}$) between 8.6 and 81 GPa. Each point corresponds to a separate sample, and the heavy line shows the general trend of the data. The shear stress is determined from Eq. 1, and it is a measure of the yield strength of the sample at high pressures. The error bars represent the combined uncertainties from the measurements of h and $\partial P/\partial r$. The open circles show the strength of samples that were initially compressed to 50 GPa, unloaded, and then recompressed. The arrow marks the zero pressure strength of silica glass (*19*).

SCIENCE, VOL. 241

Anomalous shear yield stress documented in geophysics literature!

Multiscale modeling approach



Data Mining

Atomistic modeling of fused silica:

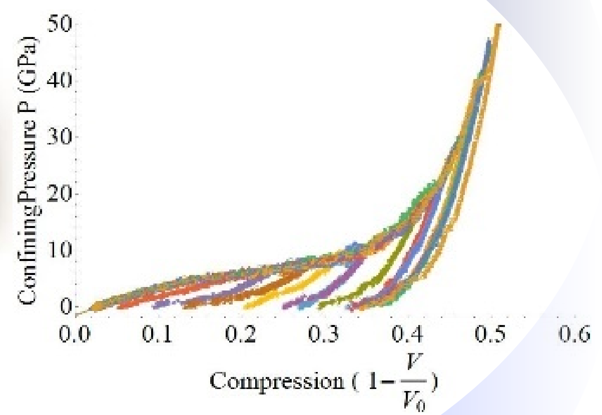
- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

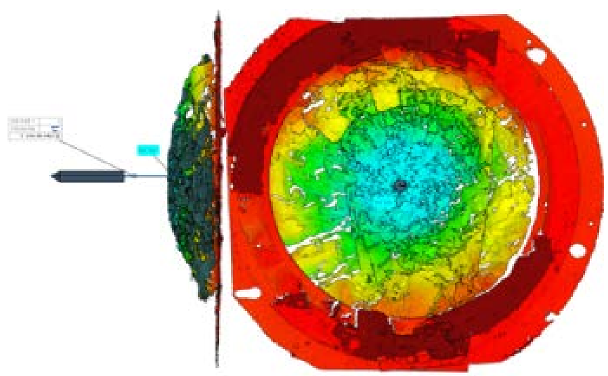
Mesoscopic modeling:

- Critical-state plasticity

Macroscopic modeling:

- Relaxation





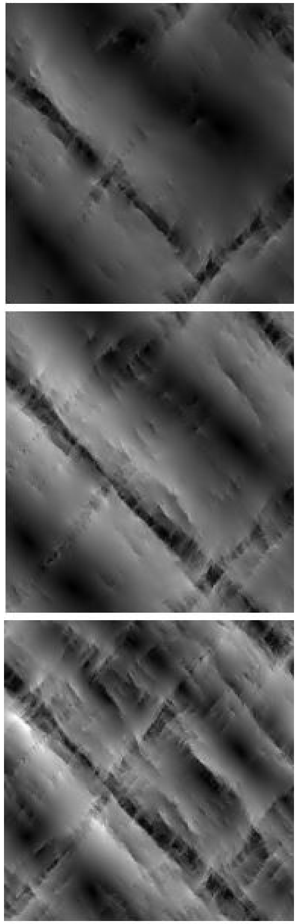
(OTM ballistic simulation of brittle target , Courtesy B. Li)

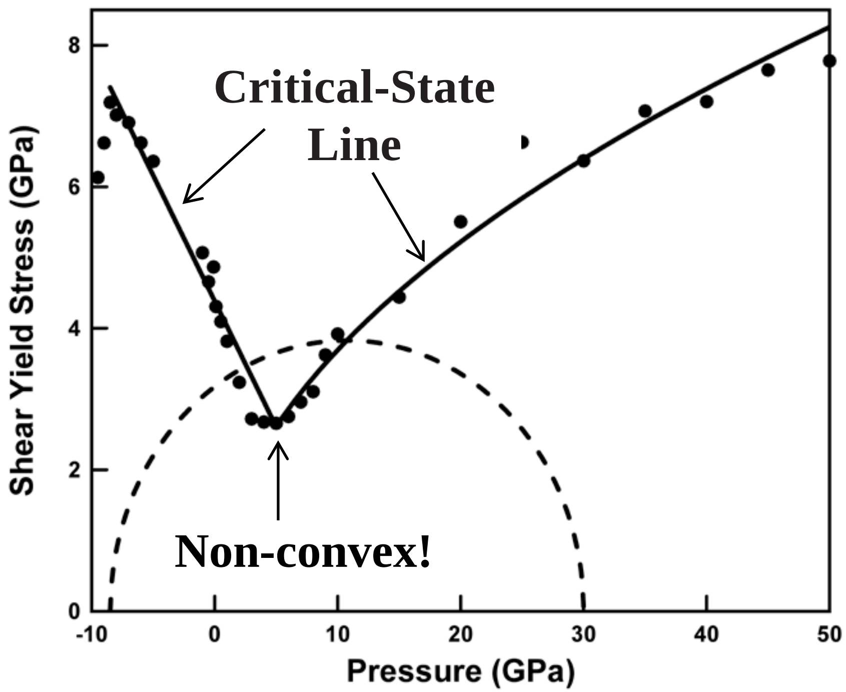
Applications

Non-convex limit analysis – Relaxation

Relaxation:

- Strong non-convexity (material instability) is exploited by the material to maximize dissipation (**relaxation**, per calculus of variations)
- Relaxation occurs through the formation of fine **microstructure**[1] (finely patterned stress and deformation fields at the microscale) ⟶





W. Schill, S. Heyden, S. Conti and M. Ortiz, *JMPS*, **113** (2018) 105-125.

Michael Ortiz
UPEN 2018

Non-convex limit analysis – Relaxation

Relaxation:

- Classical limit analysis, kinematic and static problems:

$$\inf_v \sup_\sigma \left\{ \int_\Omega \sigma \cdot \nabla v \, dx \ : \ \sigma(x) \in K, \ \ v(x) = g(x) \text{ on } \partial\Omega \right\}$$

- Reformulation for non-convex elastic domain *K*:

$$\sup_\sigma \inf_v \left\{ \int_\Omega \sigma \cdot \nabla v \, dx \ : \ \sigma(x) \in K, \ \ v(x) = g(x) \text{ on } \partial\Omega \right\}$$

- Reduced static problem:

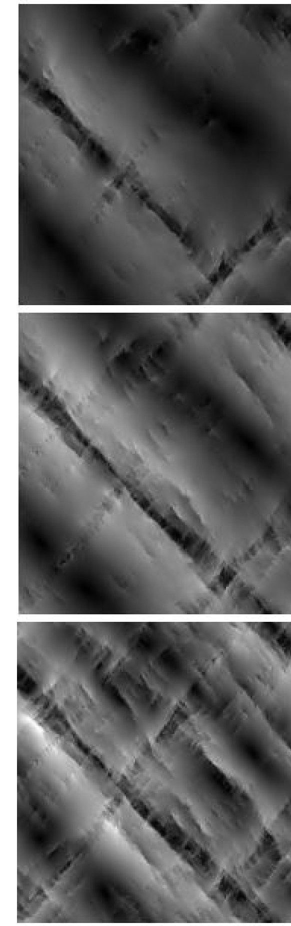
$$\sup_\sigma \left\{ \int_{\partial\Omega} \sigma\nu \cdot g \, d\mathcal{H}^2 \ : \ \sigma(x) \in K, \ \operatorname{div} \sigma(x) = 0 \text{ in } \Omega \right\}$$

- Supremum non-attained for strongly non-convex *K*!
- Div-quasiconvex envelop of *K*:

$$\bar{K} = \{ \sigma \ : \ \xi_h \rightharpoonup \sigma, \ \xi_h(x) \in K, \ \operatorname{div} \xi_h(x) = 0 \text{ in } \Omega \}$$

- Relaxed static problem (attained):

$$\sup_\sigma \left\{ \int_{\partial\Omega} \sigma\nu \cdot g \, d\mathcal{H}^2 \ : \ \sigma(x) \in \bar{K}, \ \operatorname{div} \sigma(x) = 0 \text{ in } \Omega \right\}$$



ξ_h

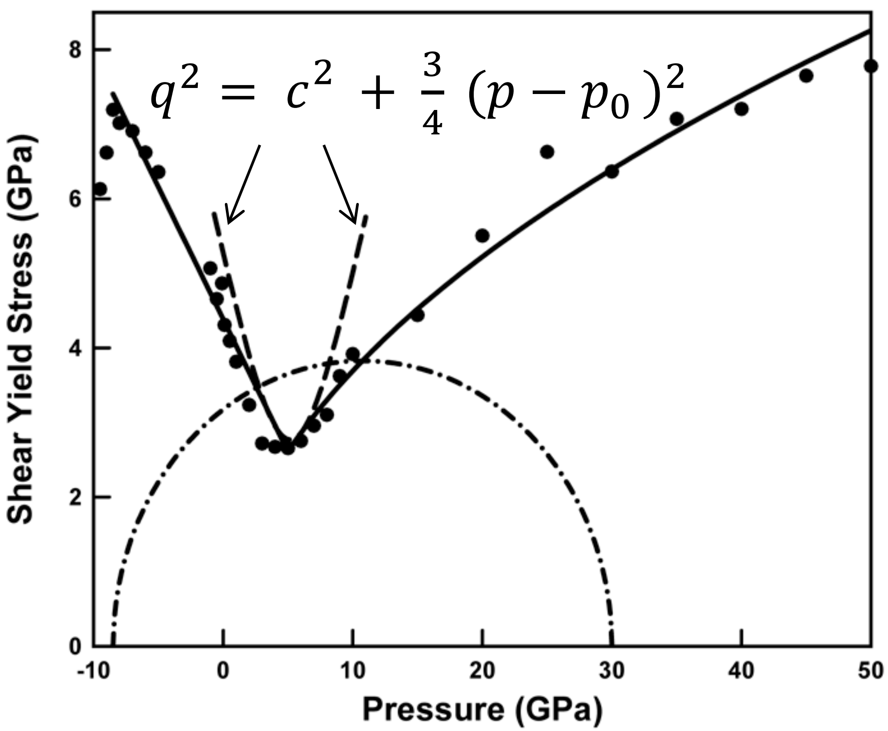
W. Schill, S. Heyden, S. Conti and M. Ortiz, *JMPS*, **113** (2018) 105-125.

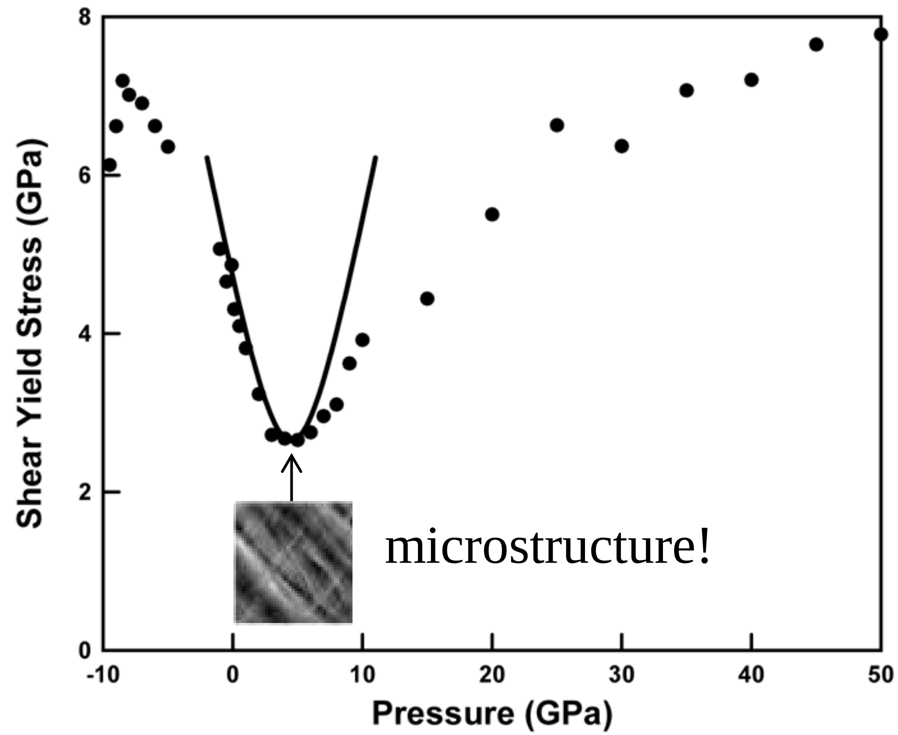
Michael Ortiz
UPEN 2018

Non-convex limit analysis – Relaxation

Div-quasiconvex envelop of glass elastic domain:

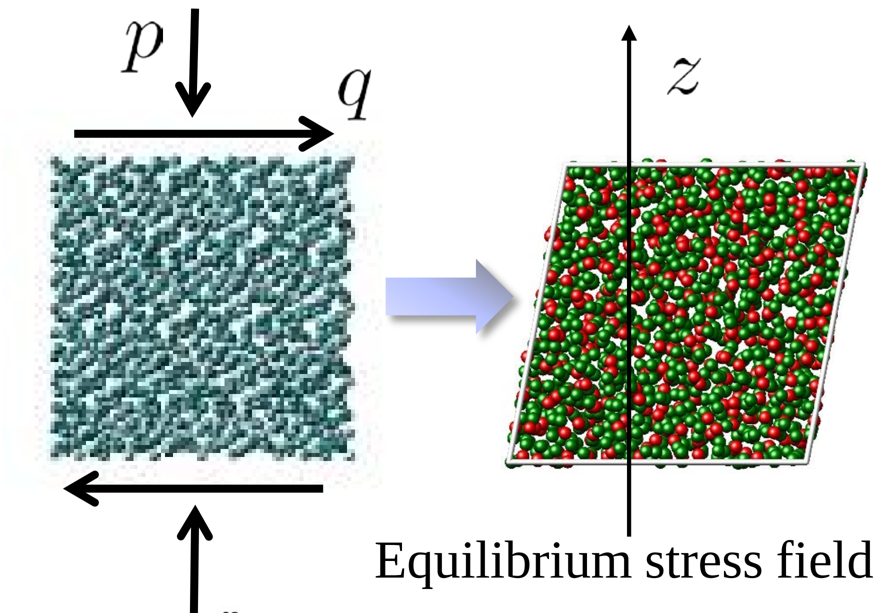
- **Theorem** (Tartar'85). *The function* $f(\sigma) = 2|\sigma|^2 - \mathrm{tr}(\sigma)^2$ *is div-quasiconvex.*
- **Theorem**. *The set* $\{\sigma : q^2 \leq c^2 + \frac{3}{4}(p - p_0)^2\}$ *is div-quasiconvex.*
- **Theorem** (CMO'17) *The div-quasiconvex envelop of K is:*

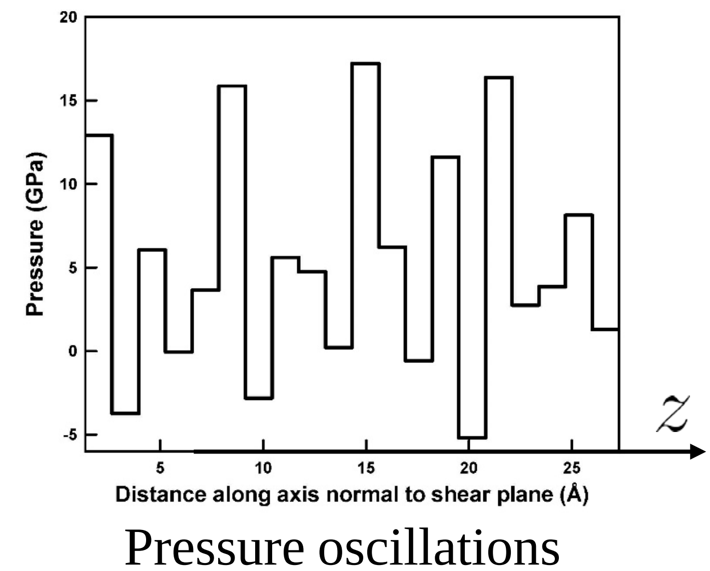


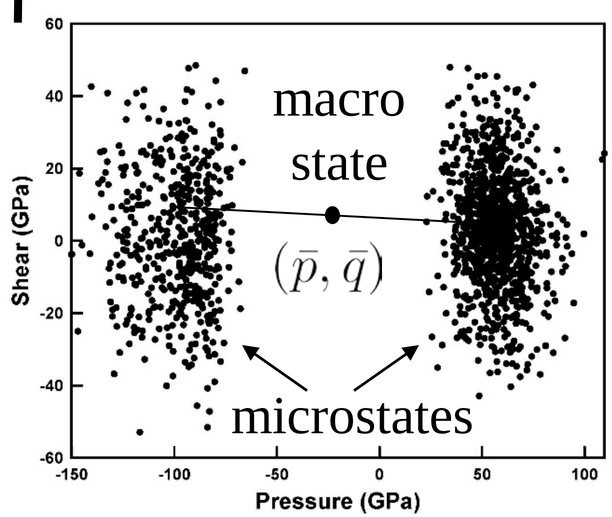


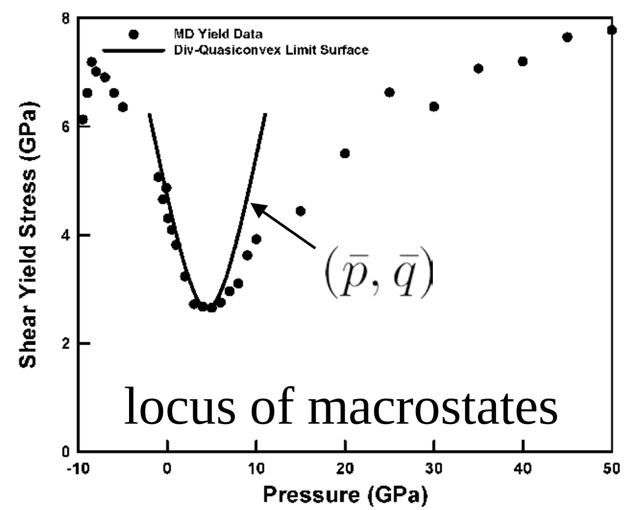
L. Tartar "Estimations nes des coefficients homogeneises". In Ennio De Giorgi colloquium (Paris, 1983), vol. 125 of Res. Notes in Math., pp. 168-187, Pitman, Boston, MA, 1985.

Critical-state plasticity – Relaxation







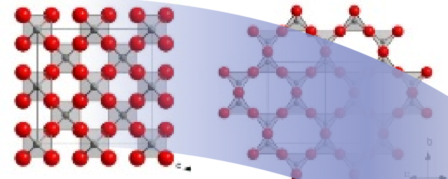


W. Schill, S. Heyden, S. Conti and M. Ortiz, *JMPS*, **113** (2018) 105-125.

Multiscale modeling approach

Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature



Data Mining

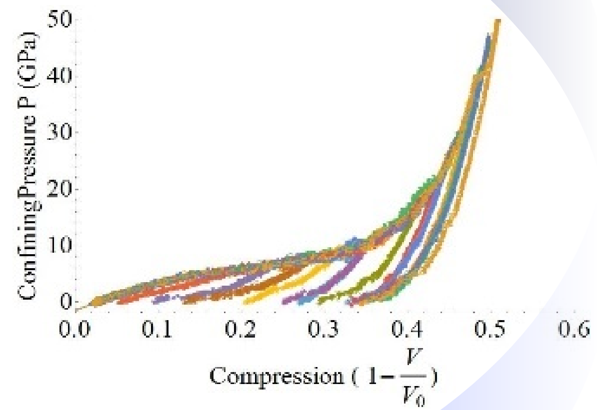
Mesoscopic modeling:

- Critical-state plasticity

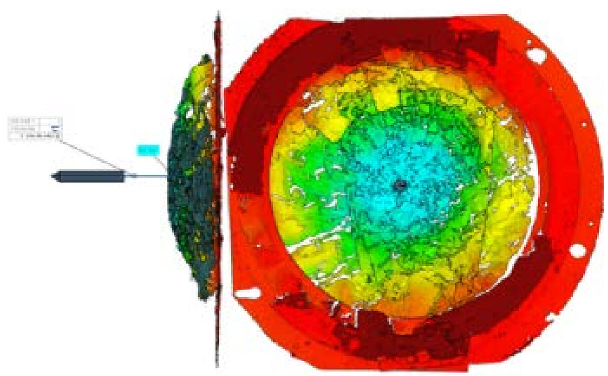
Macroscopic modeling:

- Relaxation

Continuum Models

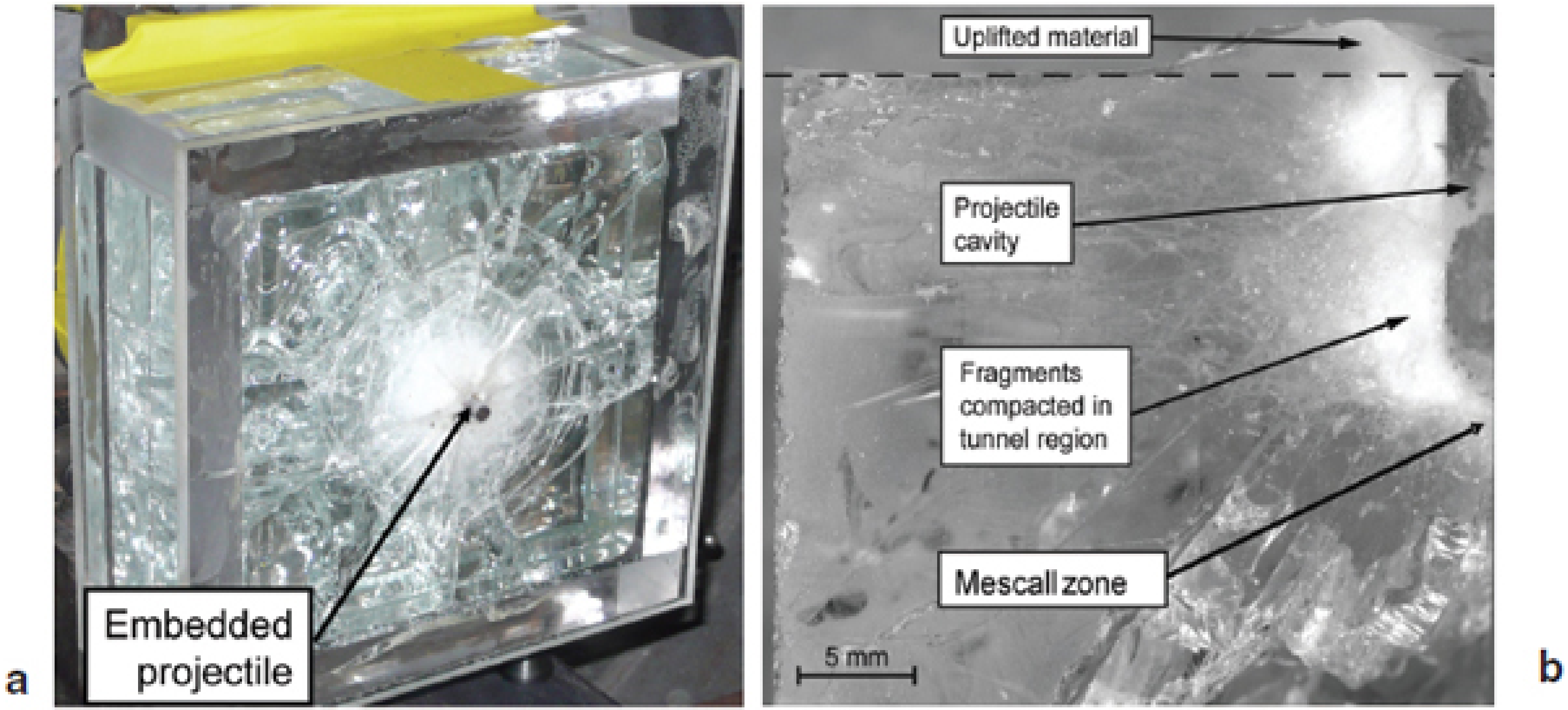


(OTM ballistic simulation of brittle target , Courtesy B. Li)



Applications: Solvers!

Recall: Glass as protection material



A soda lime glass target impacted by steel rod at 300 m/s[1].

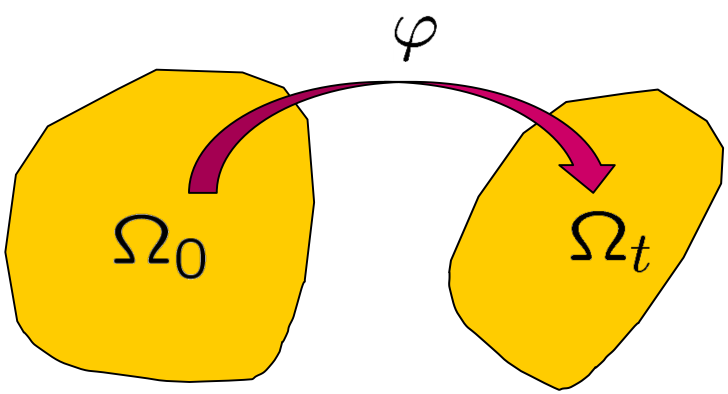
[1]Shockey, D., Simons, J. and Curran D., *Int. J. Appl. Ceramic Tech.*, **7**(5):566-573, 2010.

Optimal transportation problems

- Mass + linear-momentum transport (Eulerian):

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho\, v) = 0, & \text{in } [0,T] \times \Omega_t \,, \\ \partial_t (\rho v) + \nabla \cdot (\rho\, v \otimes v) = \nabla \cdot \sigma, & \text{in } [0,T] \times \Omega_t \,, \\ \sigma = \sigma(\text{deformation history}), & \text{in } [0,T] \times \Omega_t \,. \end{cases}$$

- Lagrangian reformulation:



$$\begin{cases} \partial_t \varphi = v \circ \varphi, \\ \rho \circ \varphi = \rho_0 / \det(\nabla \varphi). \end{cases}$$

Geometrically exact!

Optimal transportation — Time-discrete

- Semidiscrete action: $A_d(\varphi_1, \ldots, \varphi_{N-1}) =$

$$\sum_{k=0}^{N-1} \Big\{ \underbrace{\frac{1}{2} \frac{d_W^2(\rho_k, \rho_{k+1})}{(t_{k+1} - t_k)^2}}_{\text{inertia}} - \underbrace{\frac{1}{2}[U(\varphi_k) + U(\varphi_{k+1})]}_{\text{potential energy}} \Big\} (t_{k+1} - t_k)$$

- Discrete Euler-Lagrange equations: $\delta A_d = 0 \Rightarrow$

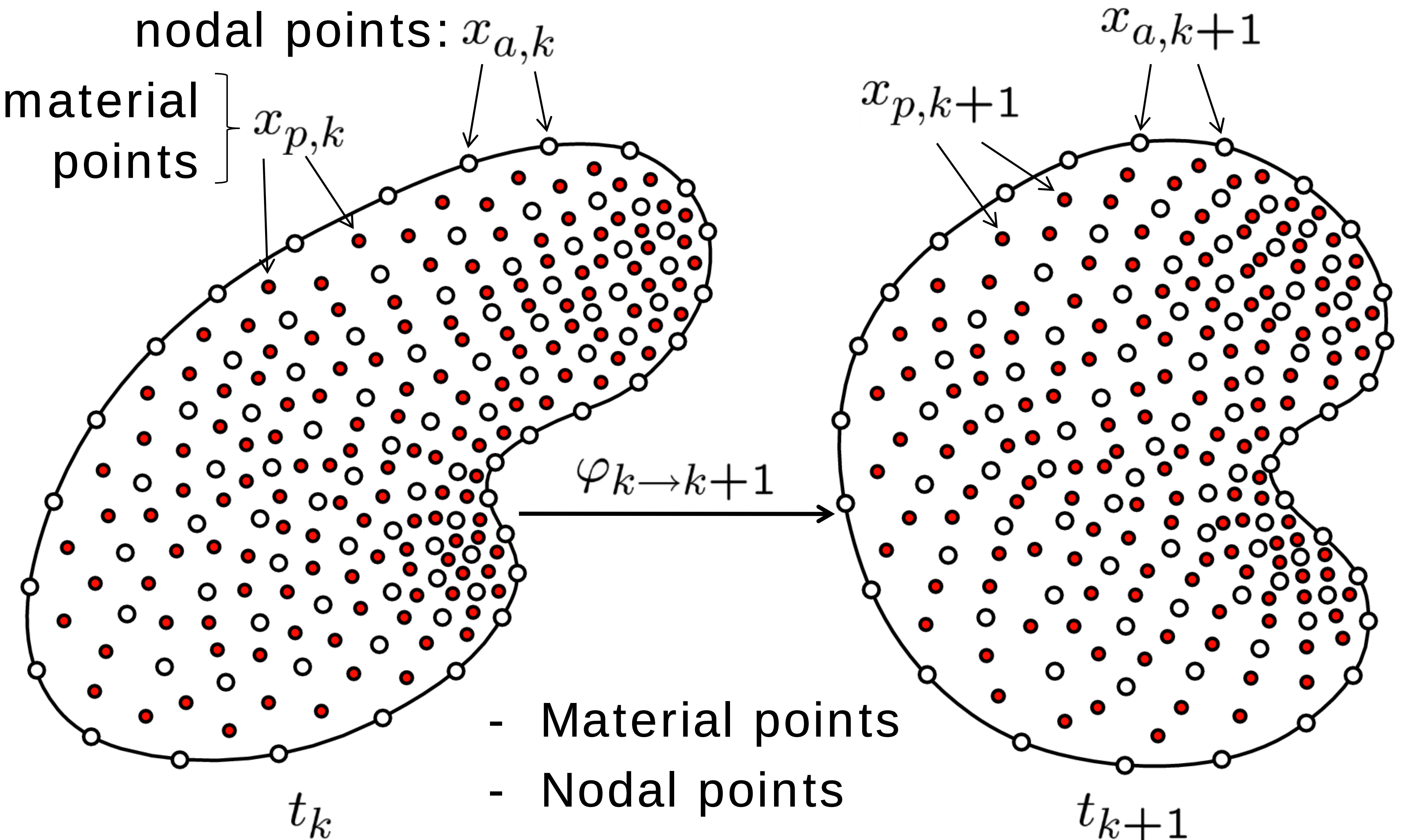
$$\frac{2\rho_k}{t_{k+1} - t_{k-1}} \left(\frac{\varphi_{k \to k+1} - x}{t_{k+1} - t_k} + \frac{\varphi_{k \to k-1} - x}{t_k - t_{k-1}} \right) = \nabla \cdot \sigma_k + \rho_k b_k$$

$$\rho_{k+1} \circ \varphi_{k \to k+1} = \rho_k / \det \left(\nabla \varphi_{k \to k+1} \right)$$

Geometrically exact!

Li, B., Habbal, F. and Ortiz, M., *IJNME*, **83**(12):1541–1579, 2010.

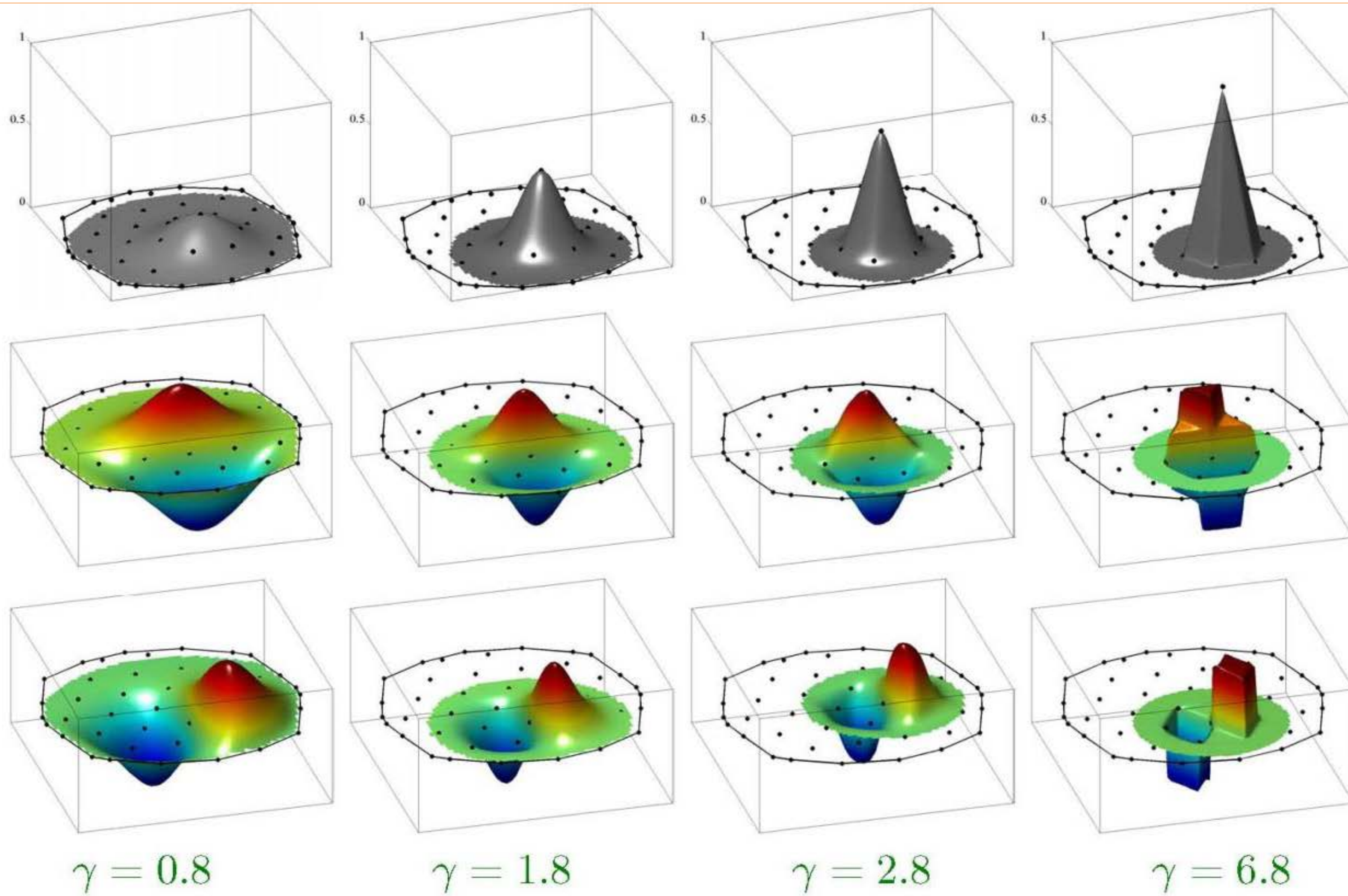
Optimal Transportation Meshfree (OTM)



Michael Ortiz
UPEN 2018

Li, B., Habbal, F. and Ortiz, M., *IJNME*, **83**(12):1541–1579, 2010.

Max-ent interpolation



Max-ent shape functions, $\gamma = \beta h^2$

Arroyo, M. and Ortiz, M., *IJNME*, **65** (2006) 2167.

Michael Ortiz
UPEN 2018

OTM Solver — Flow chart

(i) Explicit nodal coordinate update:

$$x_{k+1} = x_k + (t_{k+1} - t_k)(v_k + \frac{t_{k+1} - t_{k-1}}{2} M_k^{-1} f_k)$$

(ii) Material point update:

position: $x_{p,k+1} = \varphi_{k\to k+1}(x_{p,k})$

deformation: $F_{p,k+1} = \nabla\varphi_{k\to k+1}(x_{p,k}) F_{p,k}$

volume: $V_{p,k+1} = \det \nabla\varphi_{k\to k+1}(x_{p,k}) V_{p,k}$

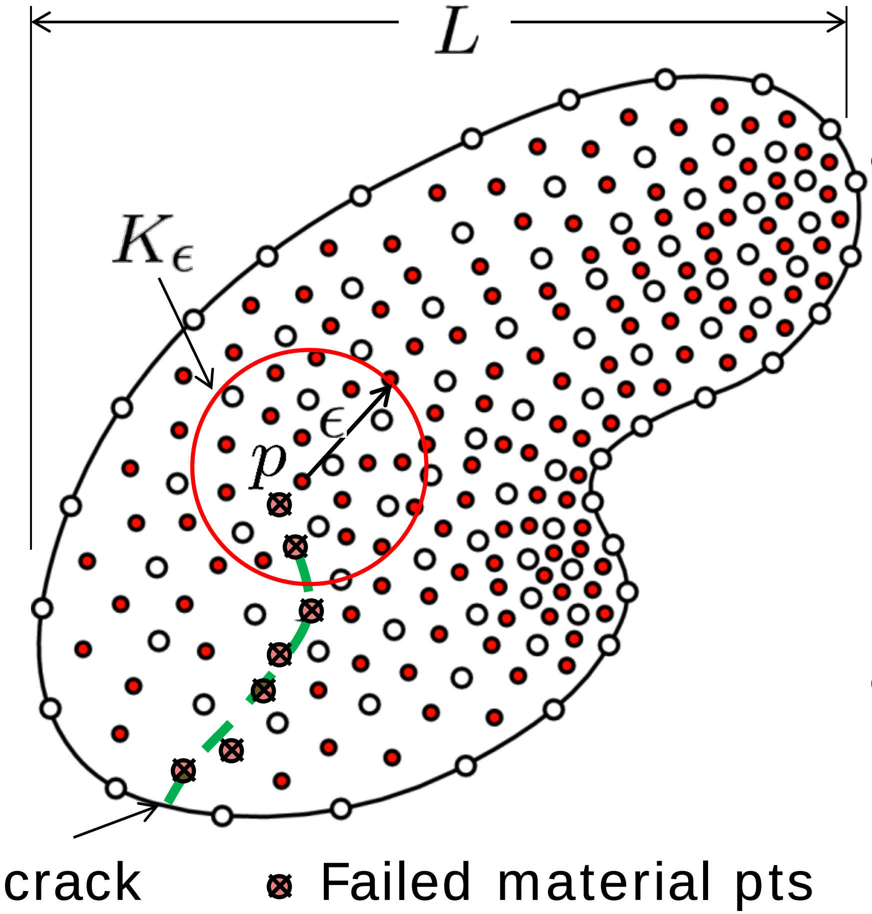
density: $\rho_{p,k+1} = m_p / V_{p,k+1}$

(iii) Constitutive update at material points

(iv) Reconnect nodal and material points (range searches), recompute max-ext shape functions

Li, B., Habbal, F. and Ortiz, M., *IJNME*, **83**(12):1541–1579, 2010.

Fracture Solver – Material-point erosion



Schematic of ϵ-neighborhood construction

- ϵ-neighborhood construction: Choose $h \ll \epsilon \ll L$
- Erode material point p if

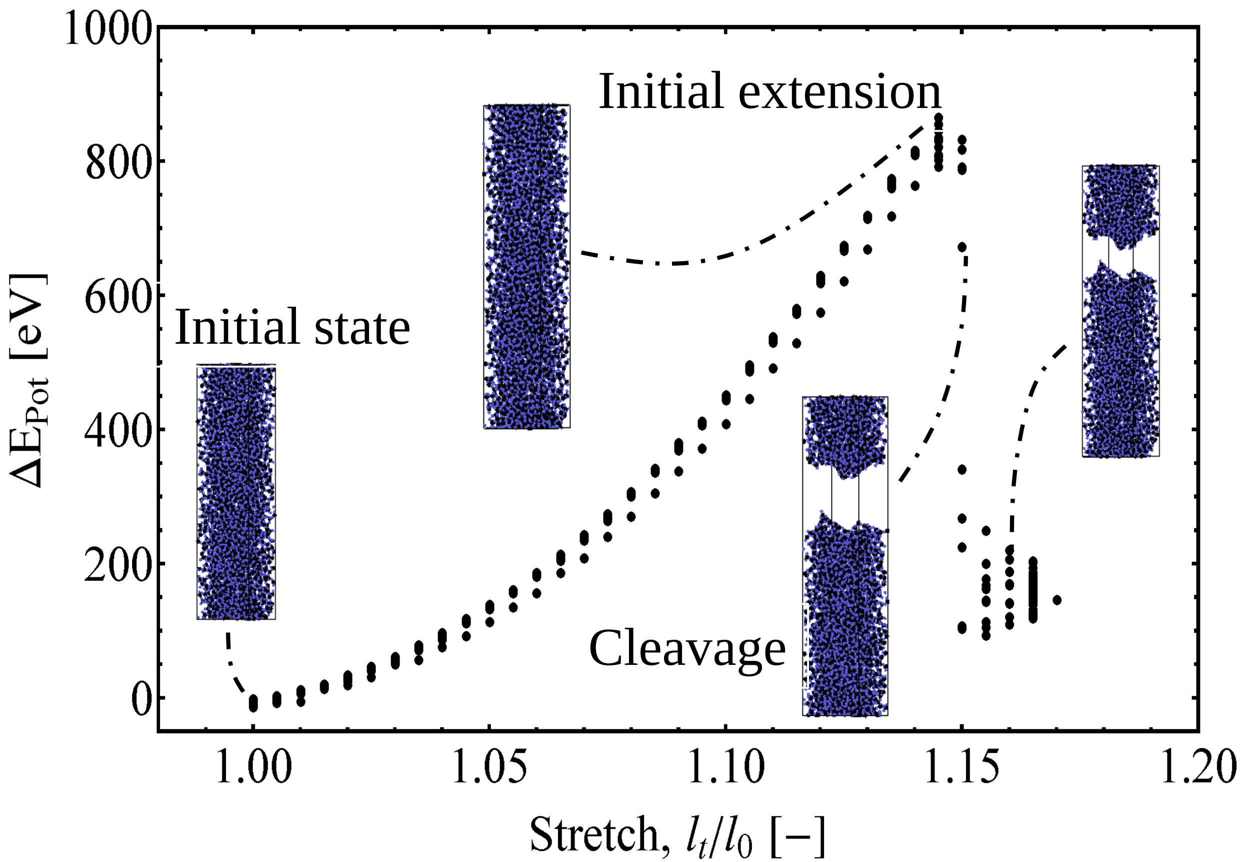
$$G_{p,h,\epsilon} \sim \frac{E_p\, h\, \epsilon}{|K_\epsilon|} \geq G_c$$

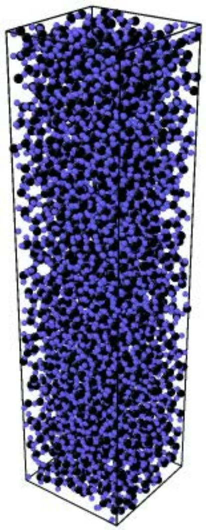
- Proof of convergence to Griffith fracture:
  - *Schmidt, B., Fraternali, F. & MO, SIAM J. Multiscale Model. Simul.*, **7**(3):1237-1366, 2009.

Fracture of SiO_2

Tensile test, brittle fracture, specific fracture energy:

- Common reported values (experimental and MD): G = 1-10 J/m^2



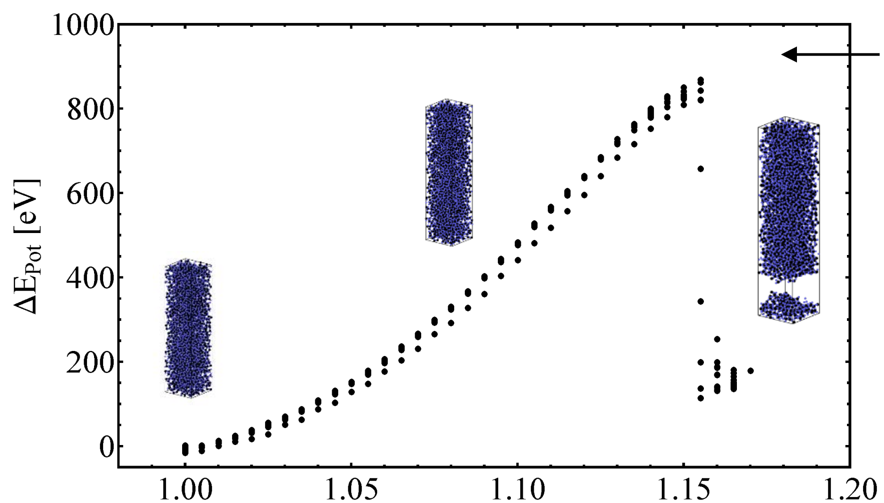


$\gamma = (E_{final} - E_{initial})/A \qquad G = 2\gamma = 3.1969\,\frac{J}{m^2}$

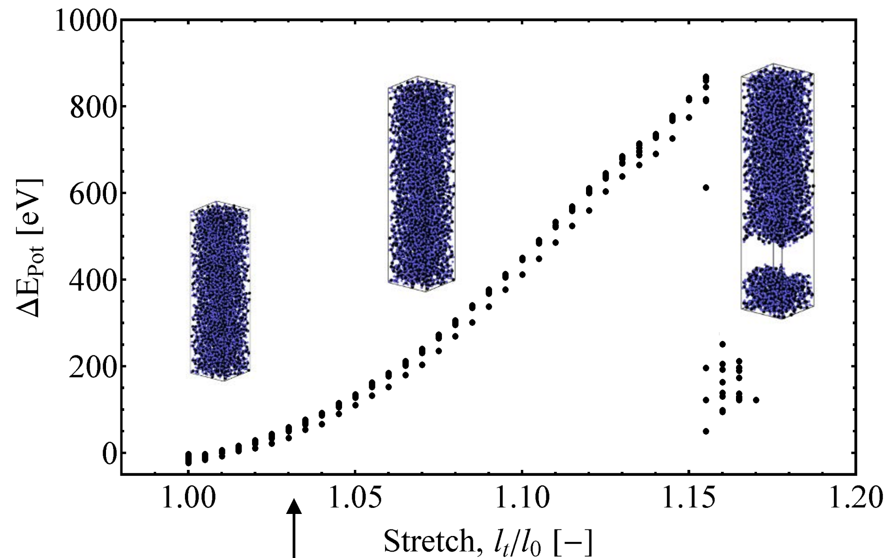
Fracture of SiO_2

Tensile test, brittle fracture, specific fracture energy:

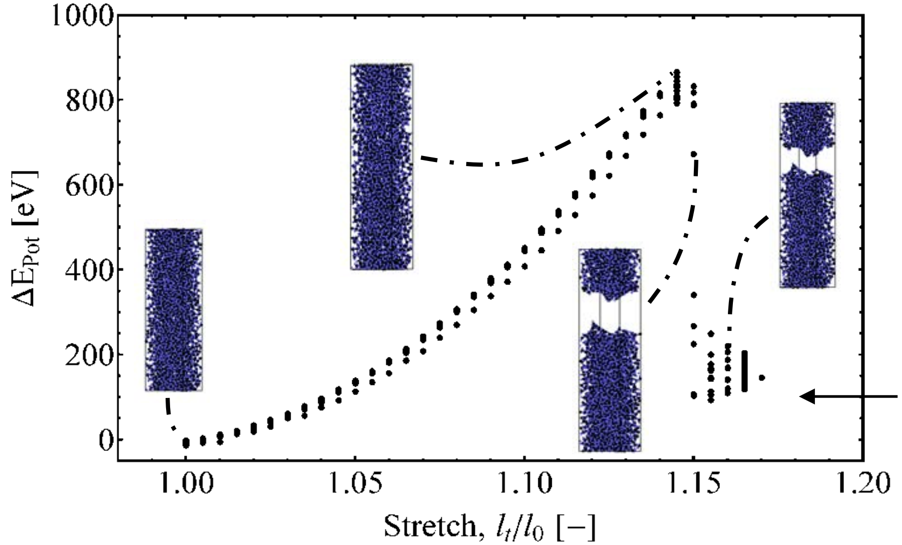
- Variability with respect of initial conditions, area, width



$$G = 2\gamma = 2.9387\,\frac{J}{m^2}$$

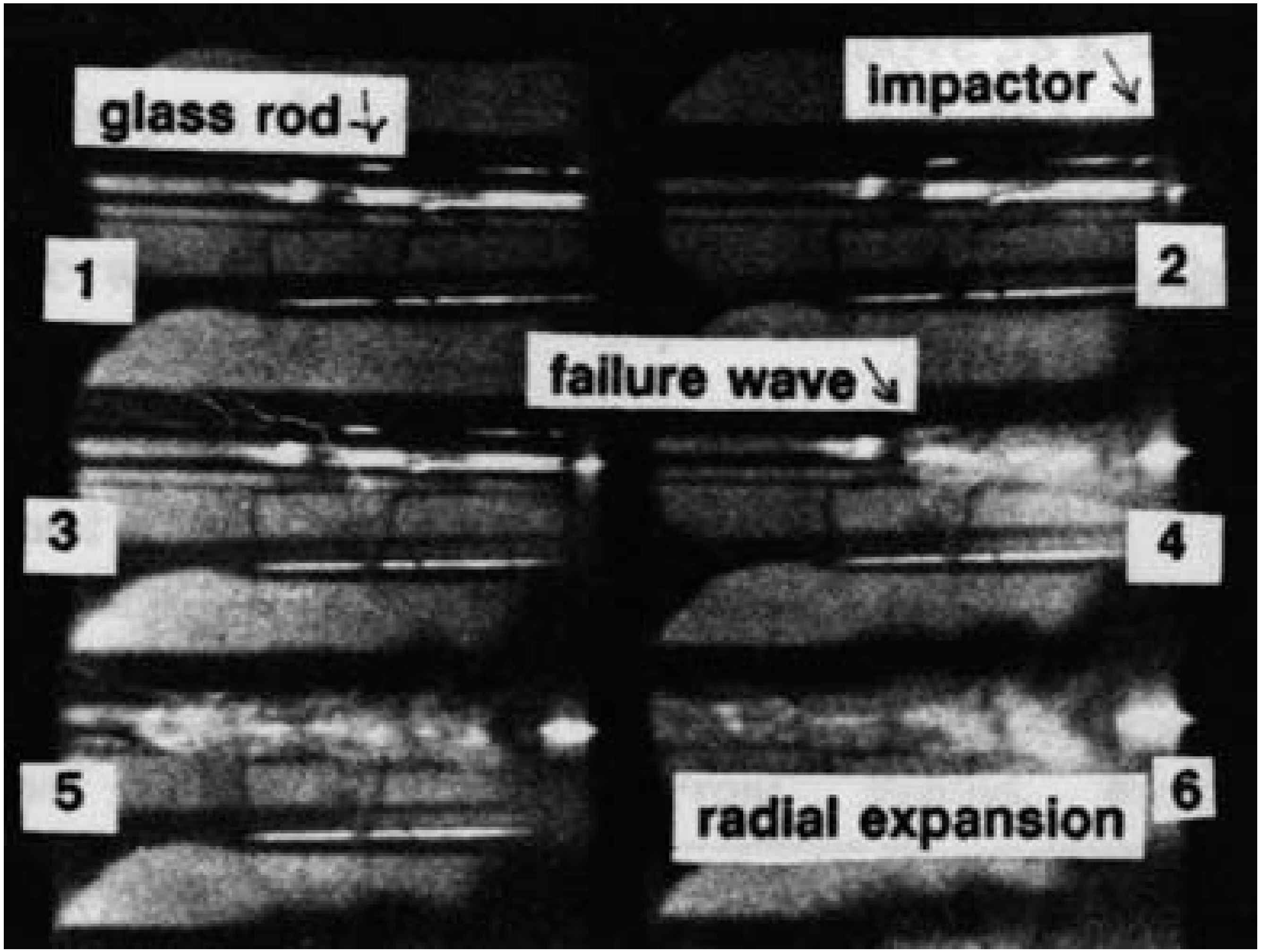


$$G = 2\gamma = 3.03192\,\frac{J}{m^2}$$



$$G = 2\gamma = 3.1969\,\frac{J}{m^2}$$

Application: Failure waves in glass rods



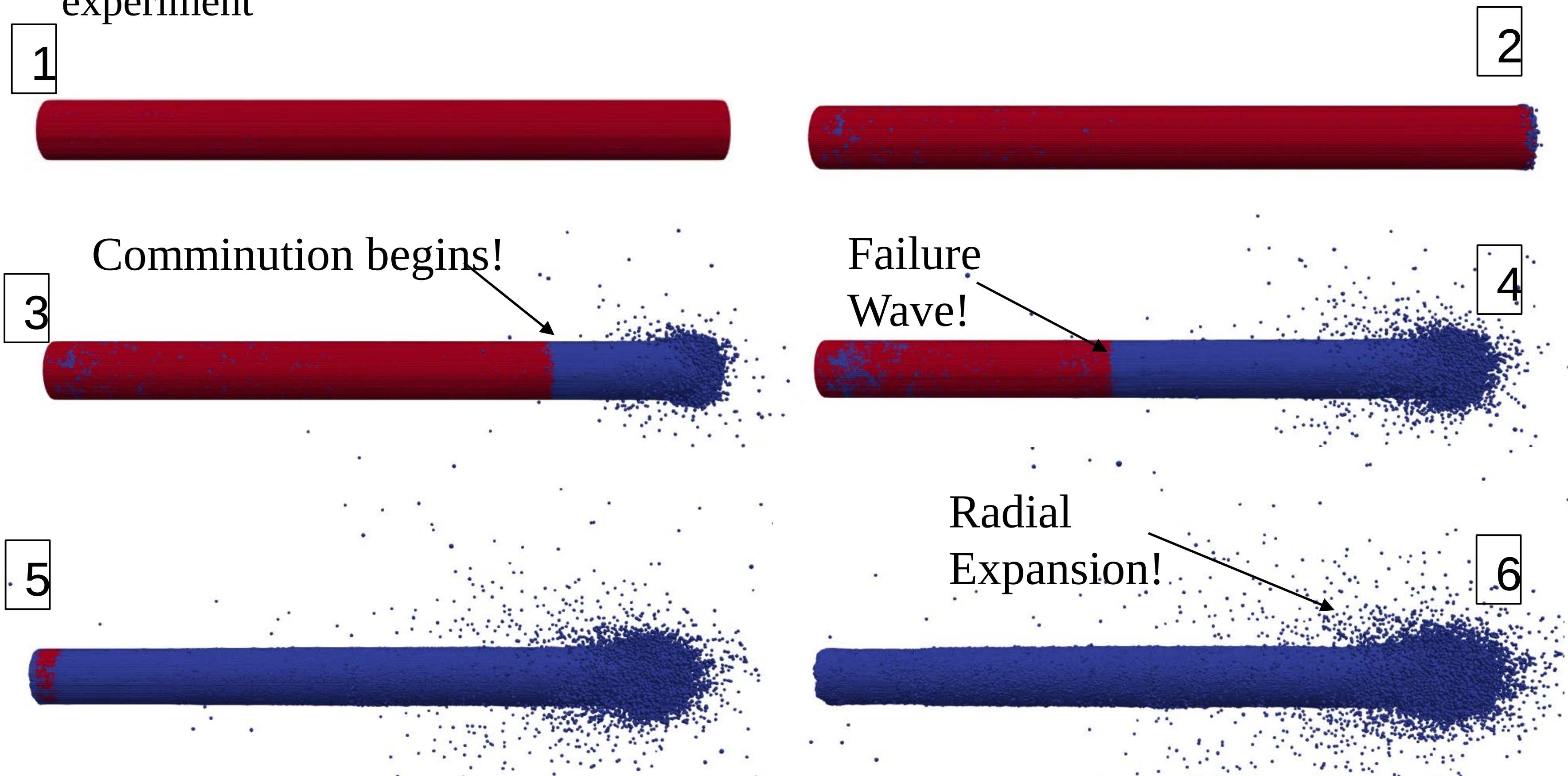
Failure wave in pyrex rod at 210 m/s.

Brar, N.S., Bless, S.J. and Rosenberg, Z., *Appl. Phys. Let.*, **59:**3396, 1991.

OTM Solver – Failure wave in glass rod

Comparison to Experiment:

- After impact, the failure wave propagates in close agreement with experiment



- $V_{failure}$ (sim) = 4.7 mm/μs
- $V_{failure}$ (exp) = 4.5 mm/μs

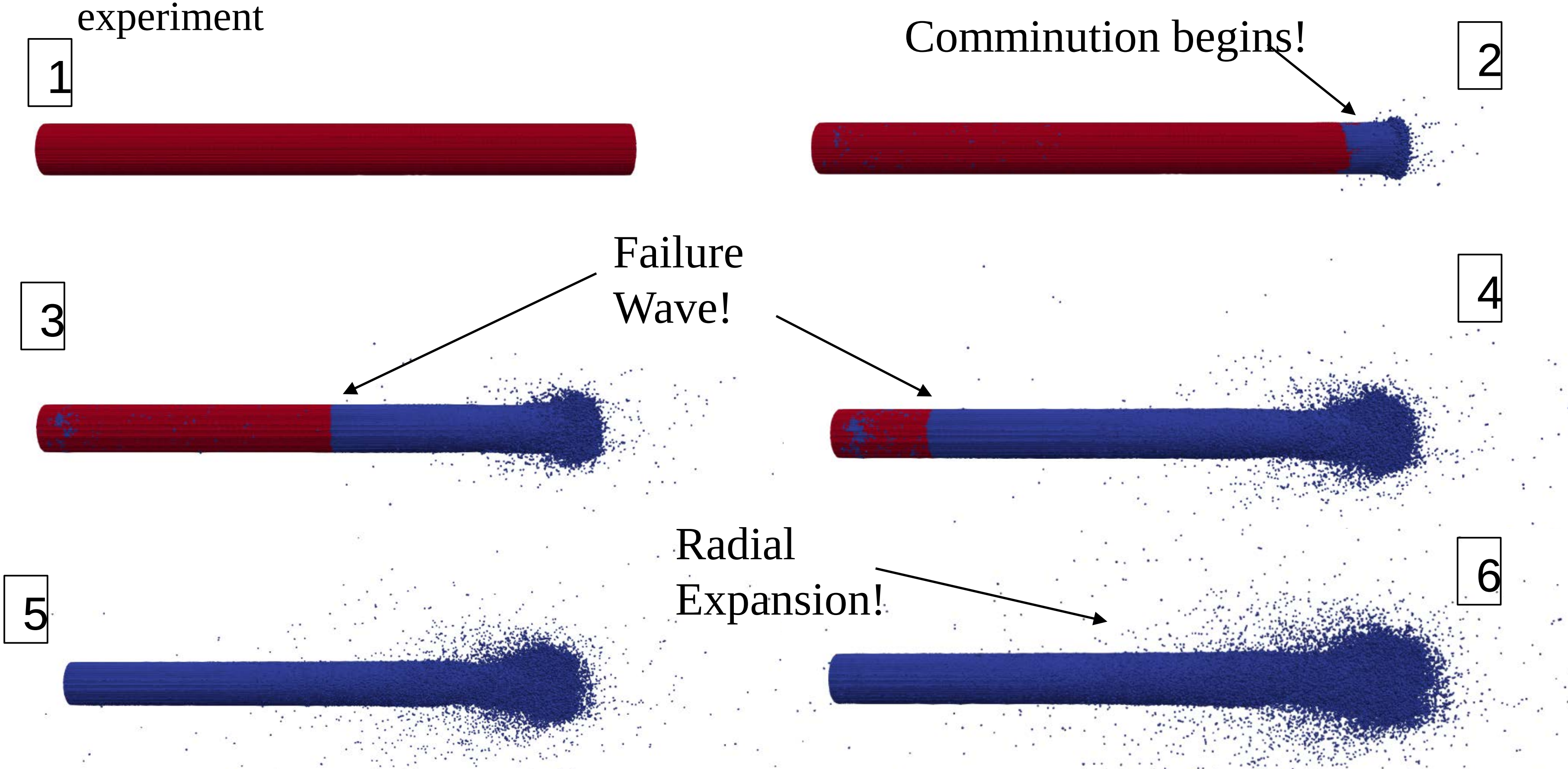
Close Agreement!

Michael Ortiz
ECCOMAS17

OTM Solver – Failure wave in glass rod

A faster impact speed: V = 336 m/s

- Again, the failure wave propagates in close agreement with experiment



- $V_{failure}$ (sim) = 5.4 mm/μs
- $V_{failure}$ (exp) = 5.2 mm/μs

} Close Agreement!

Multiscale modeling approach

Atomistic modeling of fused silica:

- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

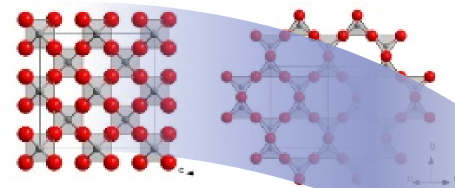
Mesoscopic modeling:

- Critical-state plasticity

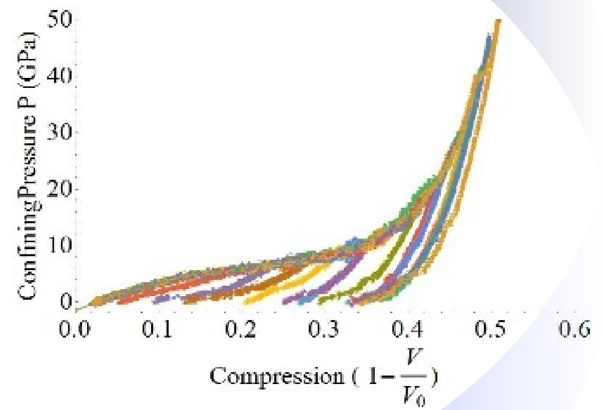
Macroscopic modeling:

- Relaxation

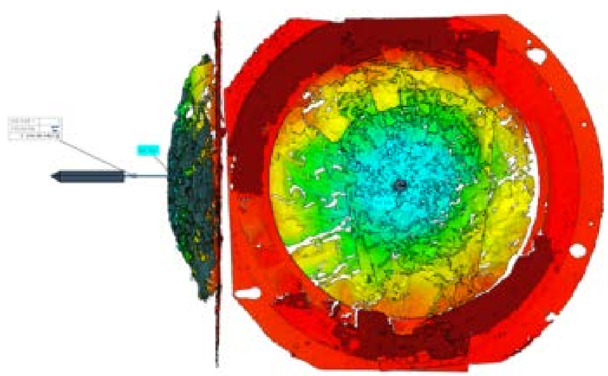
Continuum Models



Data Mining



(OTM ballistic simulation of brittle target , Courtesy B. Li)



Applications

Concluding remarks

- Fused silica glass (amorphous) lends itself ideally to multiscale modeling, atoms to solvers
- Elasticity and yielding of fused silica glass are anomalous:
  - *Shear modulus decreases with increasing pressure*
  - *Critical state line (limit elastic domain)* ***non-convex****!*
- Non-convexity of yielding can be relaxed (explicitly and in closed form) by allowing for stress patterning (under equilibrium constraint) at the microscale
- Particle solvers are powerful for applications involving complex fracture, fragmentation
- Unmodeled: Thermal EoS, thermal softening, nonlinear viscosity, shear banding...

Michael Ortiz
UPEN 2018