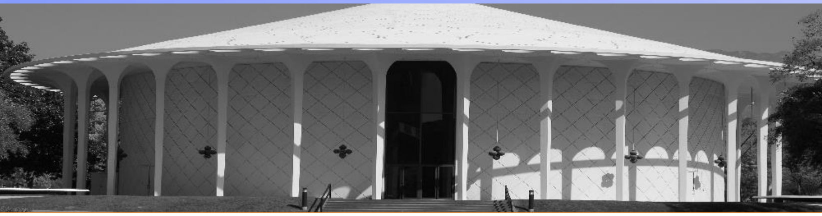
CALIFORNIA INSTITUTE OF TECHNOLOGY



universitätbonn

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

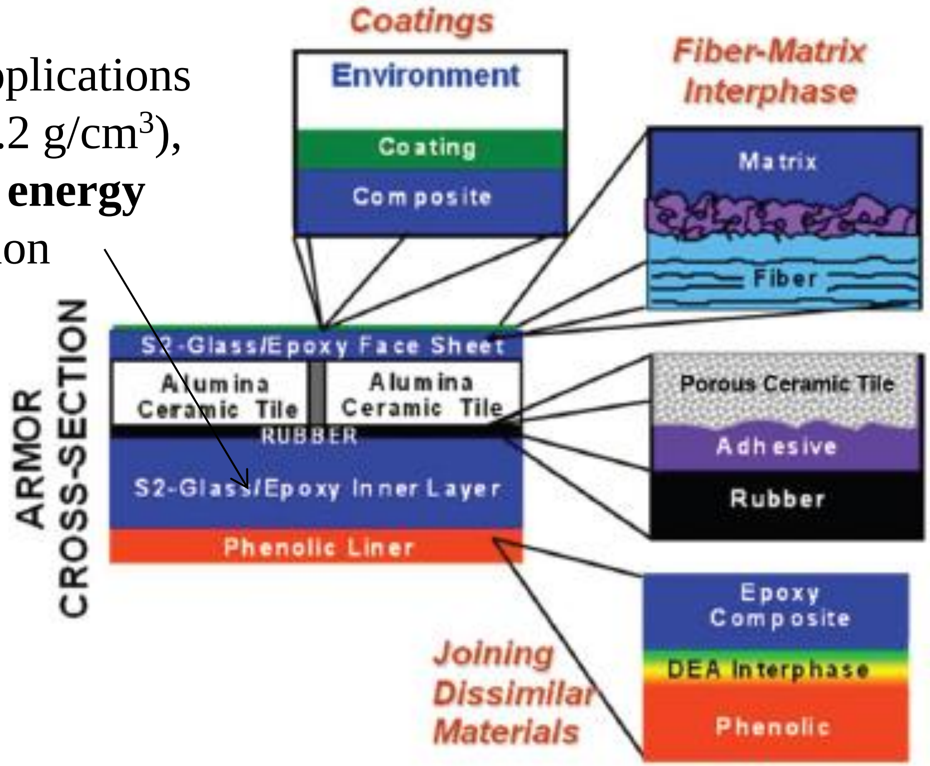
Michael Ortiz
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

ECCOMAS CMCS 2017
Computational Modeling of Complex Materials across the Scales

Espace Saint Martin, Paris, France
November 7, 2017

Glass as protection material

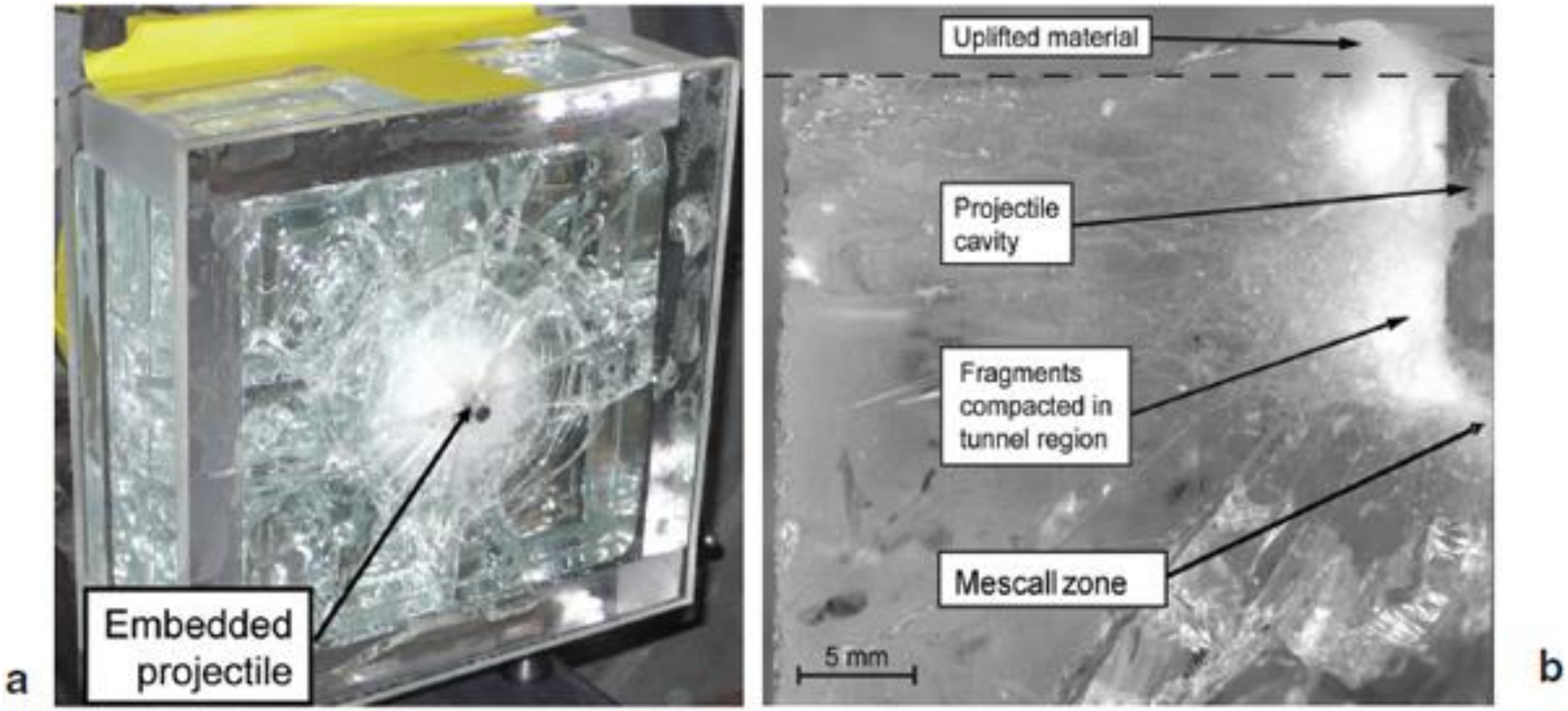
- Glass is attractive in many applications because of its **low density** (2.2 g/cm^3), **high strength** (5-6 GPa) and **energy dissipation** due to densification



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.

Glass as protection material

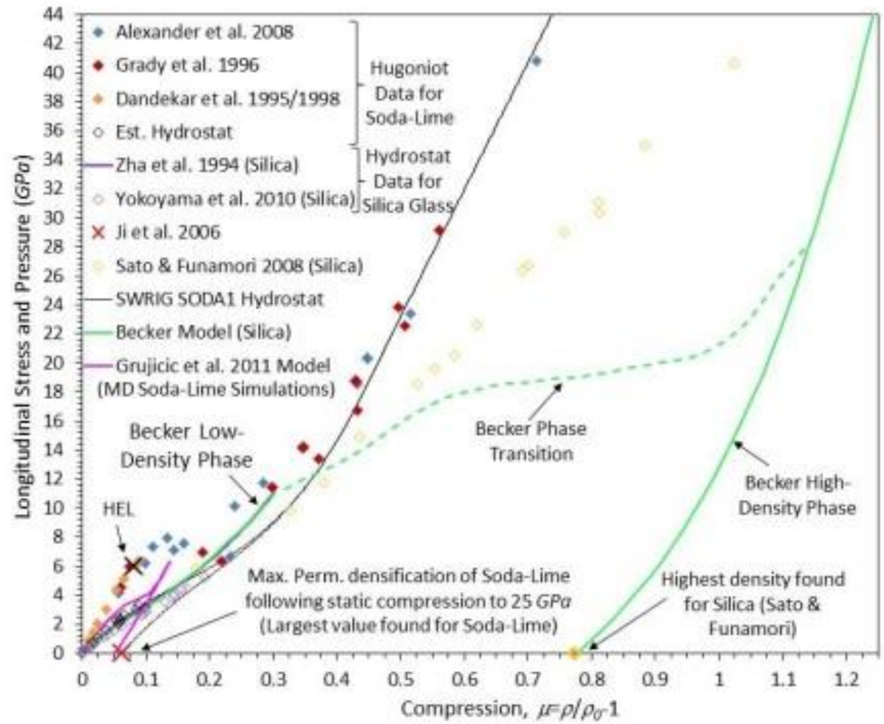


A soda lime glass target impacted by steel rod at 300 m/s[1].

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

Fused silica glass: Densification

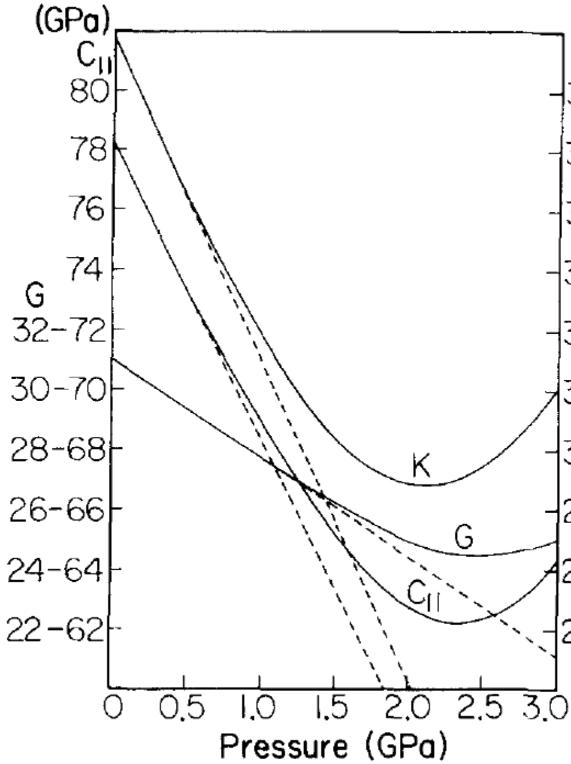
- The equation of state of glass in compression exhibits a **densification** phase transition at a pressure of 20 Gpa
- For a glass starting in its low-density phase, upon the attainment of the transition pressure the glass begins to undergo a **permanent reduction in volume**
- Reductions of up to 77% 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



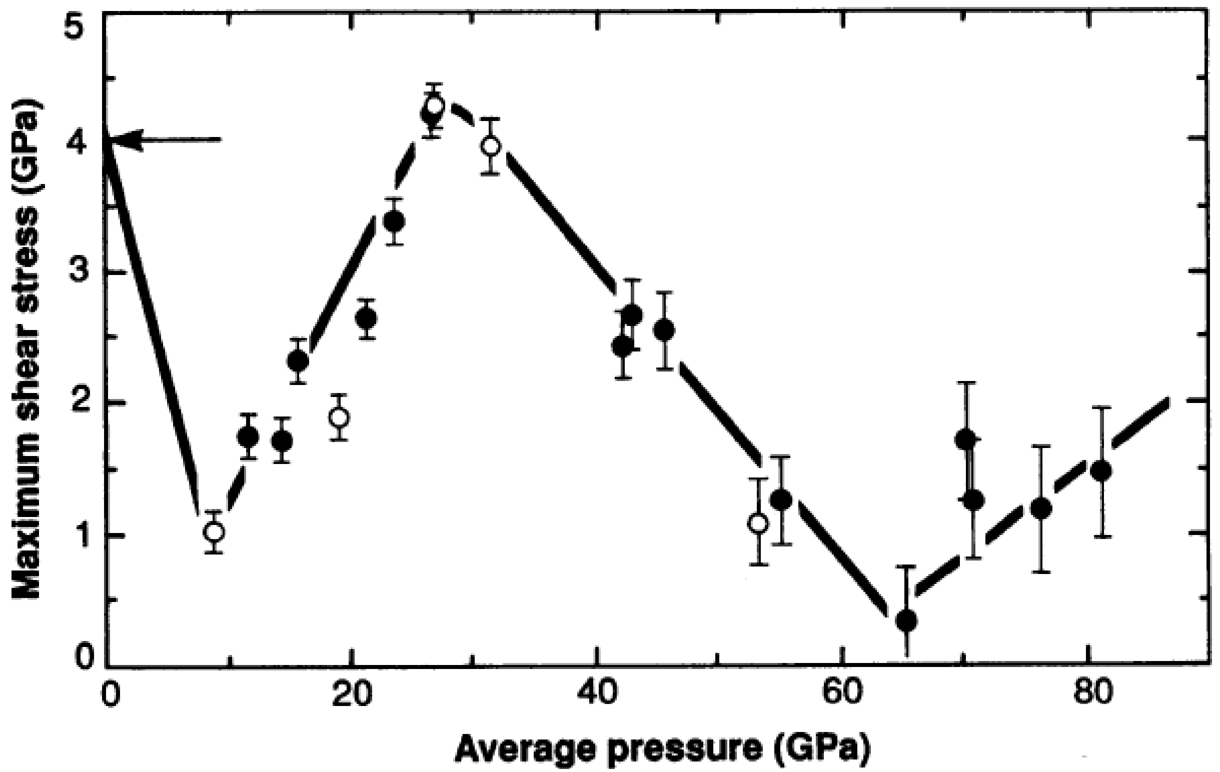
Compilation of equation-of-state data for glass (soda lime and fused silica)[1].

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

Fused silica glass: Pressure-shear



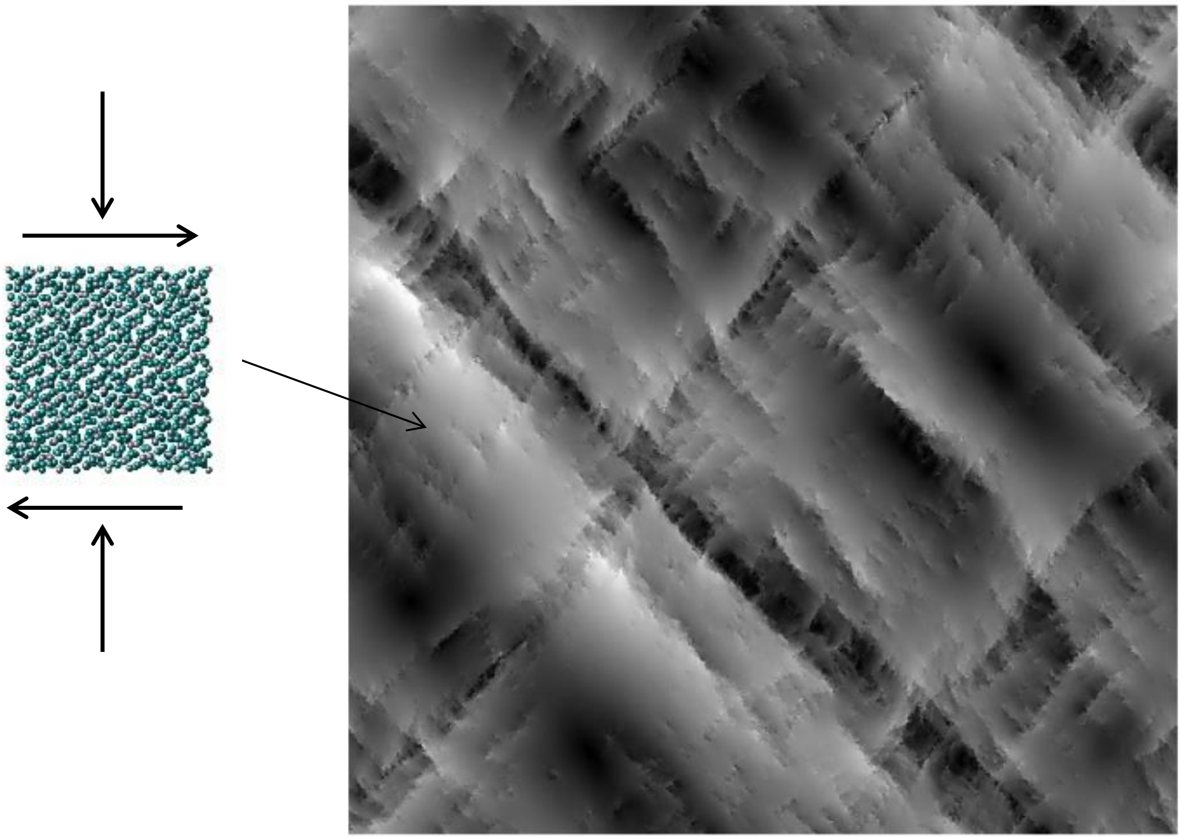
Measured elastic moduli showing *anomalous* dependence on pressure[1]



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



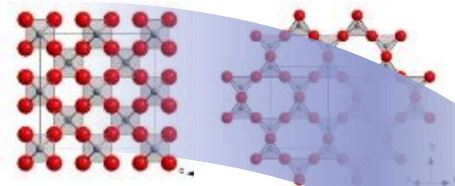
Molecular Dynamics (MD) simulation of amorphous solid showing patterning of deformation field[1]

[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



Data Mining

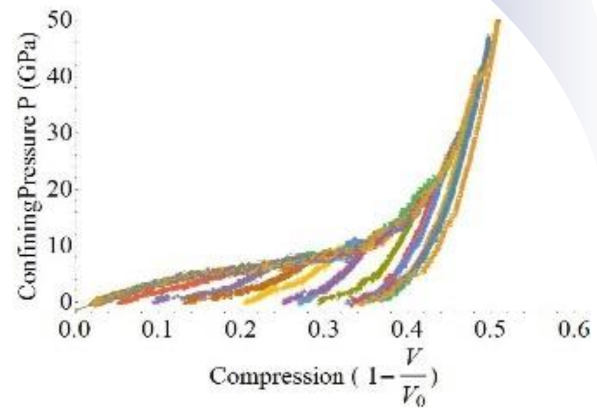
Mesoscopic modeling:

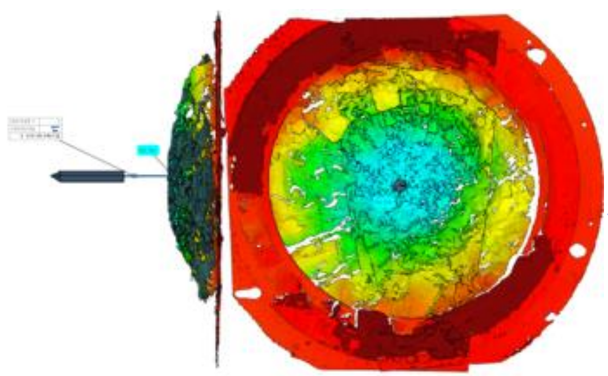
- Critical-state plasticity

Macroscopic modeling:

- Relaxation

Continuum Models

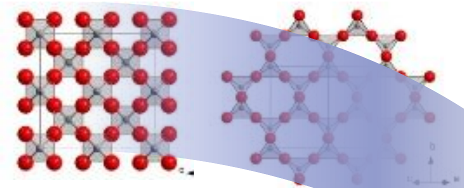




(OTM ballistic simulation of brittle target , Courtesy B. Li)

Applications

Multiscale modeling approach



Atomistic modeling of fused silica:

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

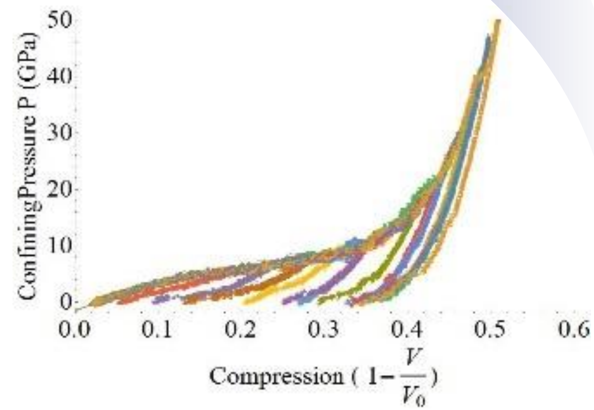
Mesoscopic modeling:

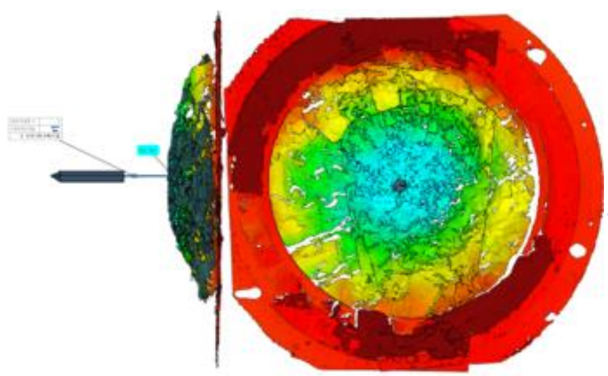
- Critical-state plasticity

Macroscopic modeling:

- Relaxation

Continuum Models





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

Applications

Michael Ortiz
CMCS 2017

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**
- Important Features: Rapid/absolute convergence, domain independence

Time integration:

- **Velocity-Verlet** time integration scheme
- Important Features: Time reversible, symplectic, one force evaluation per step

Other computational details:

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

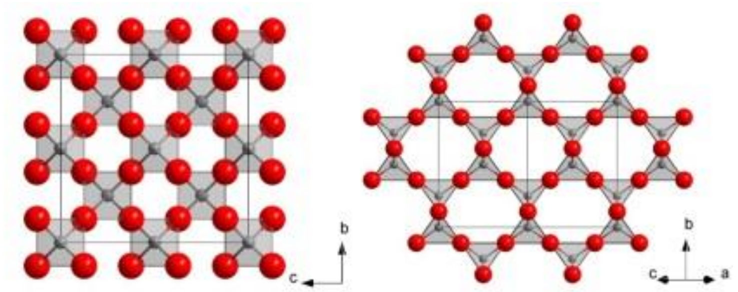
Schill, W., Hayden, S., Conti, S. and Ortiz, M., arXiv:1710.05077[cond-mat.soft] 26 Oct 2017.

RVE setup – Quenching

Starting structure: β-cristobalite

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

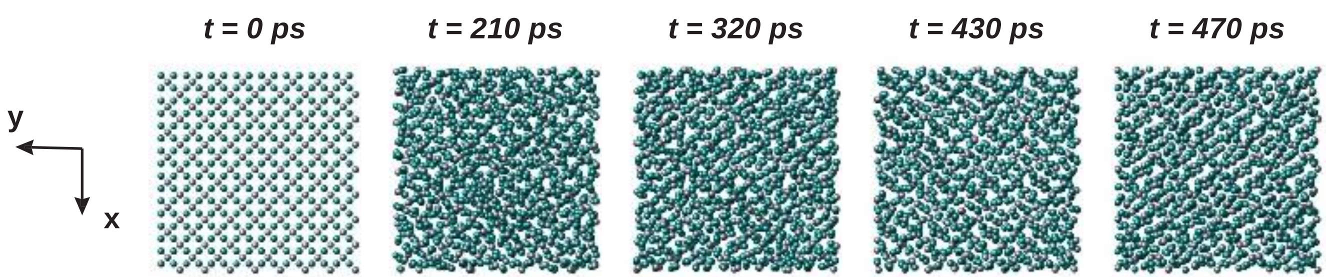
Amorphous structure of fused silica: Obtained through the **fast quenching** of a melt



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

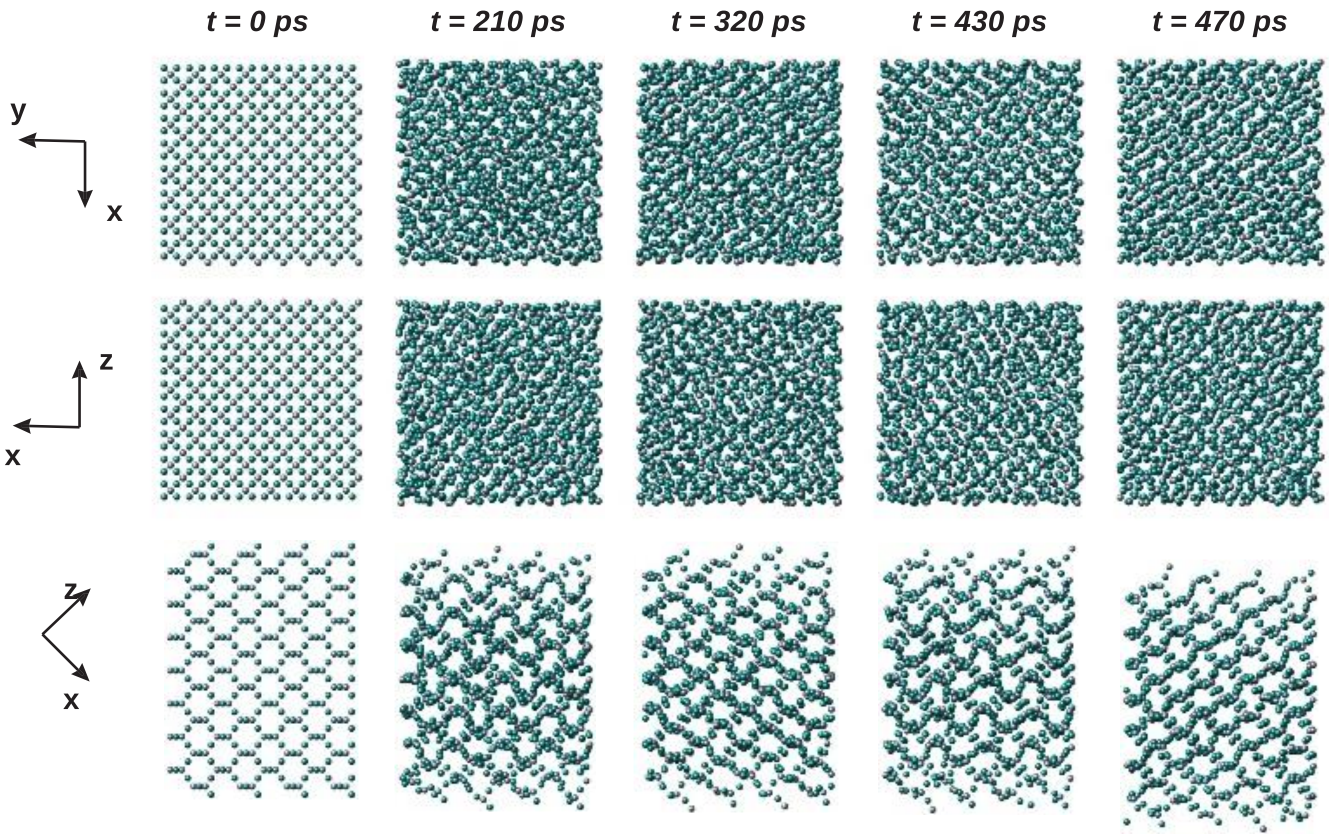
Steps taken during **quenching** process:

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



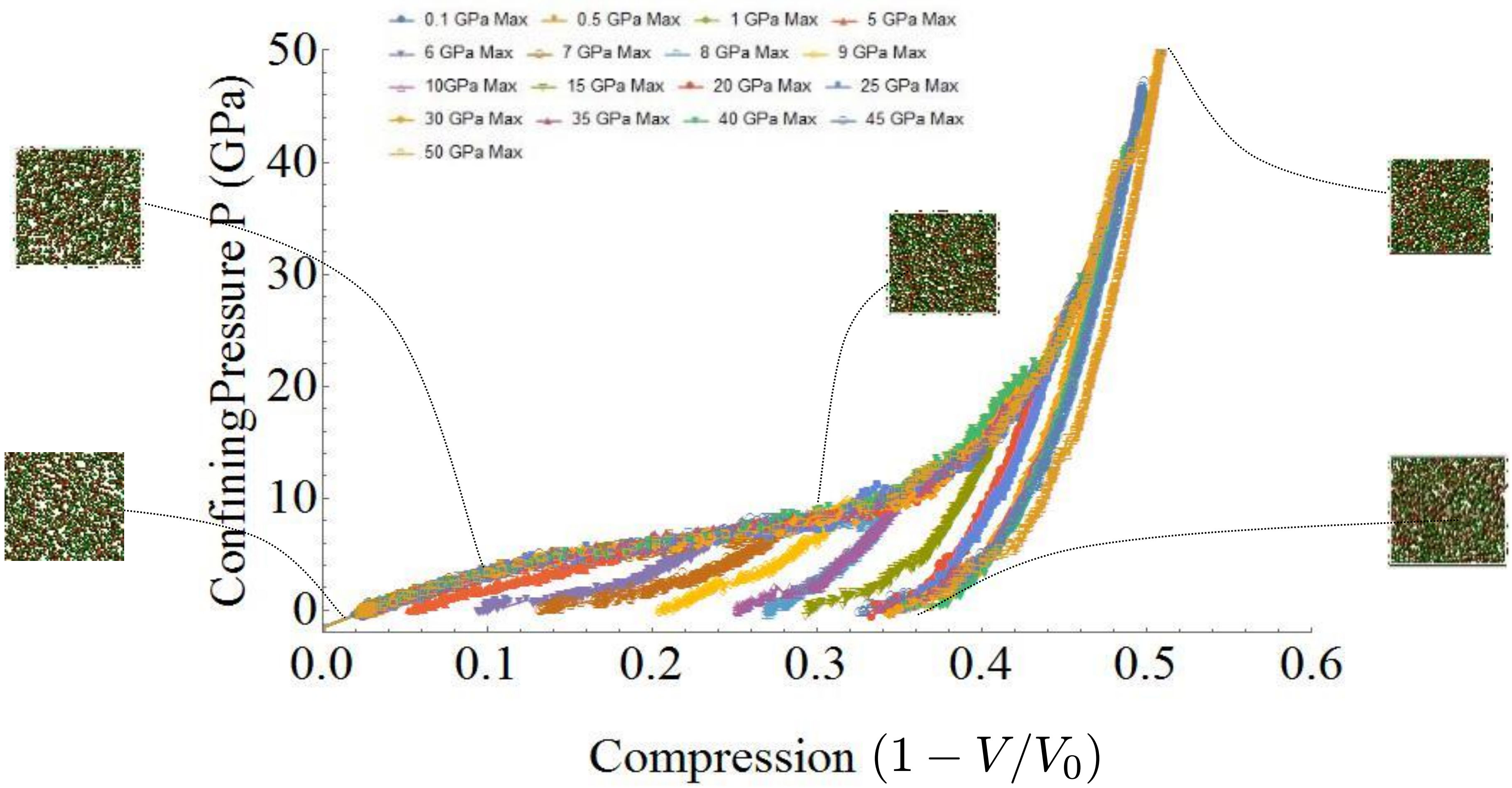
RVE setup – Quenching

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



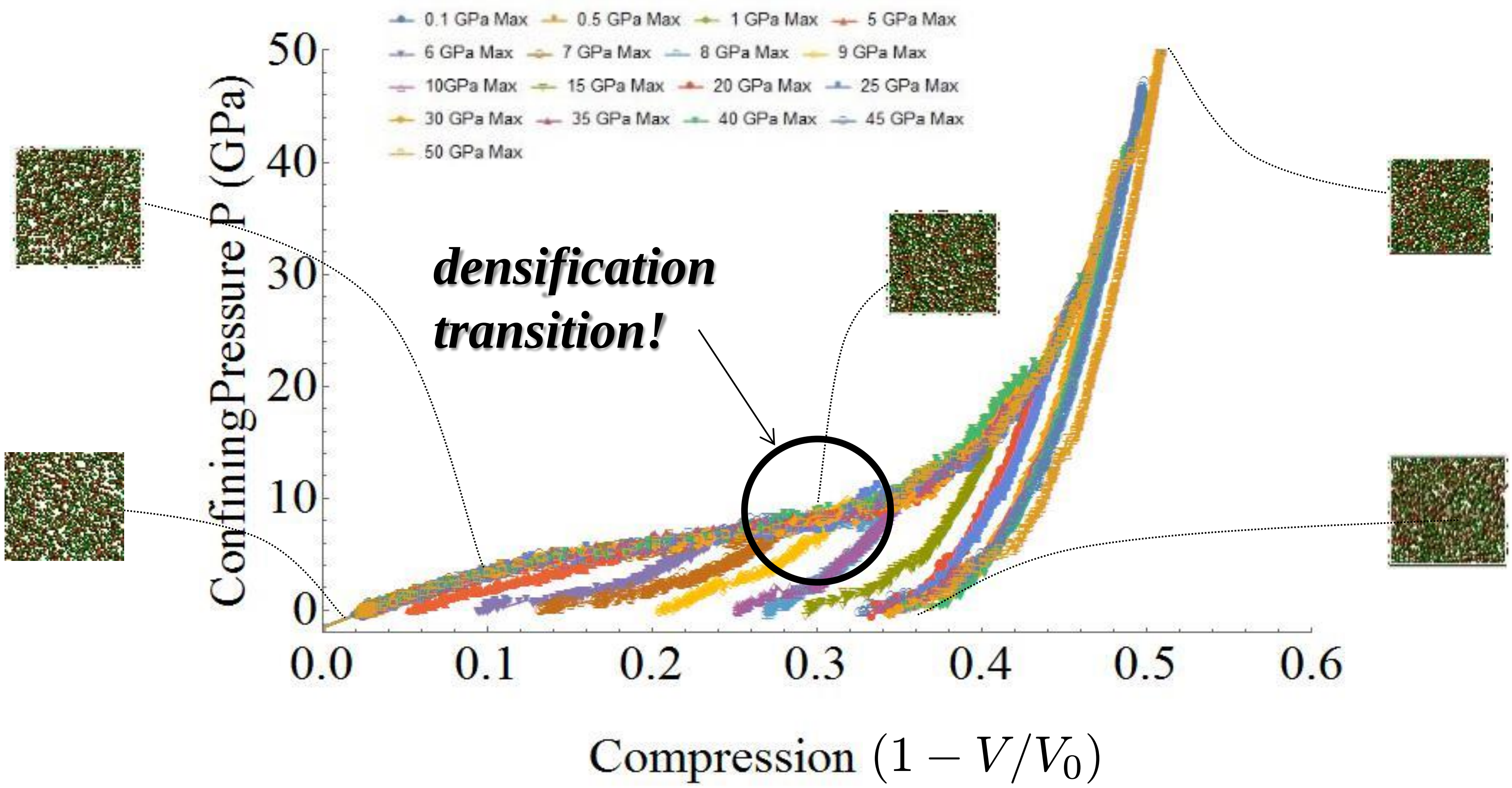
Quenching procedure for the generation of amorphous silica.T=5000K at t=0ps and T=300K at t=470ps.

Results – Volumetric compression



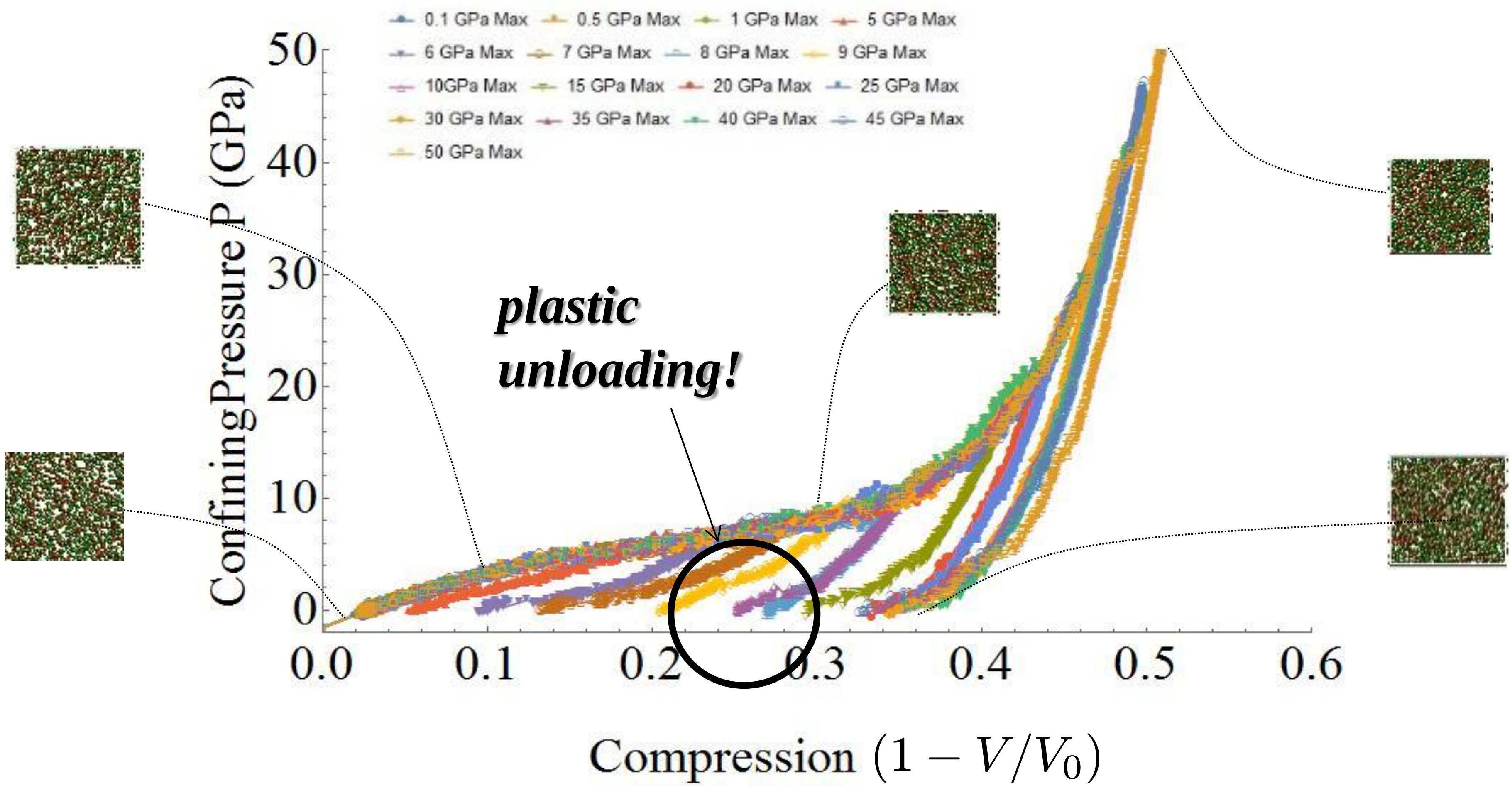
Michael Ortiz
CMCS 2017

Results – Volumetric compression



Michael Ortiz
CMCS 2017

Results – Volumetric compression

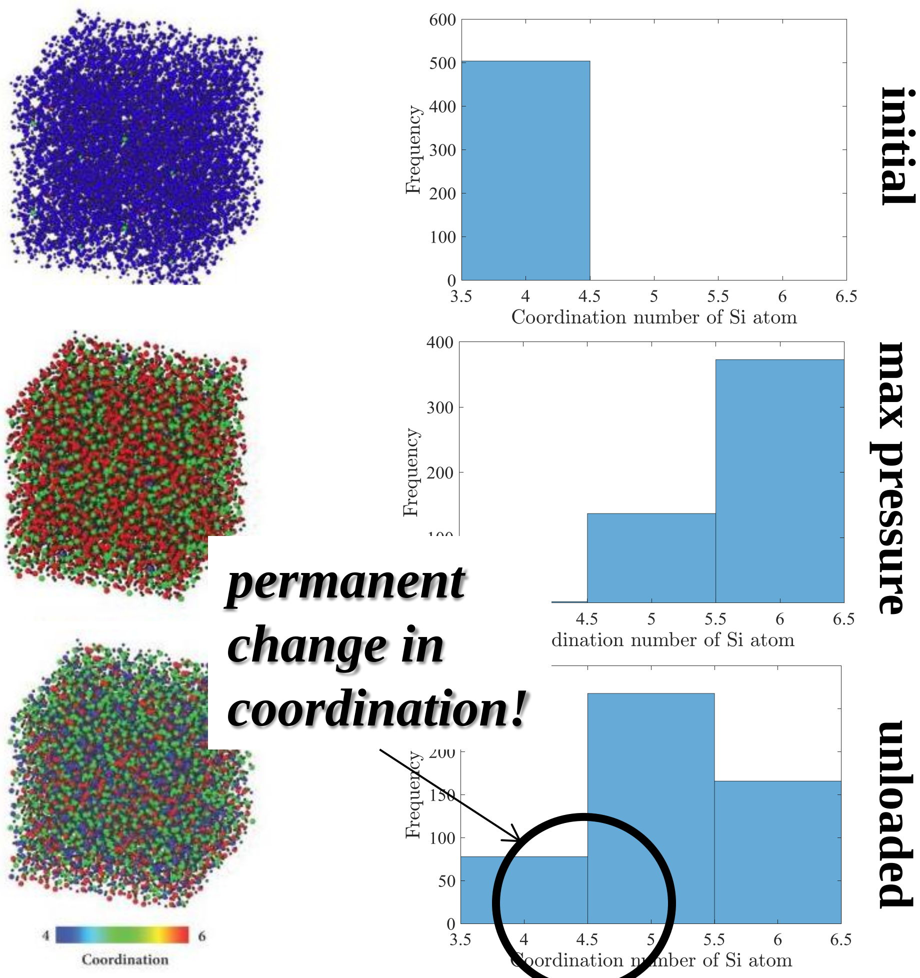


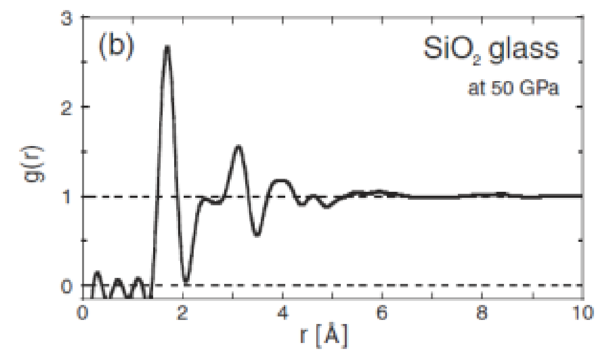
Michael Ortiz
CMCS 2017

Molecular basis of densification

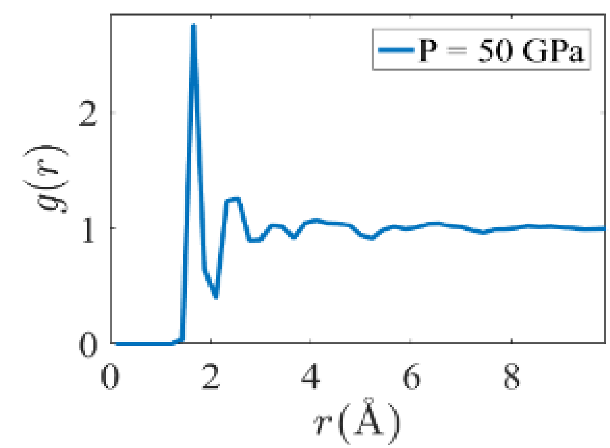
Hydrostatic compression/ decompression of amorphous silica:

- Molecular dynamics results exhibit irreversible densification at 14-20 GPa
- Molecular dynamics generated rdf are in good overall agreement with data





(Sato and Funamori, 2010)

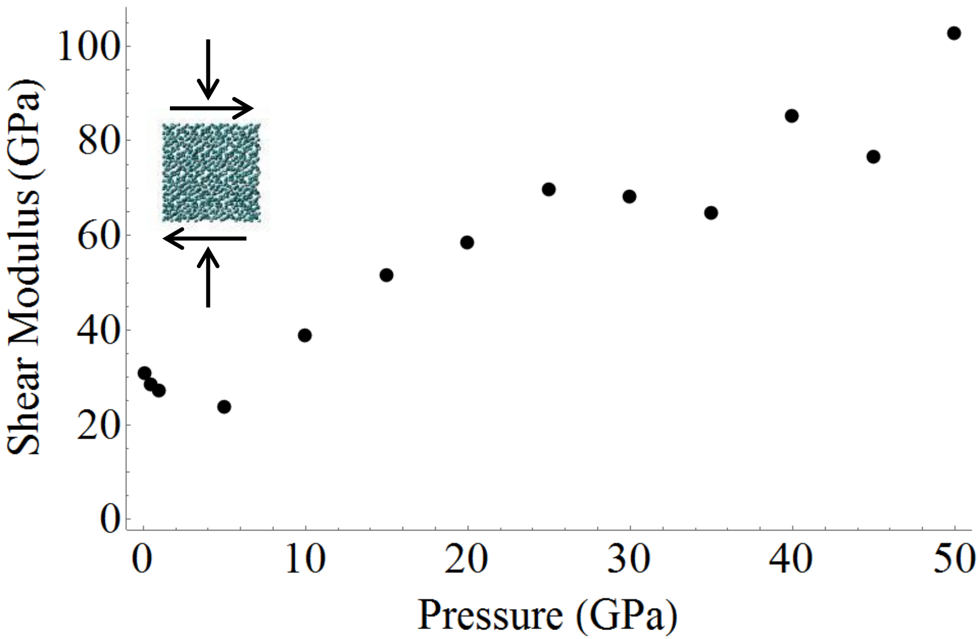


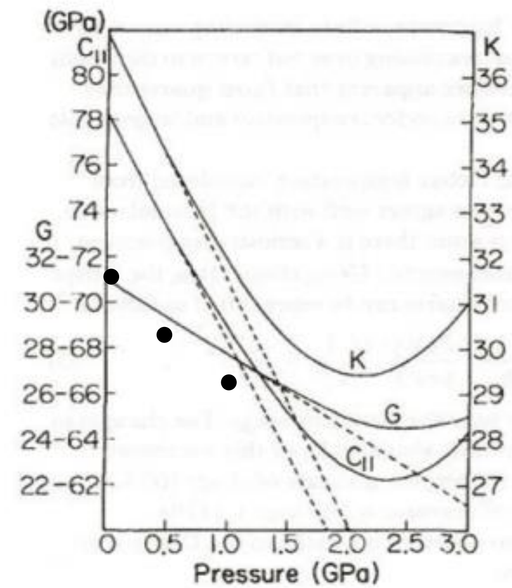
Ortiz
2017

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





Kondo et al. (1981)

Initial shear modulus *versus* pressure

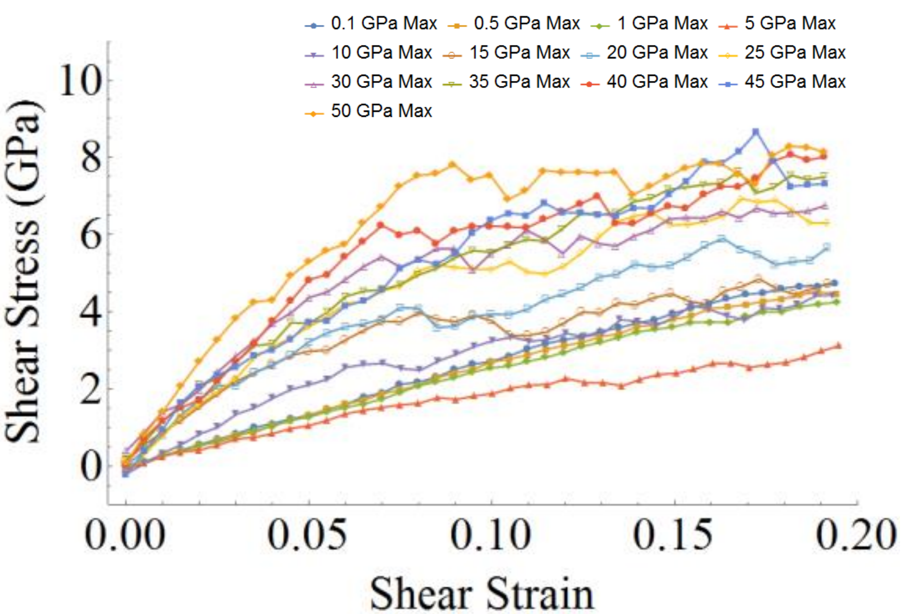
Anomalous pressure dependence of shear modulus!

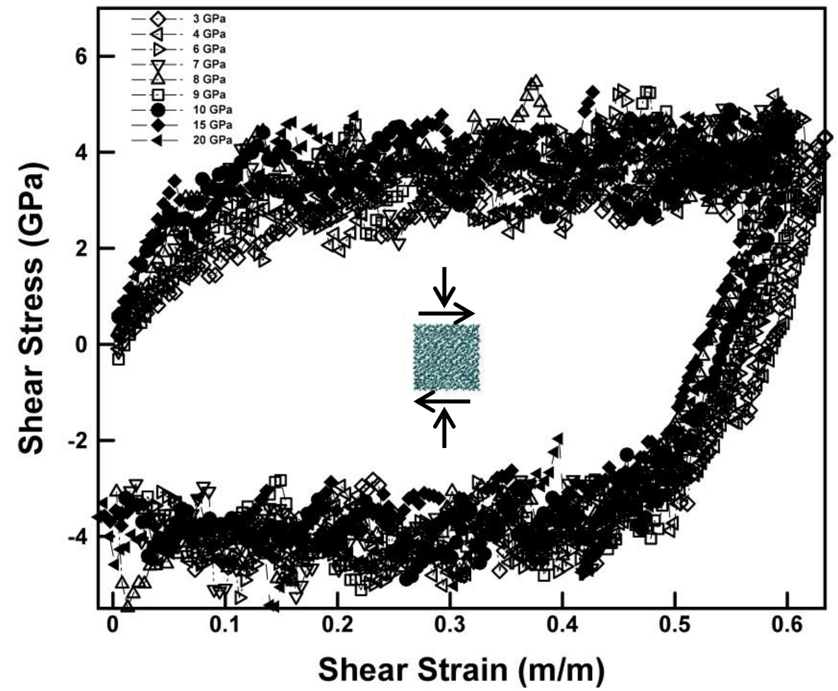
(shear modulus initially decreases with increasing pressure)

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!

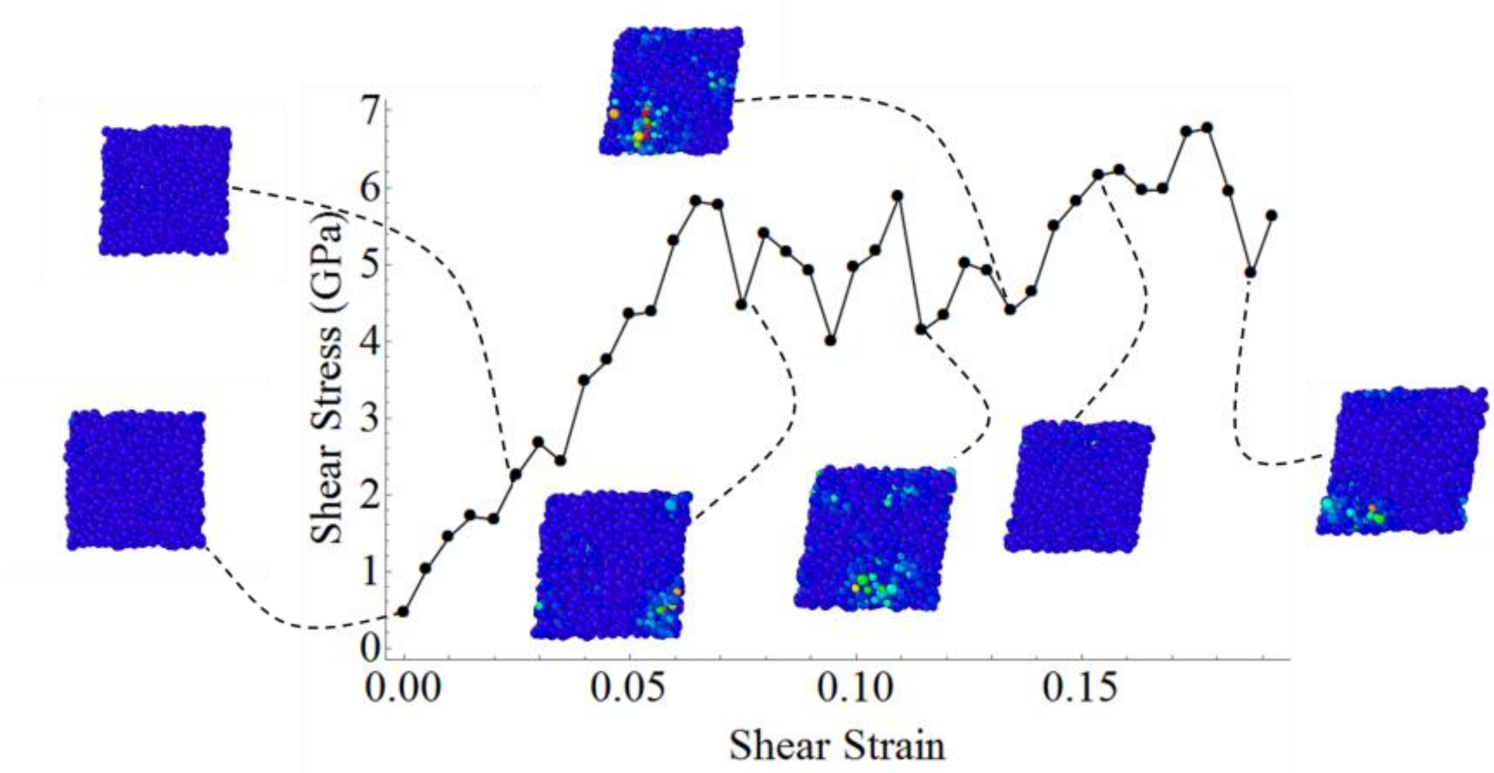
(permanent or plastic shear deformation, pressure-dependent plasticity)

Michael Ortiz
CMCS 2017

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!

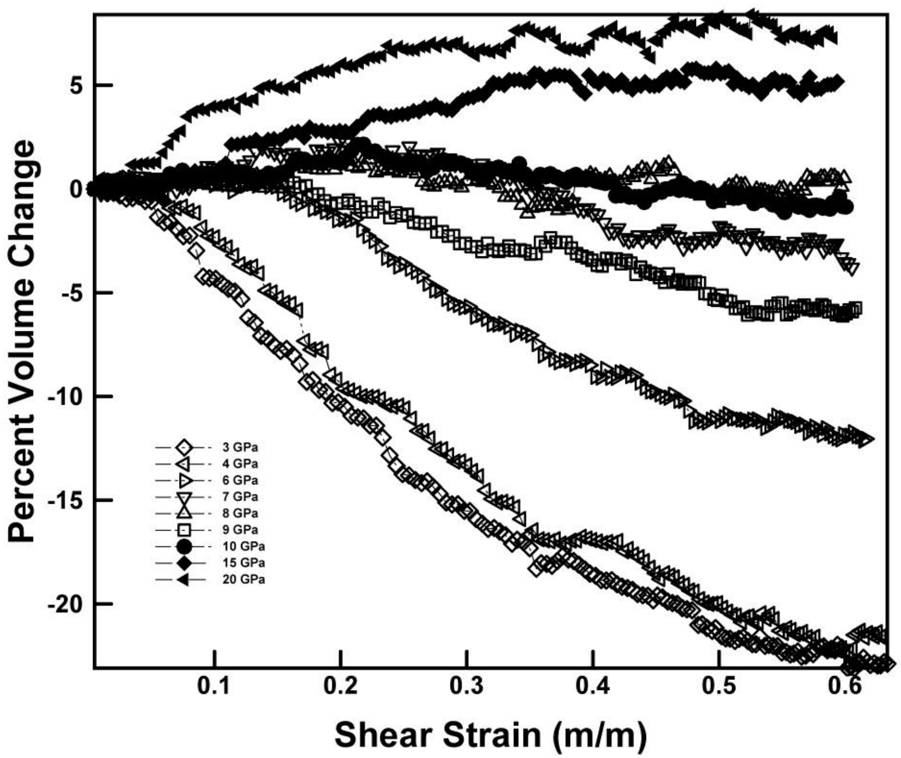
(shear deformation proceeds inhomogeneously through local bursts)

Michael Ortiz
CMCS 2017

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:

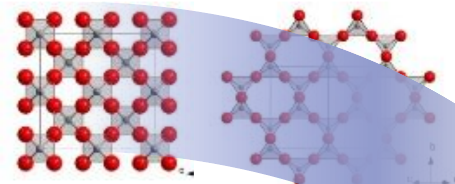
- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

Mesoscopic modeling:

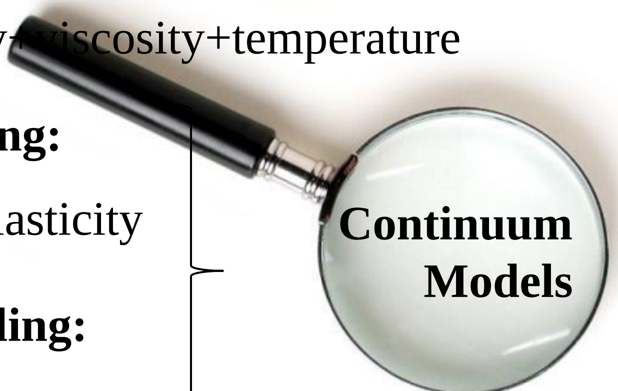
- Critical-state plasticity

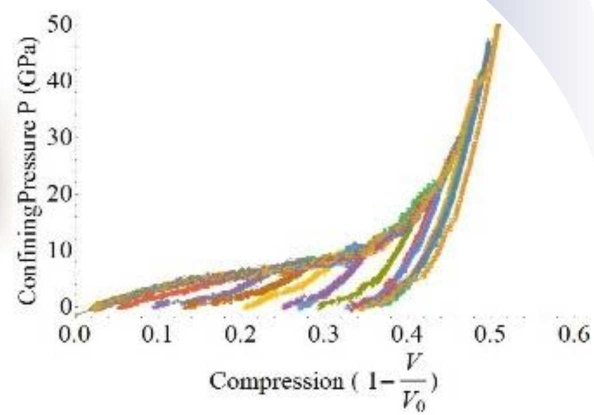
Macroscopic modeling:

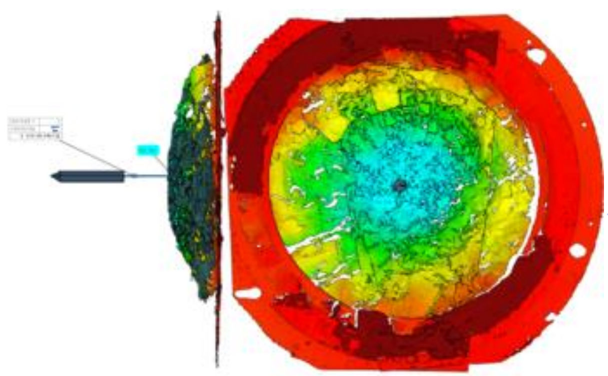
- Relaxation



Data Mining







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

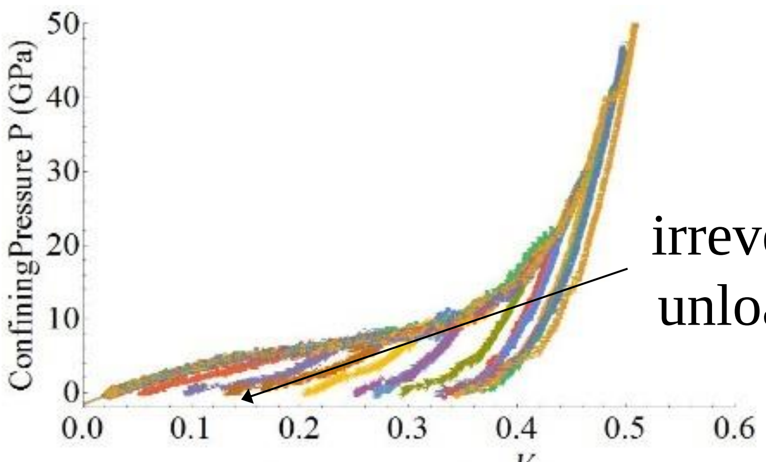
Applications

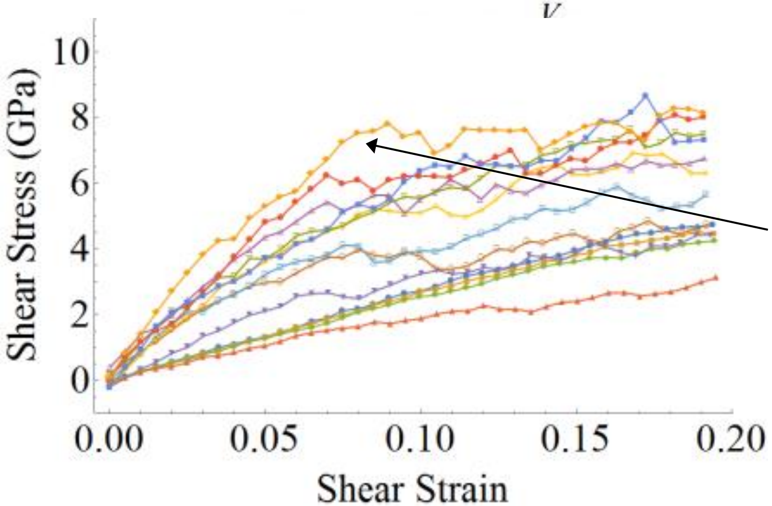
Michael Ortiz
CMCS 2017

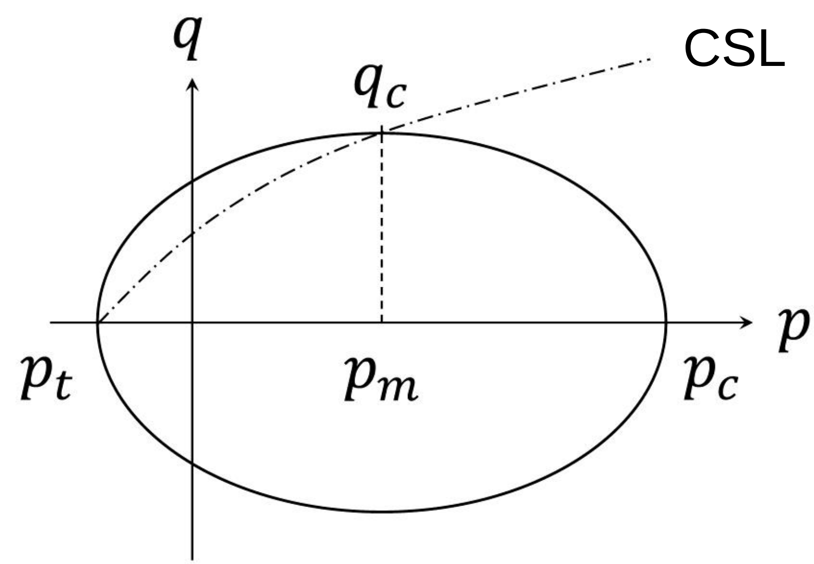
Critical-state plasticity model

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)

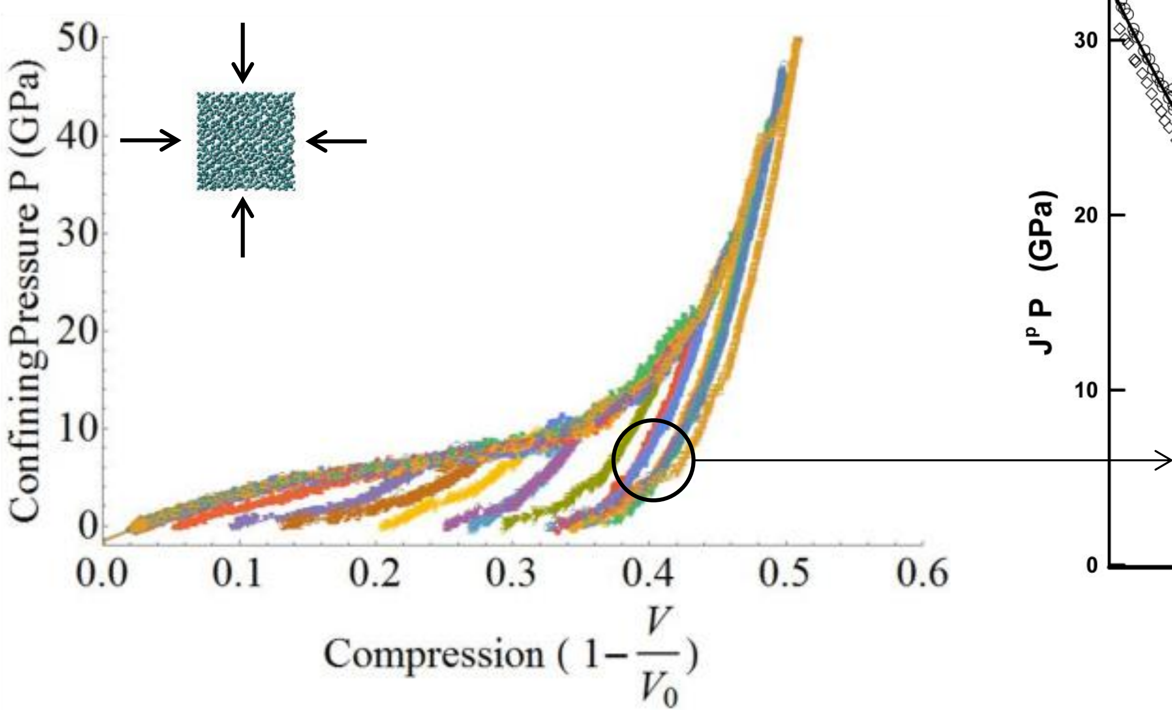
Michael Ortiz
CMCS 2017

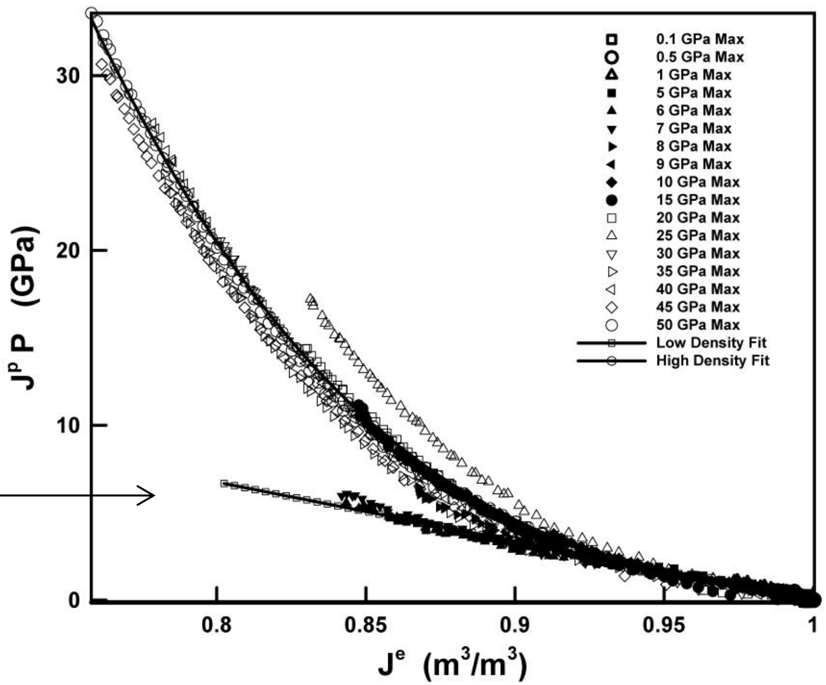
Schill, W., Hayden, S., Conti, S. and Ortiz, M., arXiv:1710.05077[cond-mat.soft] 2017.

Volumetric equation of state

Implementation Verification:

- Volumetric Compression Test Case
- Agreement with Molecular Dynamics Data is Obtained



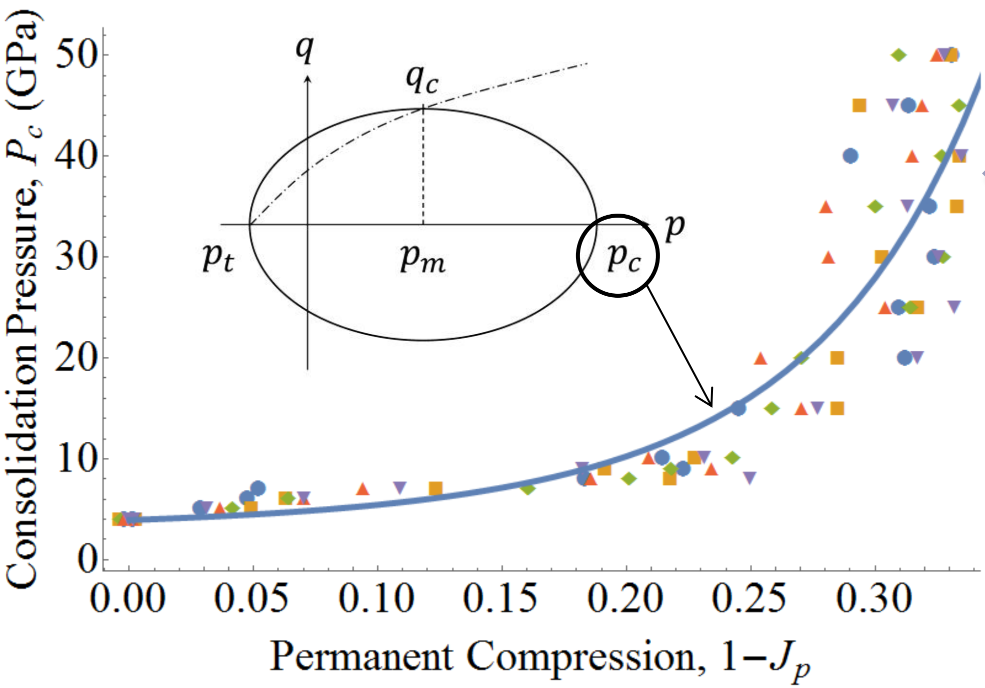


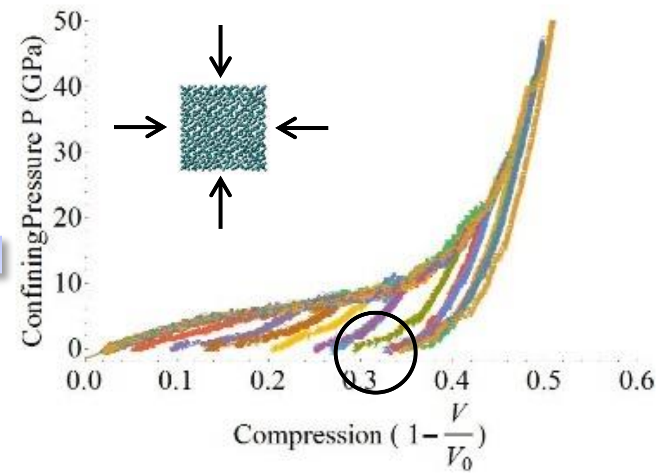
Michael Ortiz
CMCS 2017

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

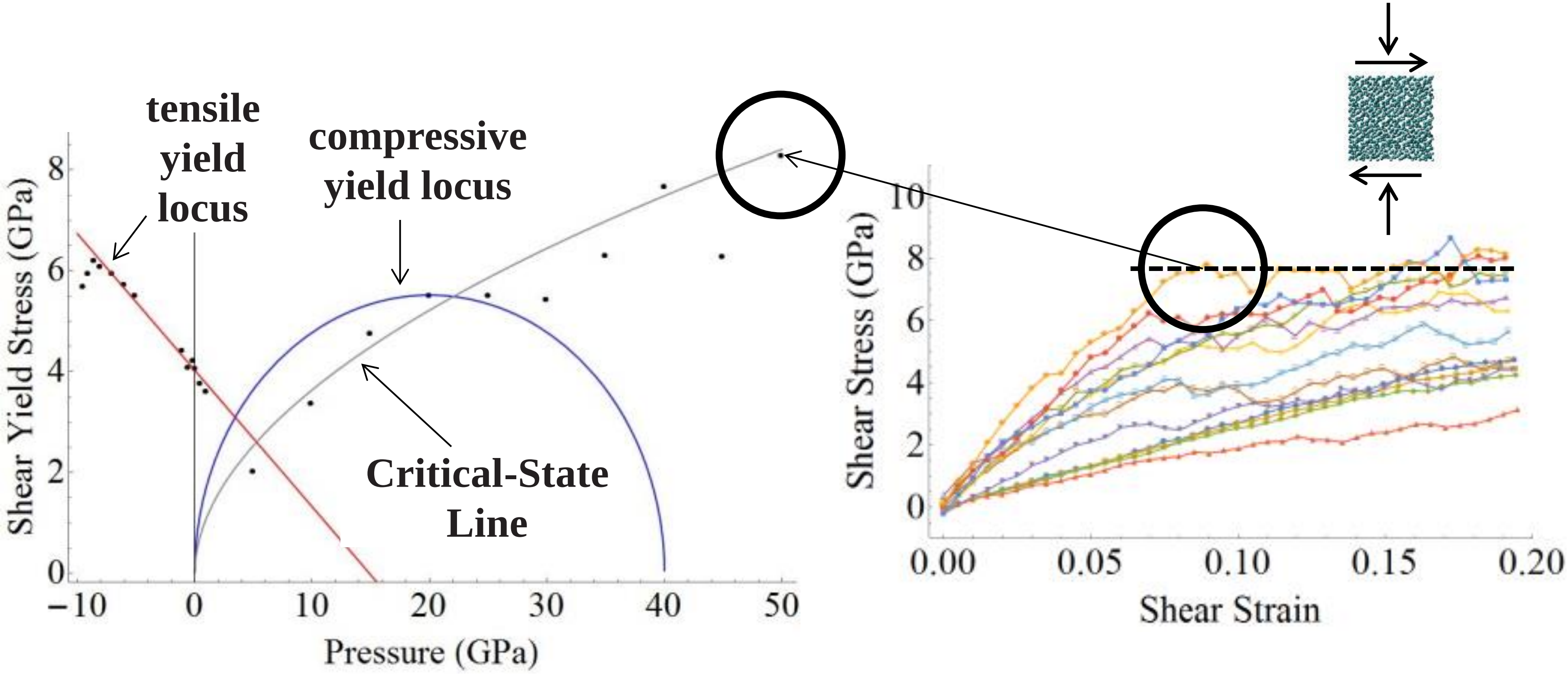
K_B	k_b	Γ
8.48613 GPa	9.2689	3.02934 GPa

Schill, W., Hayden, S., Conti, S. and Ortiz, M., arXiv:1710.05077[cond-mat.soft] 26 Oct 2017.

Critical-state plasticity model

Yield Surface:

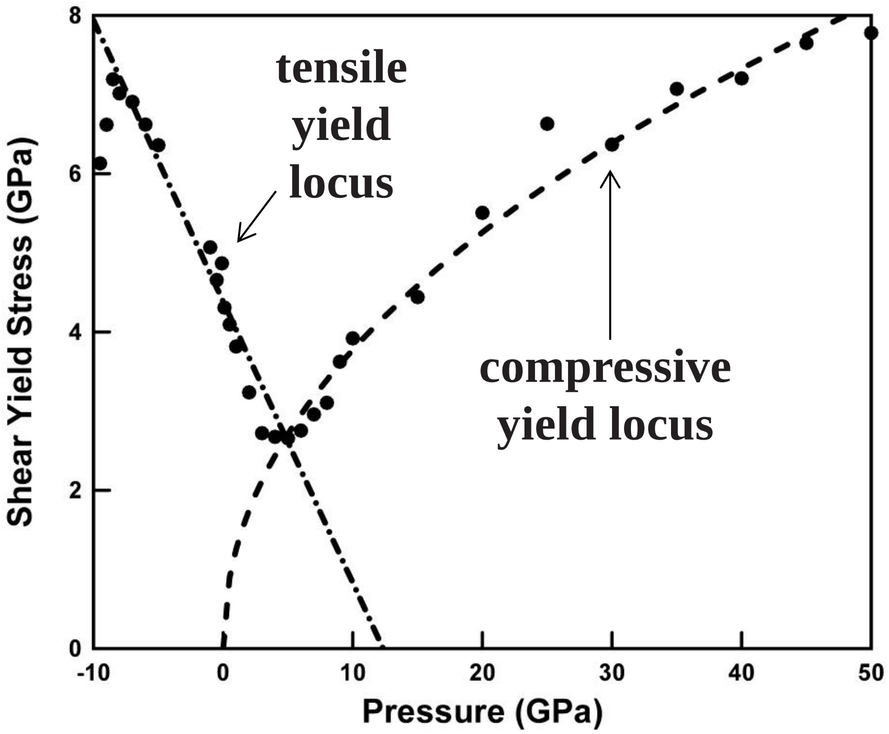
- Identify computed shear yield stress–pressure relationship as Critical Line

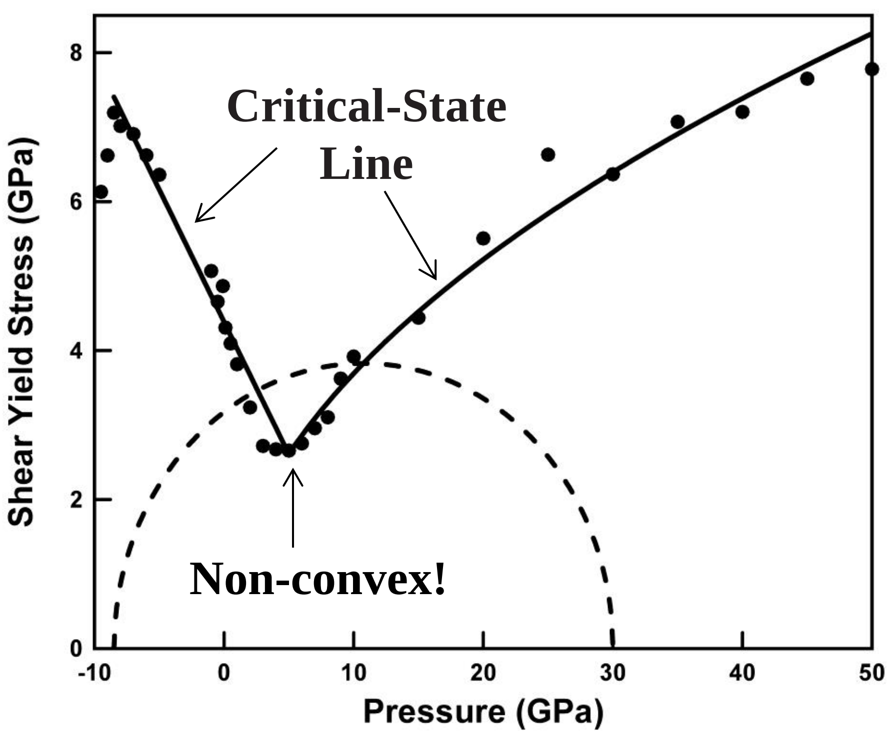


Anomalous pressure dependence of shear yield stress!
Non-convex critical-state line!

Michael Ortiz
CMCS 2017

Critical-state plasticity model





Anomalous pressure dependence of shear yield stress!
Non-convex critical-state line !

Michael Ortiz
CMCS 2017

Anomalous plasticity of fused silica

Effect of a Coordination Change on the Strength of Amorphous SiO_2

CHARLES MEADE AND RAYMOND JEANLOZ

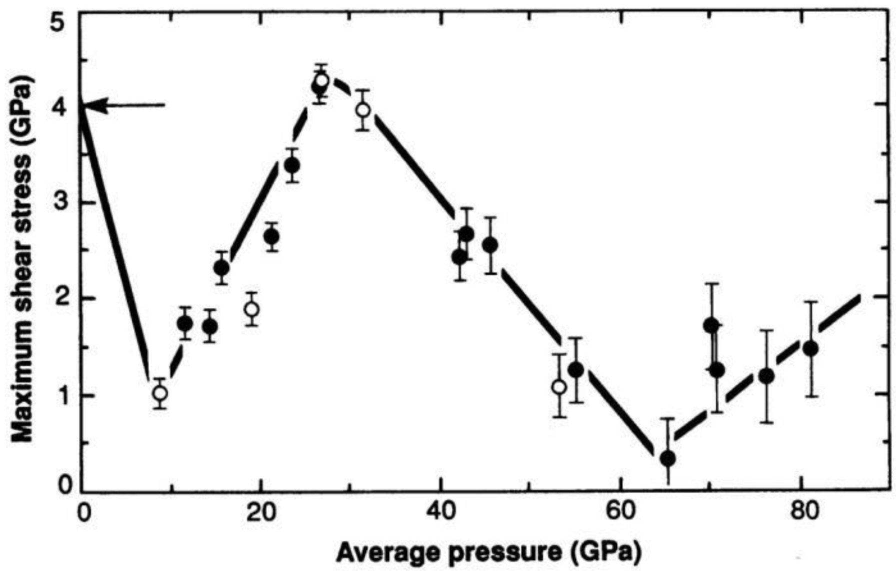


Fig. 1. Maximum shear stress in silica glass at room temperature and average pressures ($\bar{P}$) between 8.6 and 81 GPa. Each point corresponds to a separate sample, and the heavy line shows the general trend of the data. The shear stress is determined from Eq. 1, and it is a measure of the yield strength 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*).

Anomalous shear yield stress documented in geophysics literature!

Multiscale modeling approach

Atomistic modeling of fused silica:

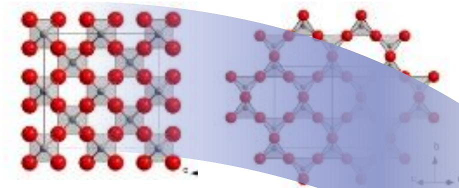
- Volumetric response (hysteretic)
- Pressure-dependent shear response
- Rate-sensitivity+viscosity+temperature

Mesoscopic modeling:

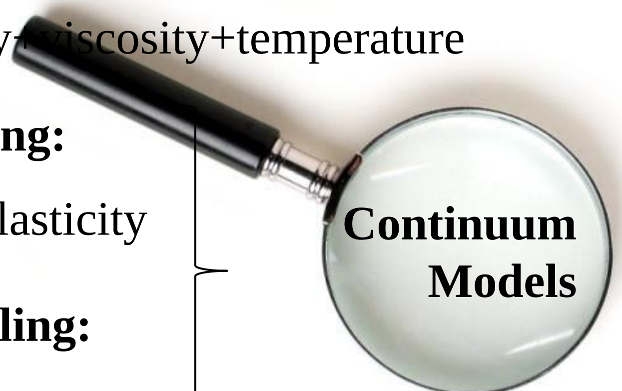
- Critical-state plasticity

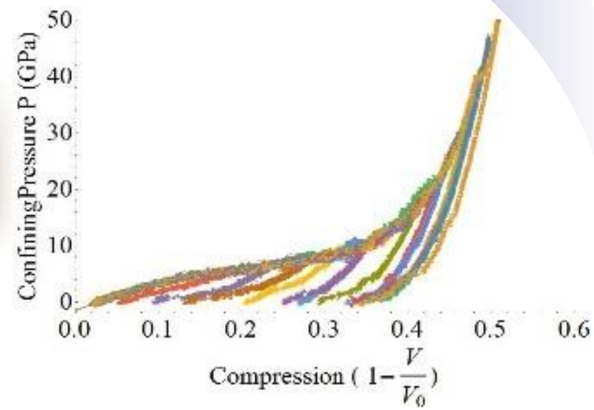
Macroscopic modeling:

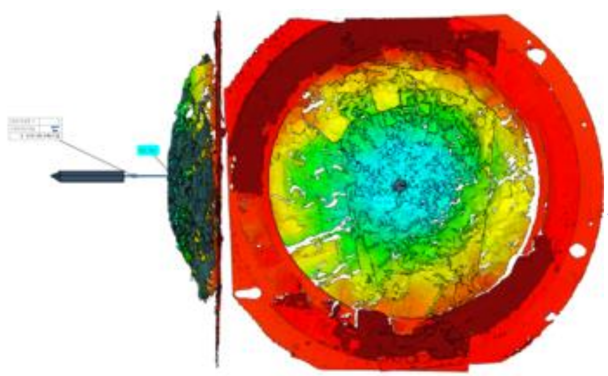
- Relaxation



Data Mining







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

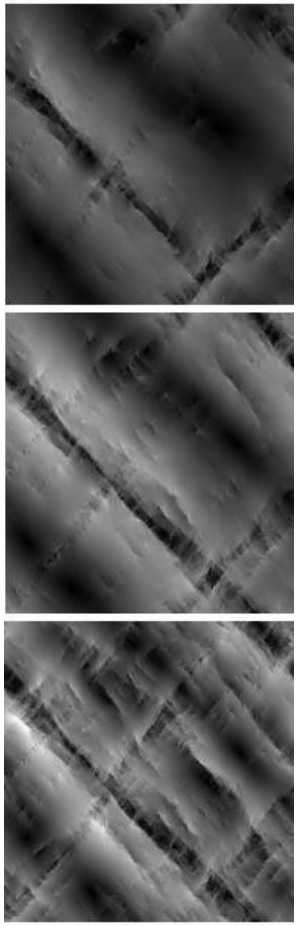
Applications

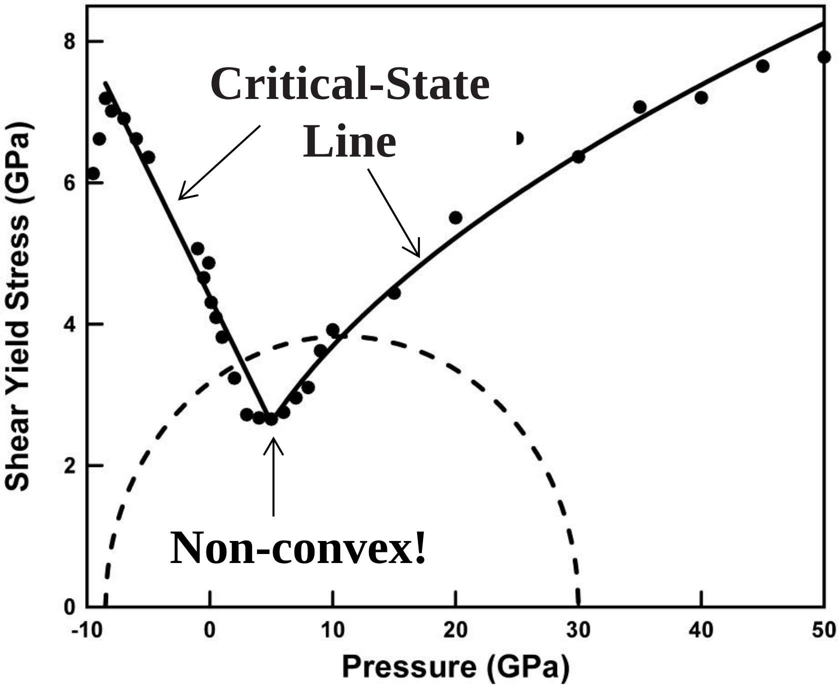
Michael Ortiz
CMCS 2017

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) ⟶



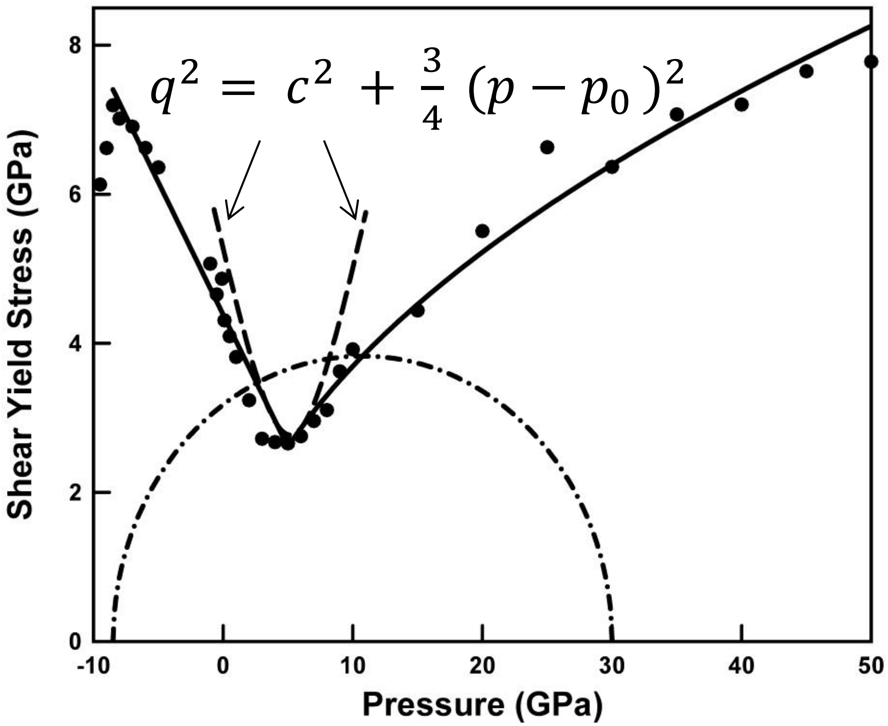


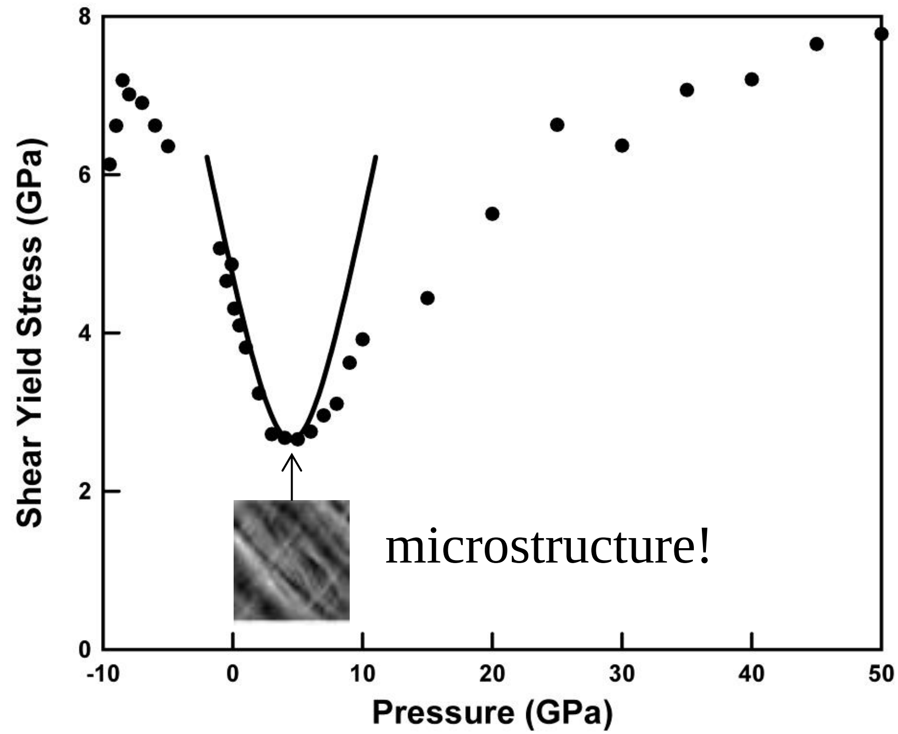
[1]C.E. Maloney and M.O. Robbins, *J. Phys.: Cond. Matter*, 20(24):244128, 2008.
Schill, W., Hayden, S., Conti, S. and Ortiz, M., arXiv:1710.05077[cond-mat.soft] 2017.

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.

Multiscale modeling approach

Atomistic modeling of fused silica:

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

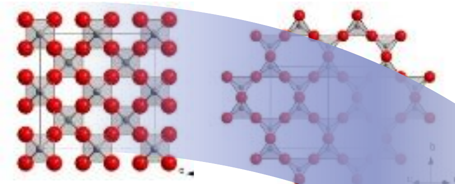
Mesoscopic modeling:

- Critical-state plasticity

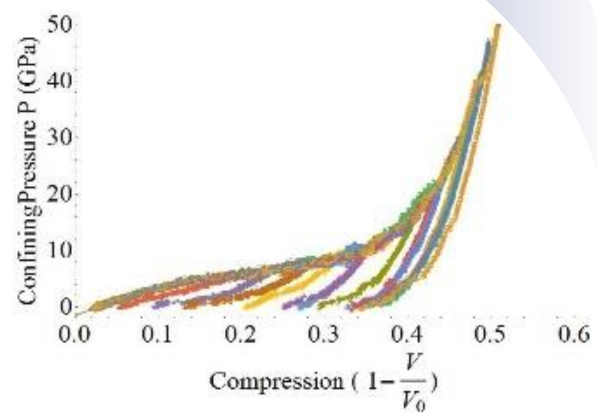
Macroscopic modeling:

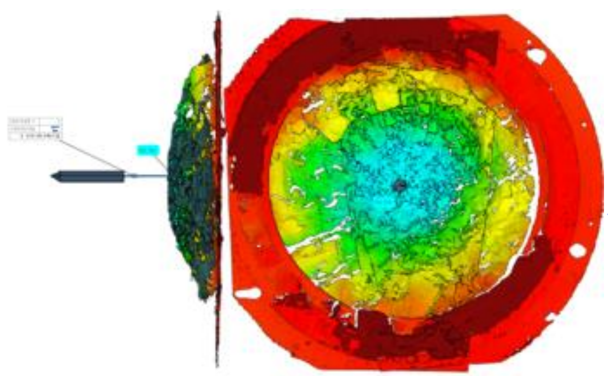
- Relaxation

Continuum Models



Data Mining

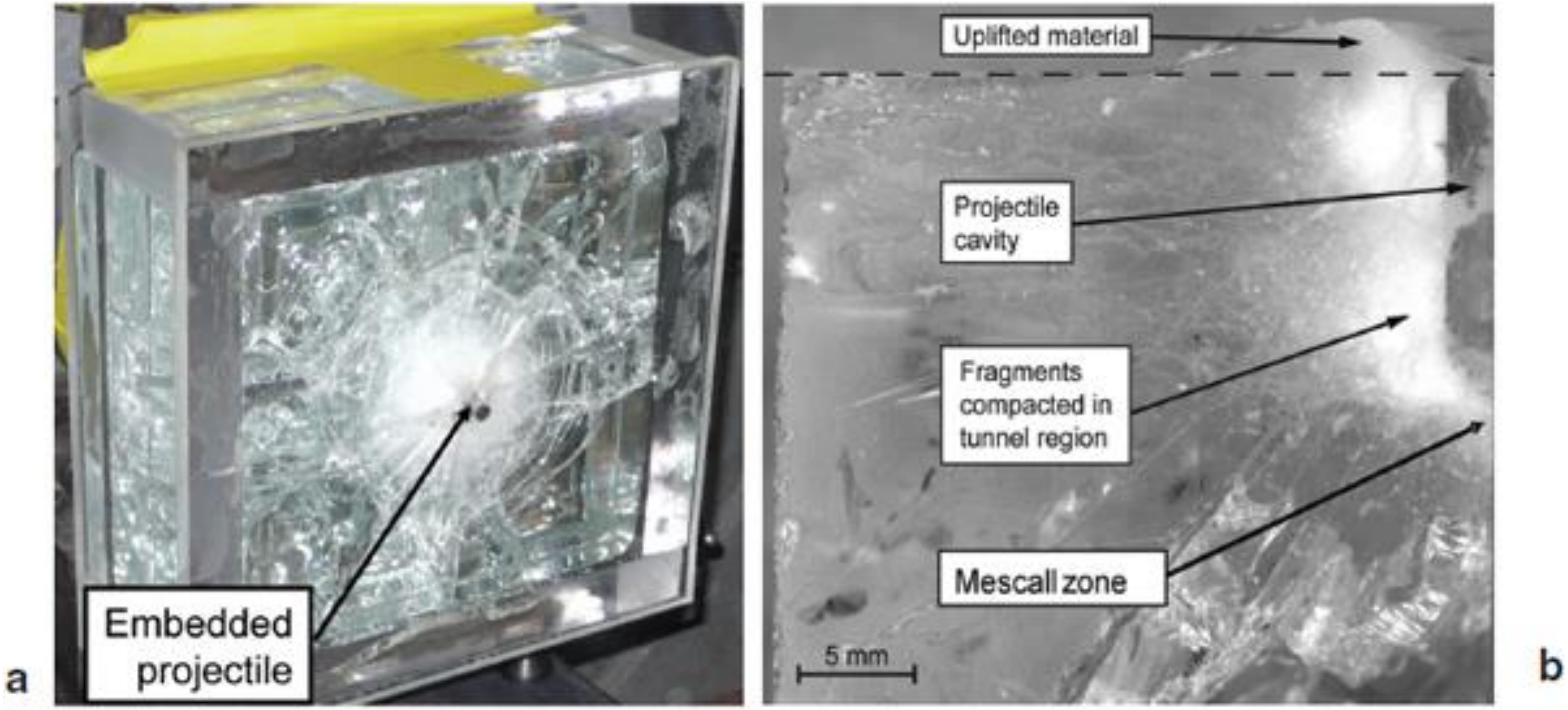




(OTM ballistic simulation of brittle target , Courtesy B. Li)

Applications: Solvers!

Recall: Glass as protection material



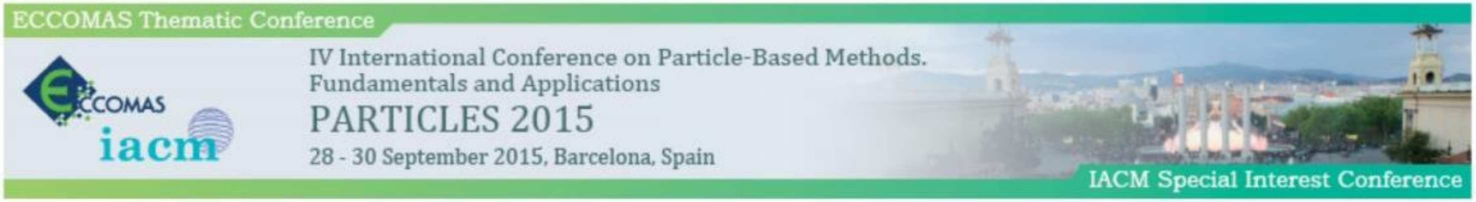
A soda lime glass target impacted by steel rod at 300 m/s[1].

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

Solvers: Fracture and fragmentation

- Solver requirements:
  - *Capable of handling geometrical and topological complexity in the crack set and its evolution*
  - *Agnostic as regards material behavior, i.e., they must apply equally well regardless of whether the material:*
    - *Is elastic or inelastic (e.g., plastic, viscoelastic…)*
    - *Undergoes small or large deformations*
    - *Deforms quasistatically or dynamically*
  - *Defined in terms of material constants measurable by means of standard fracture tests (e.g., ASTM standards)*
  - *Provably convergent, including crack set, with respect to mesh and time-step refinement (verification)*
  - *Predictive of crack initiation and growth under relevant conditions of loading, temp., environment (validation)*

Solvers: Particle + erosion methods



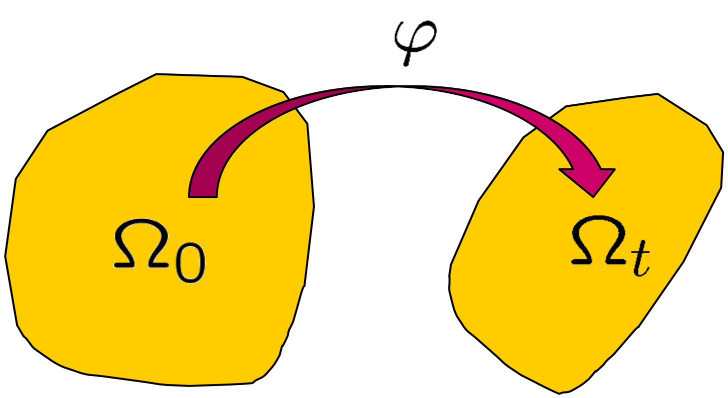
Particle methods in engineering = Transport of measures in mathematics

Optimal transportation problems

- Mass + linear-momentum transport (Eulerian):

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

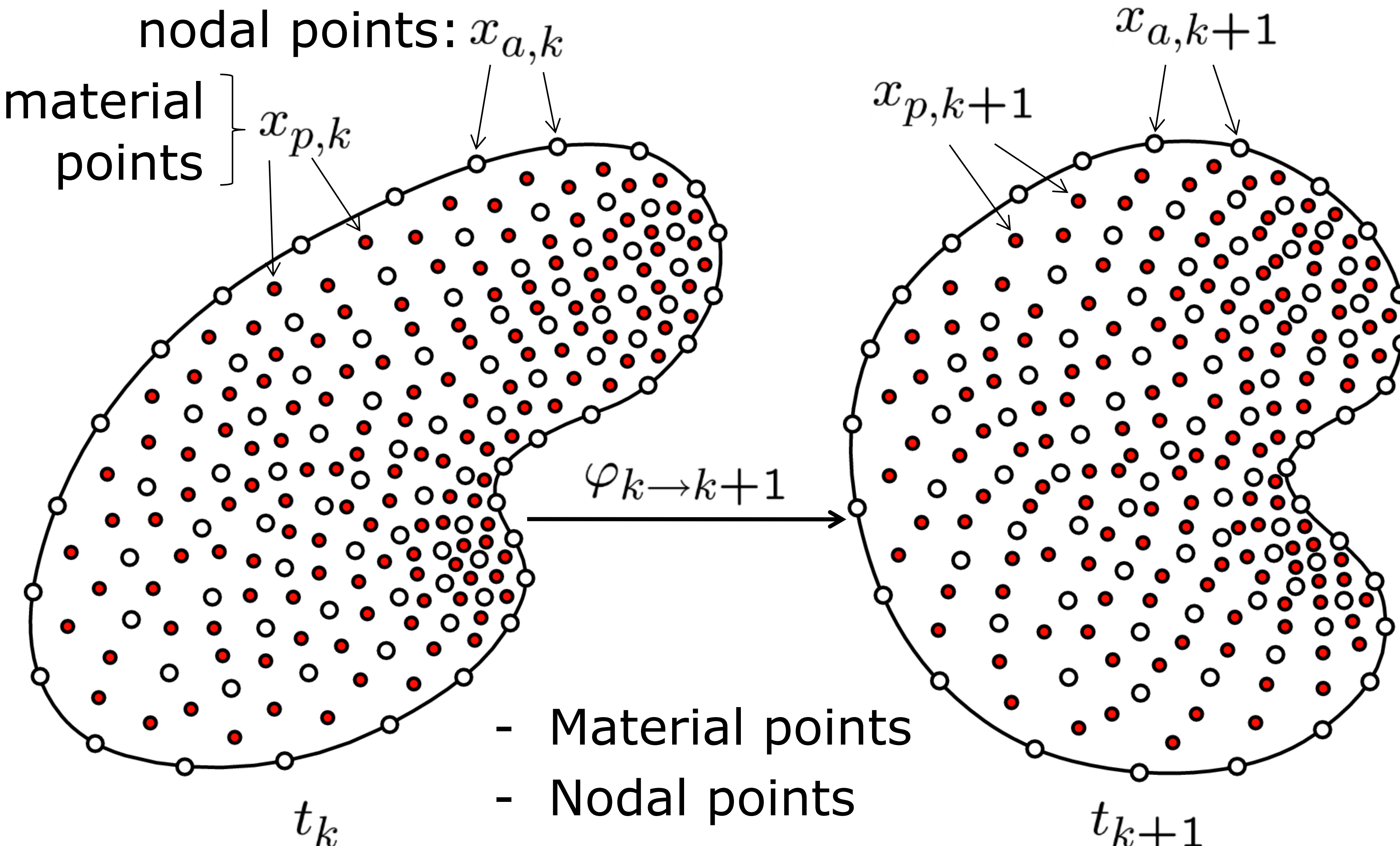
- Lagrangian reformulation:



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

Geometrically exact!

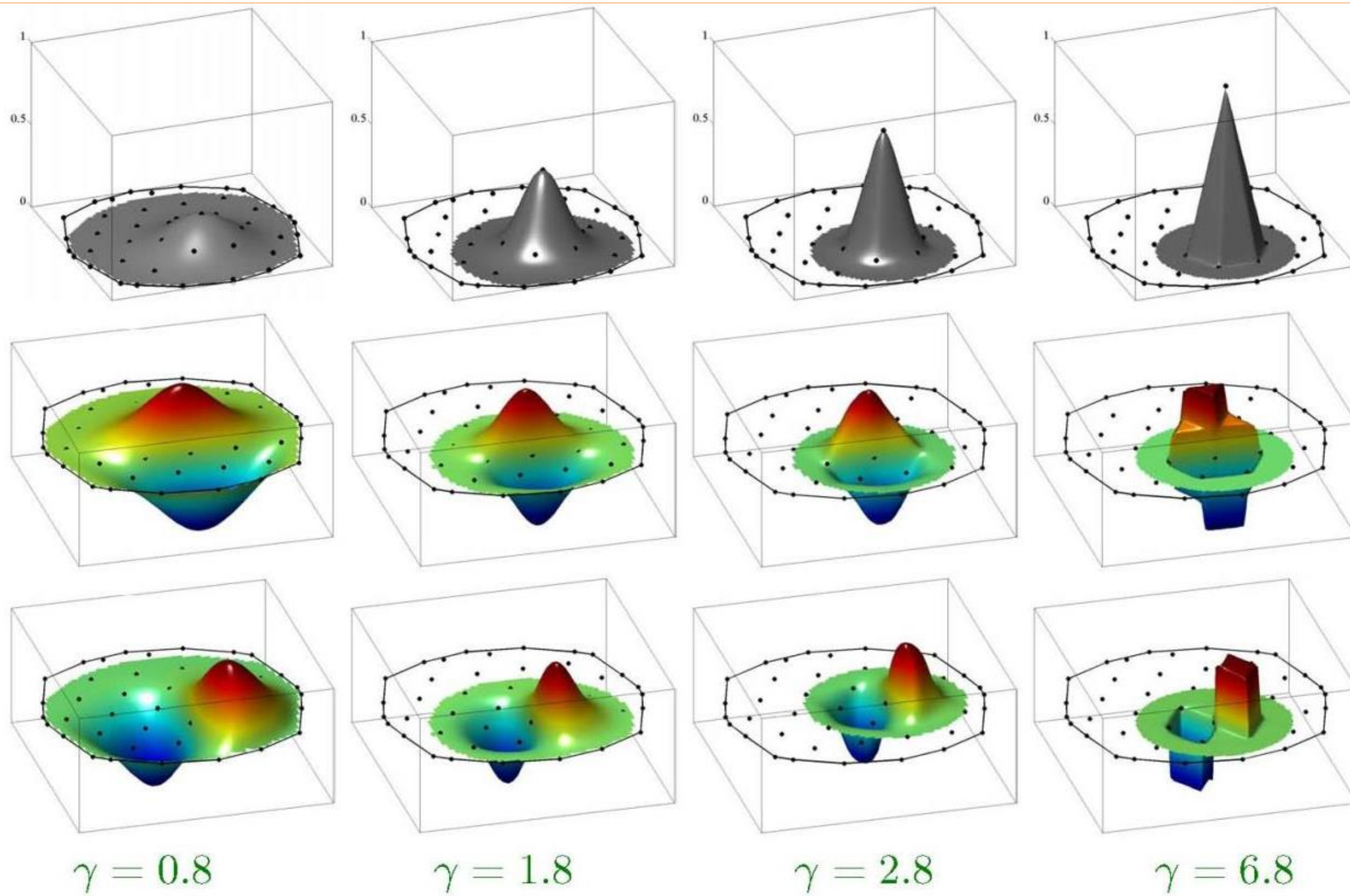
Optimal Transportation Meshfree (OTM)



Michael Ortiz
CMCS 2017

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

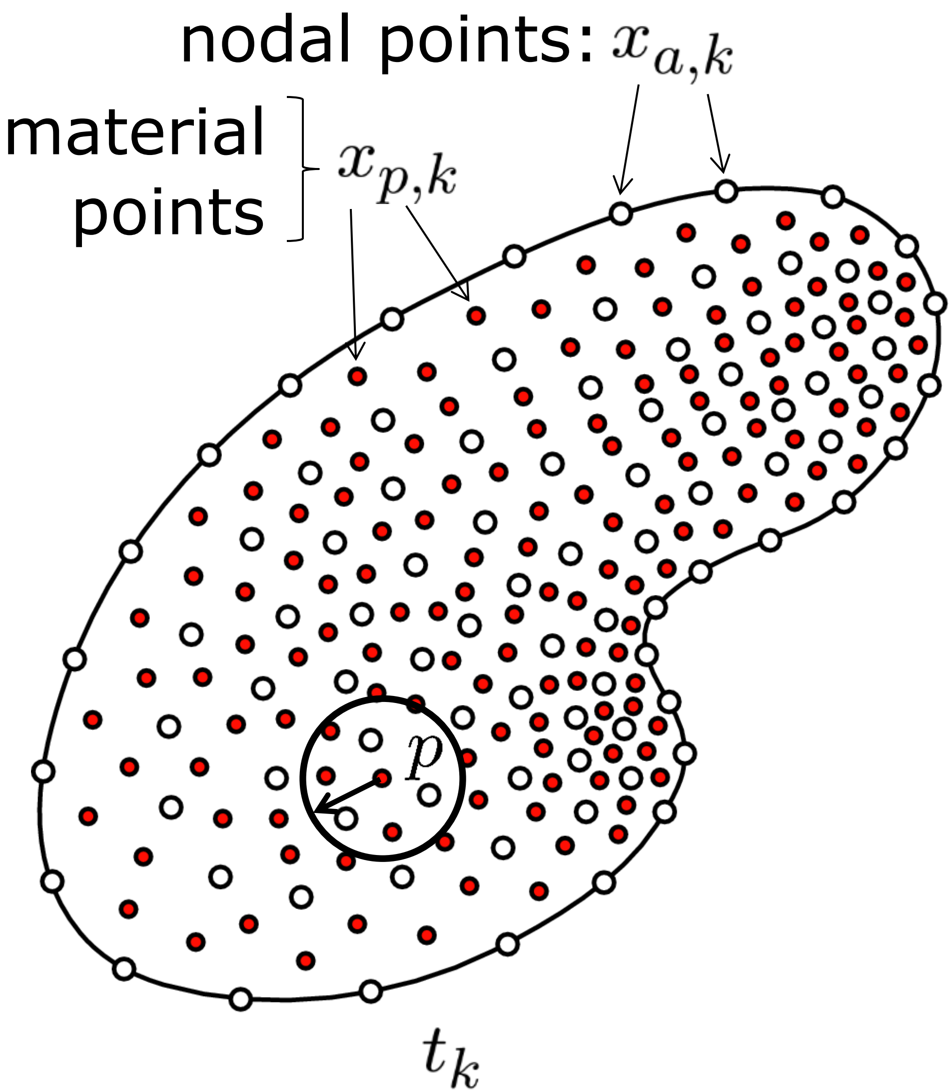
Max-ent interpolation



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

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

OTM Solver – Spatial discretization



- Max-ent interpolation at node *p* determined by nodes in its local environment
- Local environments determined 'on-the-fly' by range searches
- Local environments evolve continuously during flow (dynamic reconnection)
- Dynamic reconnection requires no remapping of history variables!

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

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

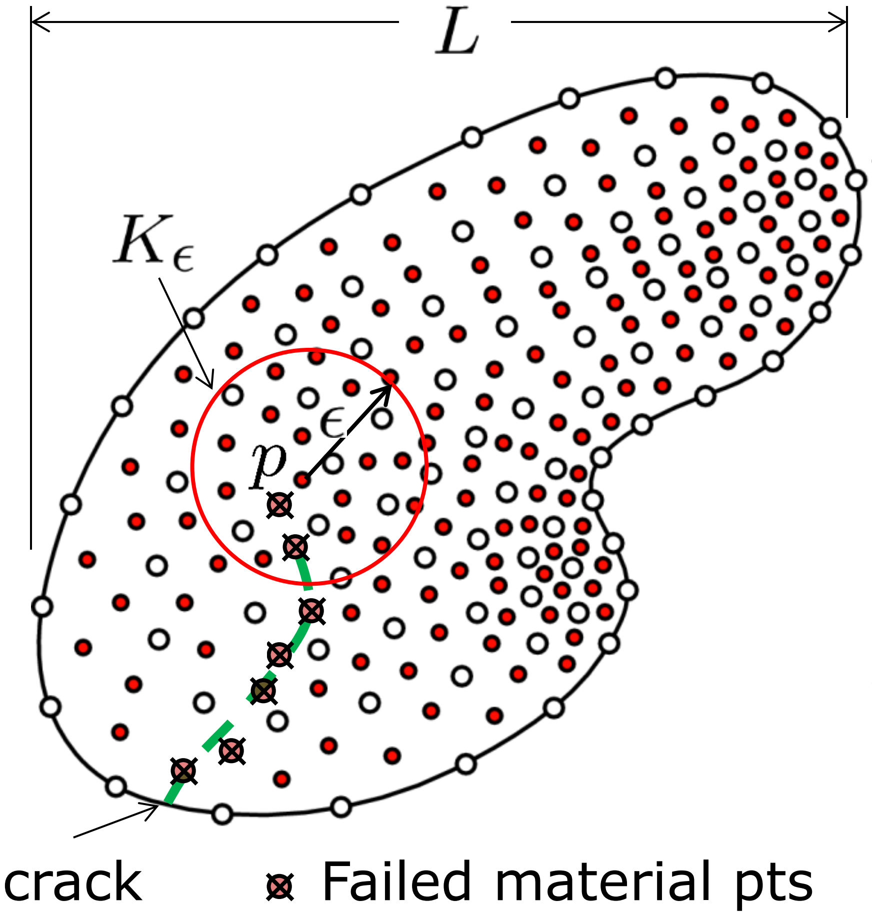
density: $\rho_{p,k+1} = m_p / V_{p,k+1}$

(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



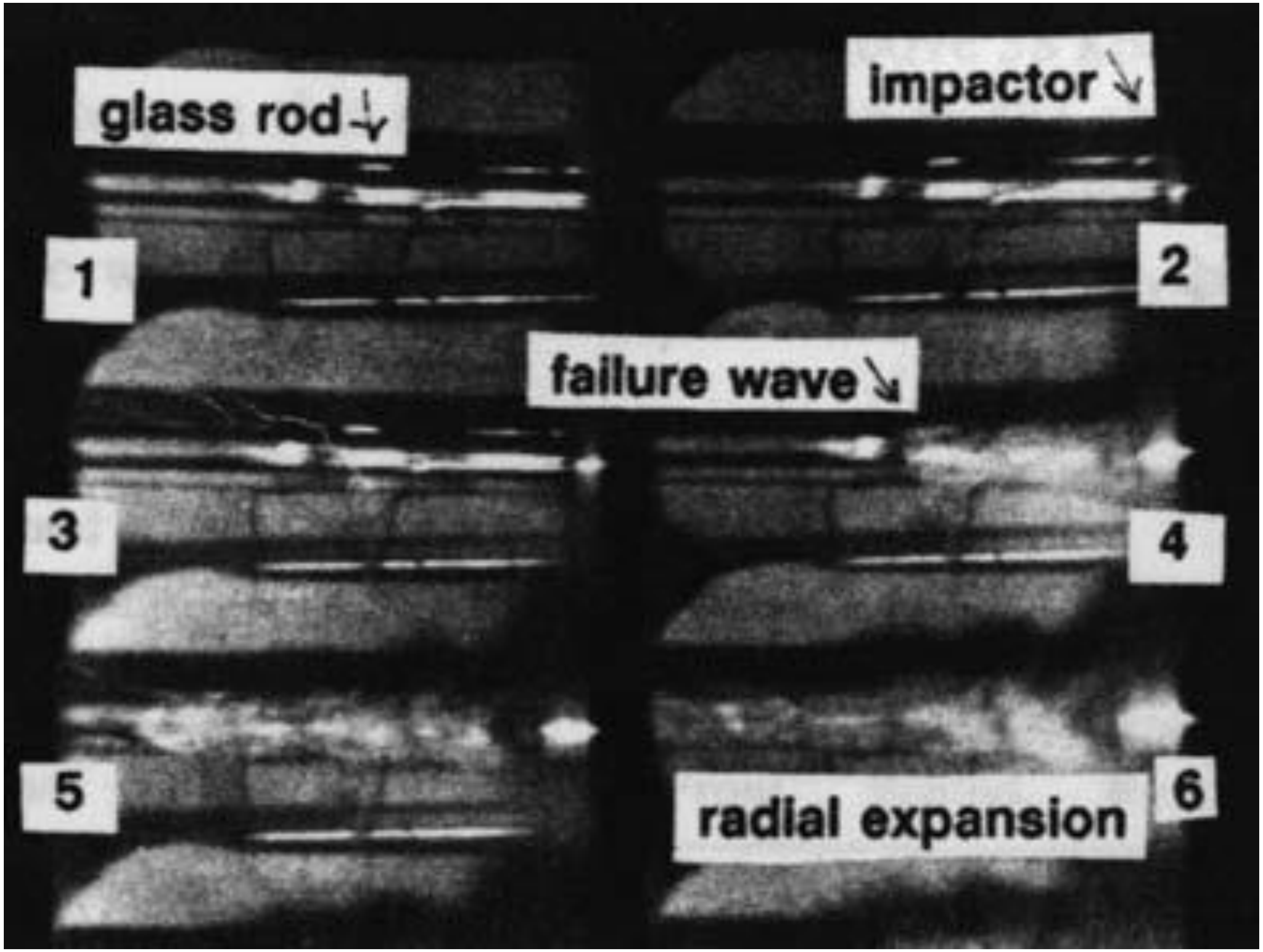
Schematic of ϵ-neighborhood construction

- 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.

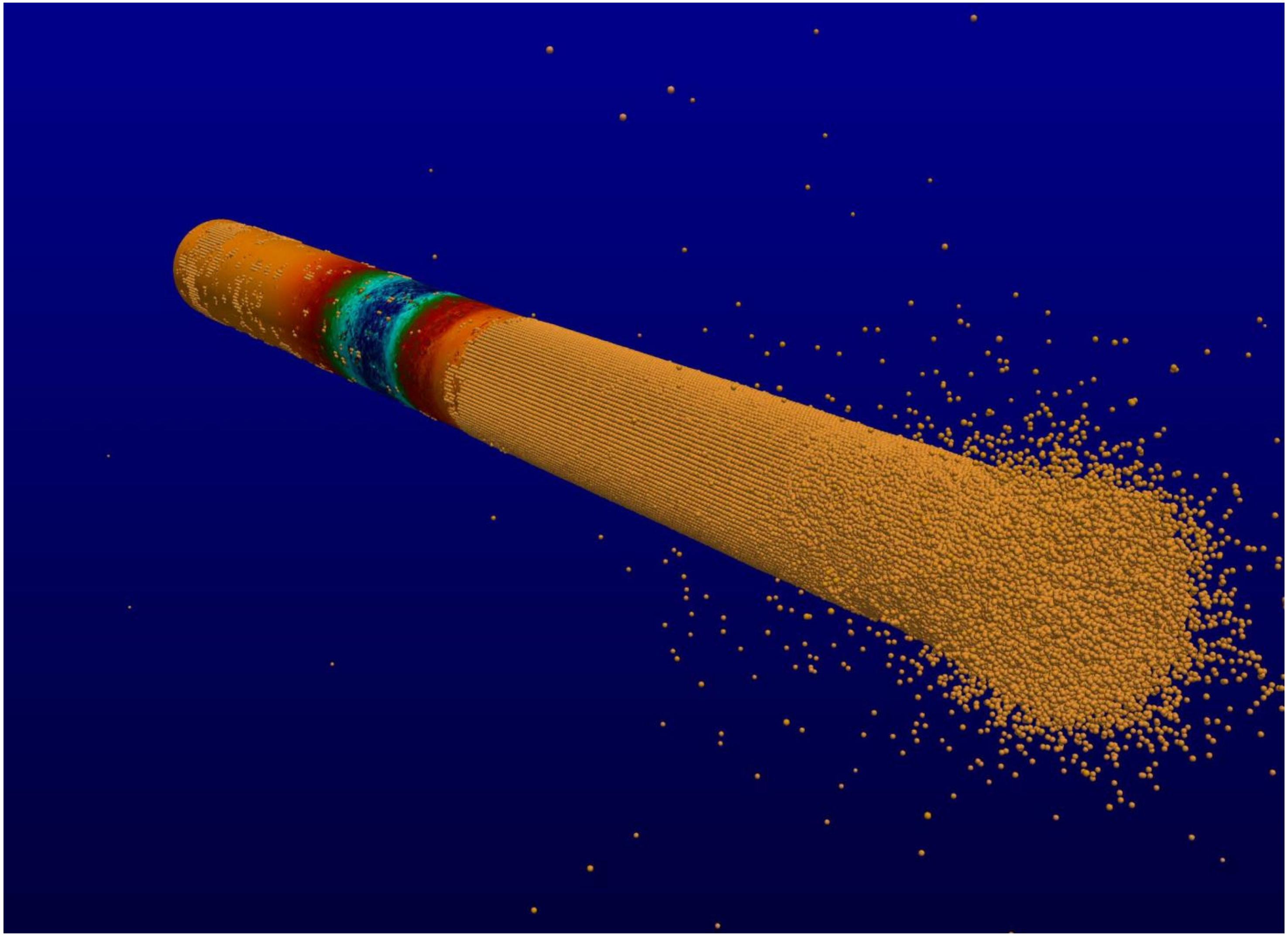
Application: Failure waves in glass rods



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



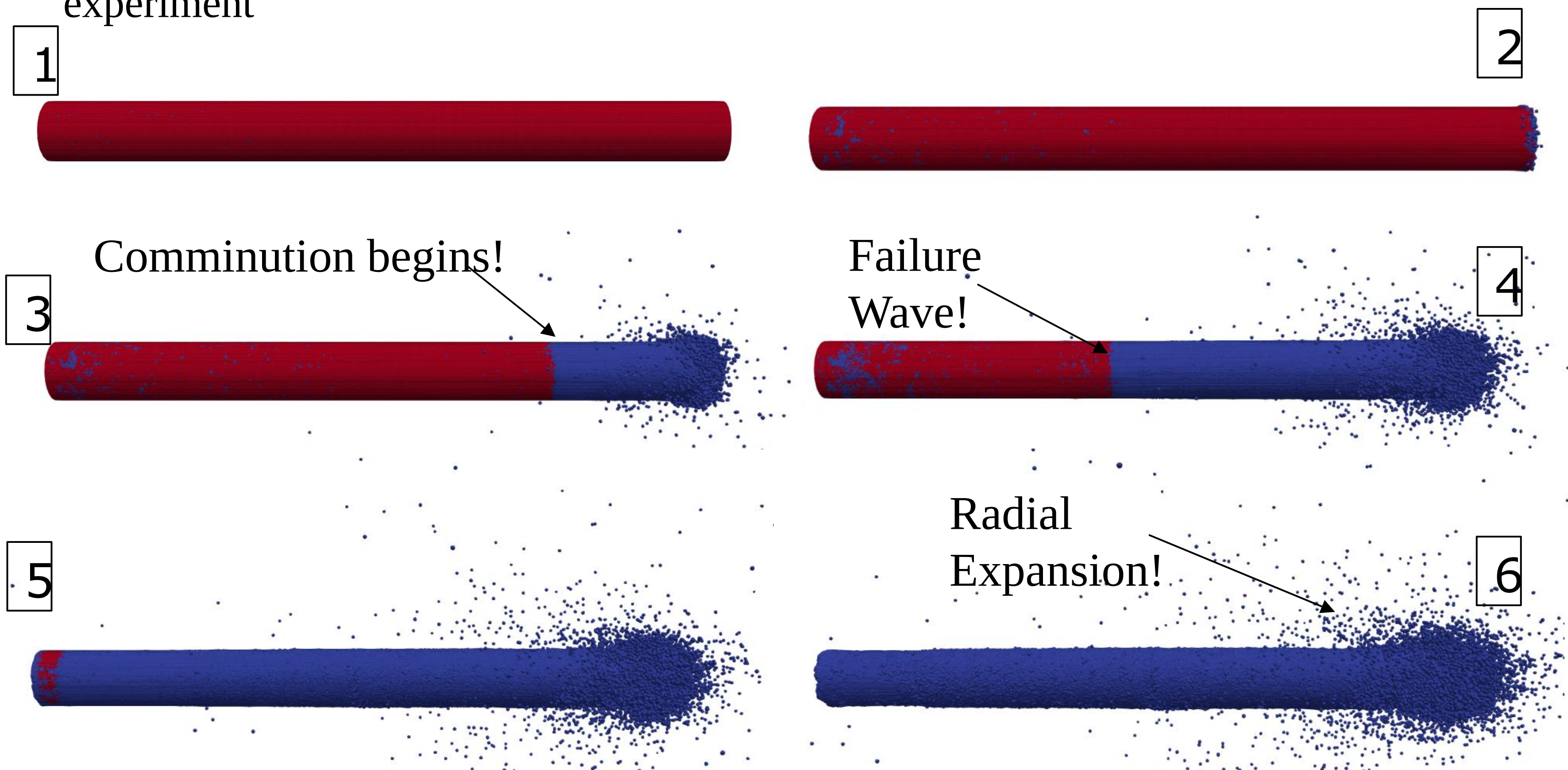
Problem Parameters: V = 210 m/s; Length, 150 mm, Diameter, 12.7 mm

Michael Ortiz
CMCS 2017

OTM Solver – Failure wave in glass rod

Comparison to Experiment:

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



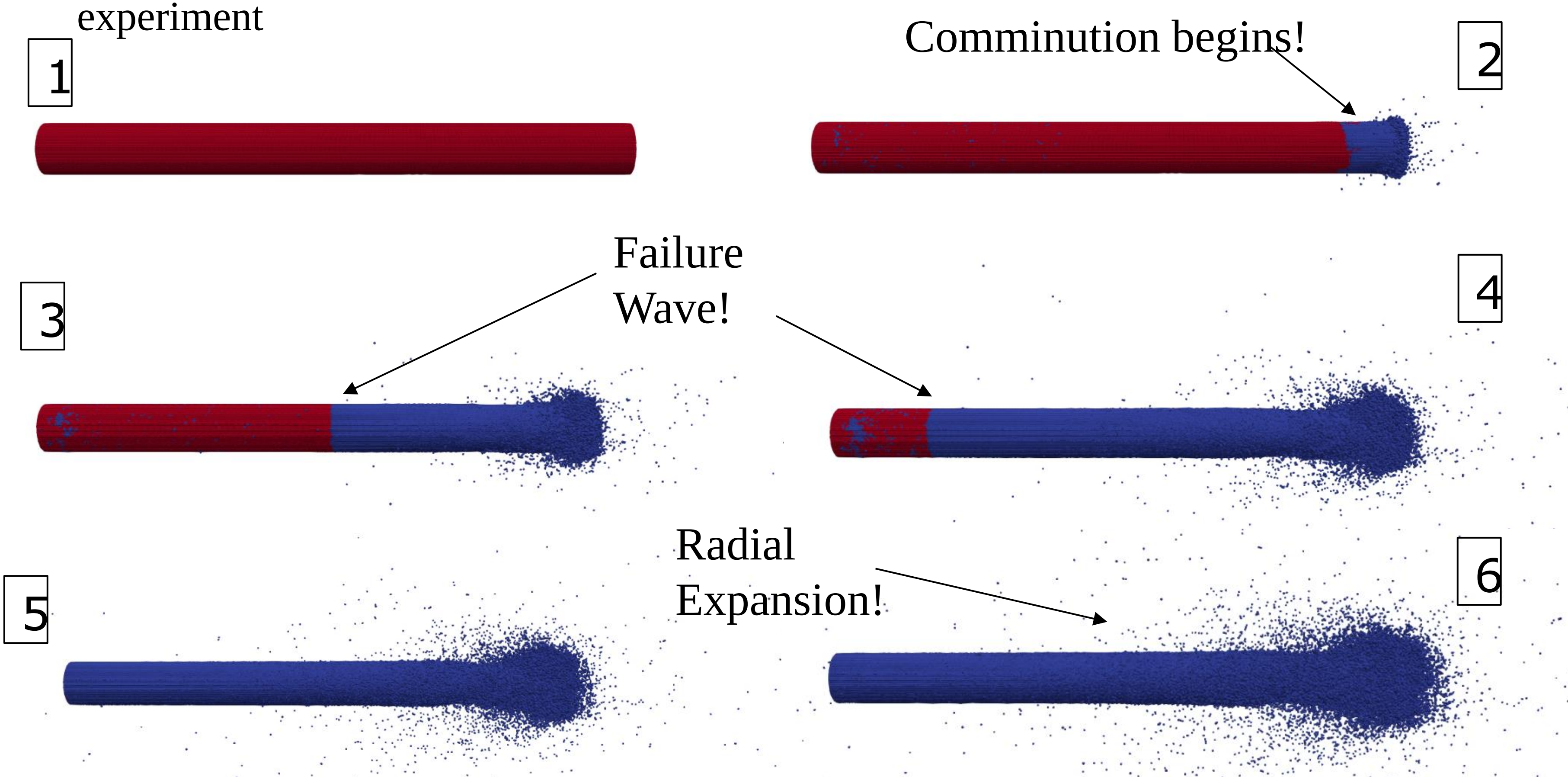
- $V_{failure}$ (sim) = 4.7 mm/μs
- $V_{failure}$ (exp) = 4.5 mm/μs

} Close Agreement!

OTM Solver – Failure wave in glass rod

A faster impact speed: V = 336 m/s

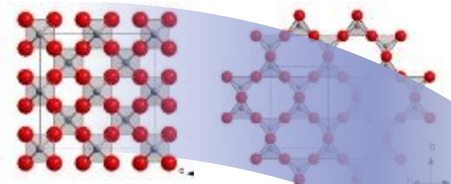
- Again, the failure wave propagates in close agreement with experiment



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

Close Agreement!

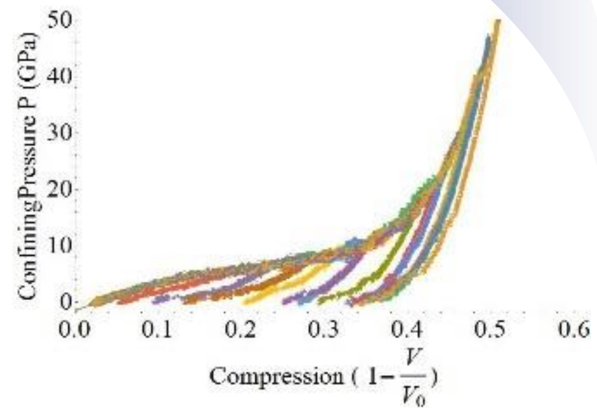
Multiscale modeling approach



Data Mining

Atomistic modeling of fused silica:

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



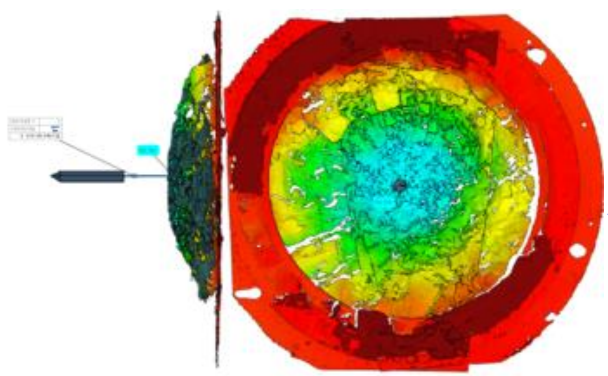
Mesoscopic modeling:

- Critical-state plasticity

Macroscopic modeling:

- Relaxation

Continuum Models



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

Applications

Acknowledgments

WS, SH and MO gratefully acknowledge support from the US Office of Naval Research through grant N000141512453, Program Officer, Roshdy G. S. Barsoum, Naval Materials Div.

SC is grateful for the support of the Deutsche Forschungsgemeinschaft through the Sonderforschungsbereich 1060 “The mathematics of emergent effects”.

MO is grateful to the Hausdorff Center for Mathematics, Rheinische Friedrich-Wilhelms Universität Bonn, for travel support

Michael Ortiz
CMCS 2017