Connecting atomistic & continuum descriptions of failure in amorphous solids

Michael L. Falk

JOHNS HOPKINS

WHITING SCHOOL *of* ENGINEERING

Bulk Metallic Glasses

Douglas Hoffman, E-Science News 1998

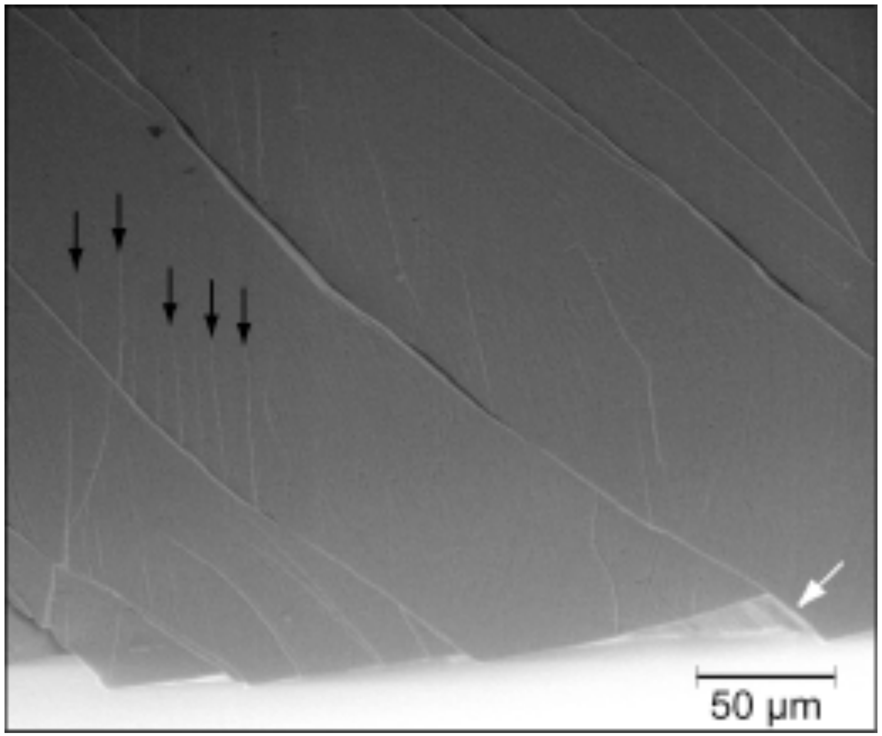
- Unique material with promising properties, but disordered structure.
- High strength.
- High formability due to lack of shrinkage upon solidification.

OMEGA WATCH AD

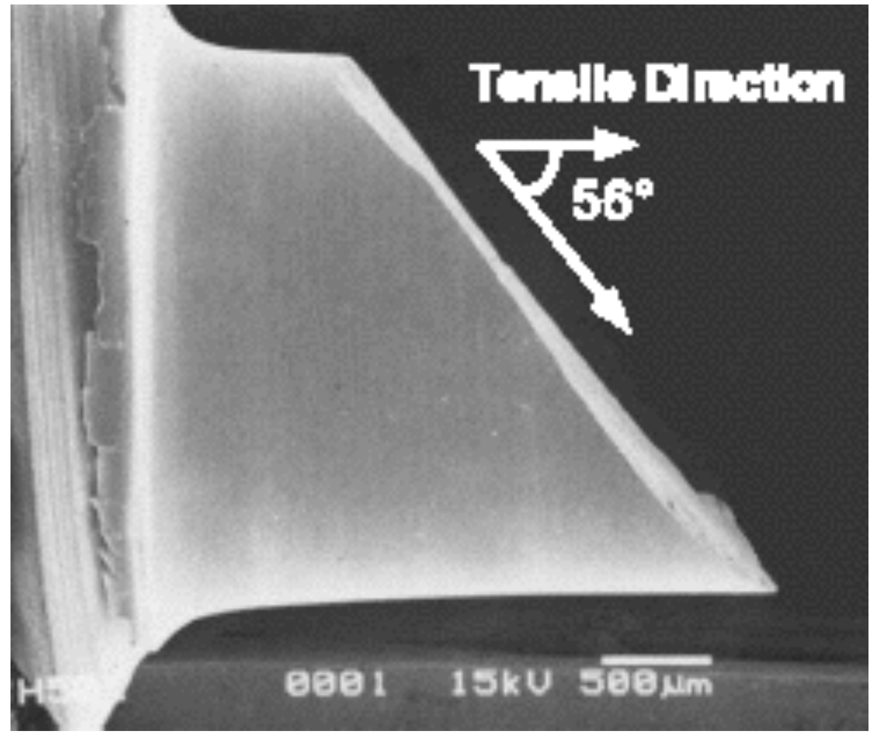
OMEGA WATCH AD

Shear Bands in Metallic Glass

strain localization (shear banding) is the primary failure mode



Electron Micrograph of Shear Bands Formed in Bending Metallic Glass
Hufnagel, El-Deiry, Vinci (2000)



Quasistatic Fracture Specimen
Mukai, Nieh, Kawamura, Inoue, Higashi (2002)

Can we use examples of shear banding to validate the effective temperature STZ theory against MD and experimental realizations?

Effective Temperature STZ Theory

- Is there an intensive thermodynamic property (called χ here) that controls the number density of deformable regions (STZs)?

$$n_{STZ} \propto e^{-e_Z/\chi}$$

- This would be an "effective temperature" that characterizes structural degrees of freedom quenched into the glass.

$$\dot{\epsilon}_{ij}^{pl} = e^{-e_Z/\chi} f_{ij}\left(s_{kl}\right)$$

$$c_0\dot{\chi} = 2s_{ij}\dot{\epsilon}_{ij}^{pl}\left(\chi_{\infty} - \chi\right) - \kappa(T)e^{-\beta/\chi}$$

Y. Shi, M.B. Katz, H. Li, MLF, Phys. Rev. Lett., 98, 185505 (2007)

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mechanical disordering

Y. Shi, M.B. Katz, H. Li, MLF, Phys. Rev. Lett., 98, 185505 (2007)

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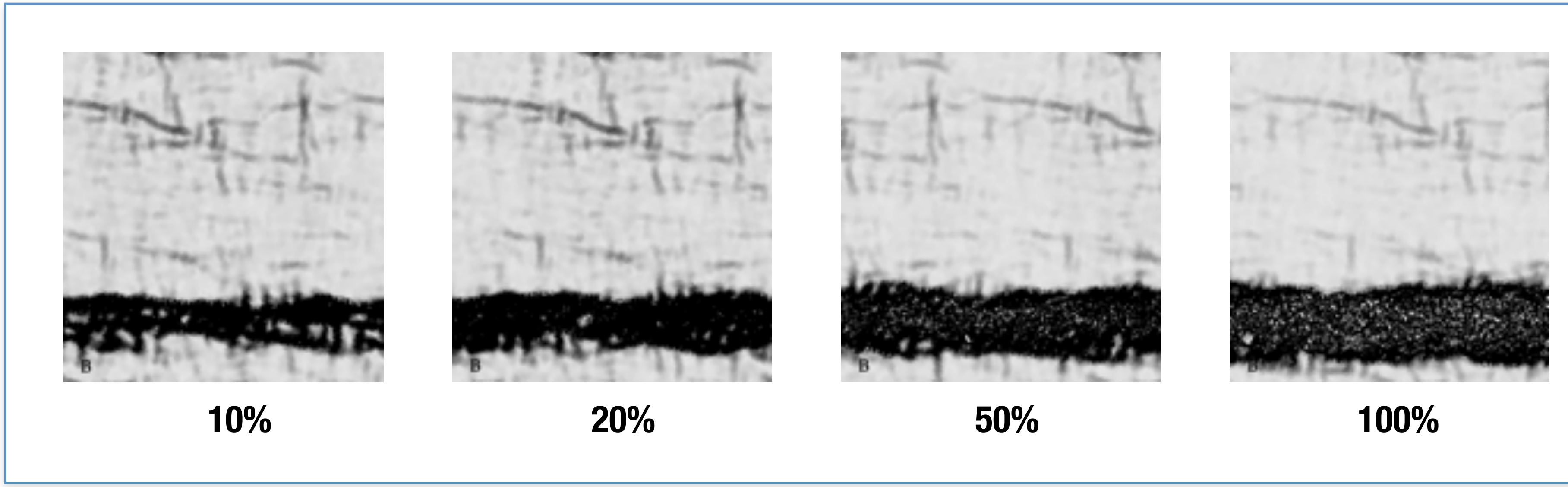
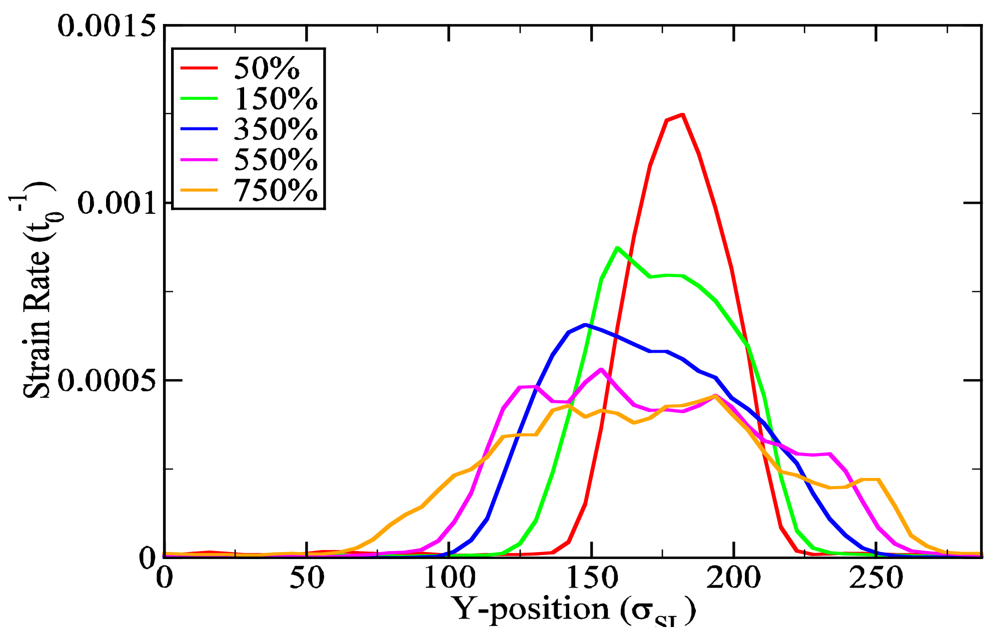
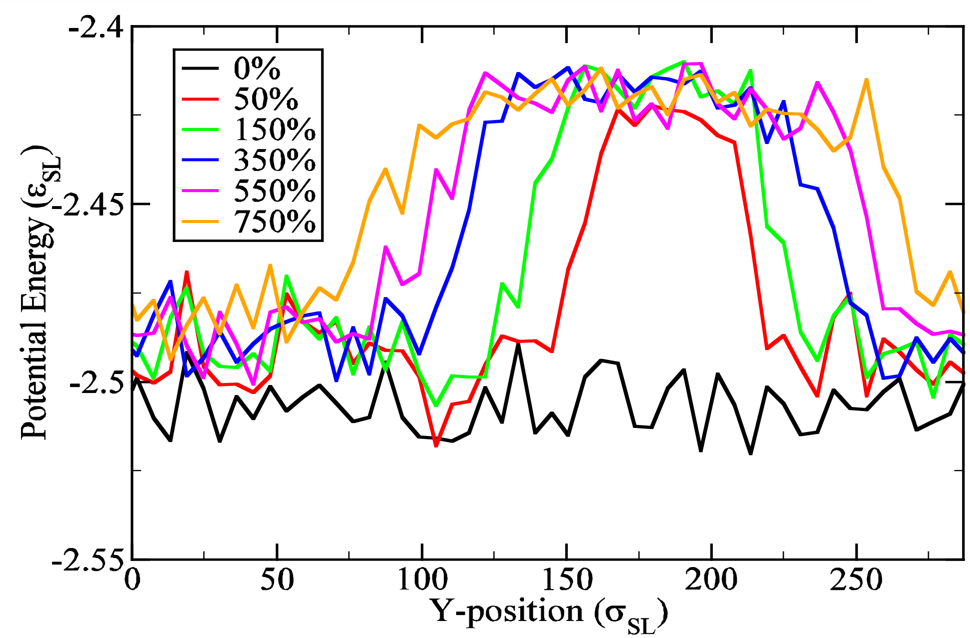
$$c_0\dot{\chi} = \underbrace{2s_{ij}\dot{\epsilon}_{ij}^{pl}\left(\chi_\infty - \chi\right)}_{\text{mechanical disordering}} - \underbrace{\kappa(T)e^{-\beta/\chi}}_{\text{thermal annealing}}$$

Y. Shi, M.B. Katz, H. Li, MLF, Phys. Rev. Lett., 98, 185505 (2007)

Development of a Shear Band







Y Shi, MB Katz, H Li, MLF, PRL, 98, 185505 (2007)

Y. Shi, M.B. Katz, H. Li, MLF, Phys. Rev. Lett., 98, 185505 (2007)

Relating χ to the microstructure

- Consider a linear relation between the χ parameter and the local internal energy

$$C_1 \chi / e_Z = PE - PE_0$$

$$\dot{\varepsilon}_{pl} = e^{-e_Z/\chi} f(s)$$

$$c_0 \dot{\chi} = 2s\dot{\varepsilon}_{pl}(\chi_\infty - \chi) - \kappa e^{-\beta/\chi}$$

- Is there an underlying scaling?

$$\frac{\dot{\varepsilon}_{pl}(y)}{\dot{\varepsilon}_b} = e^{e_Z/\chi_b - e_Z/\chi(y)}$$

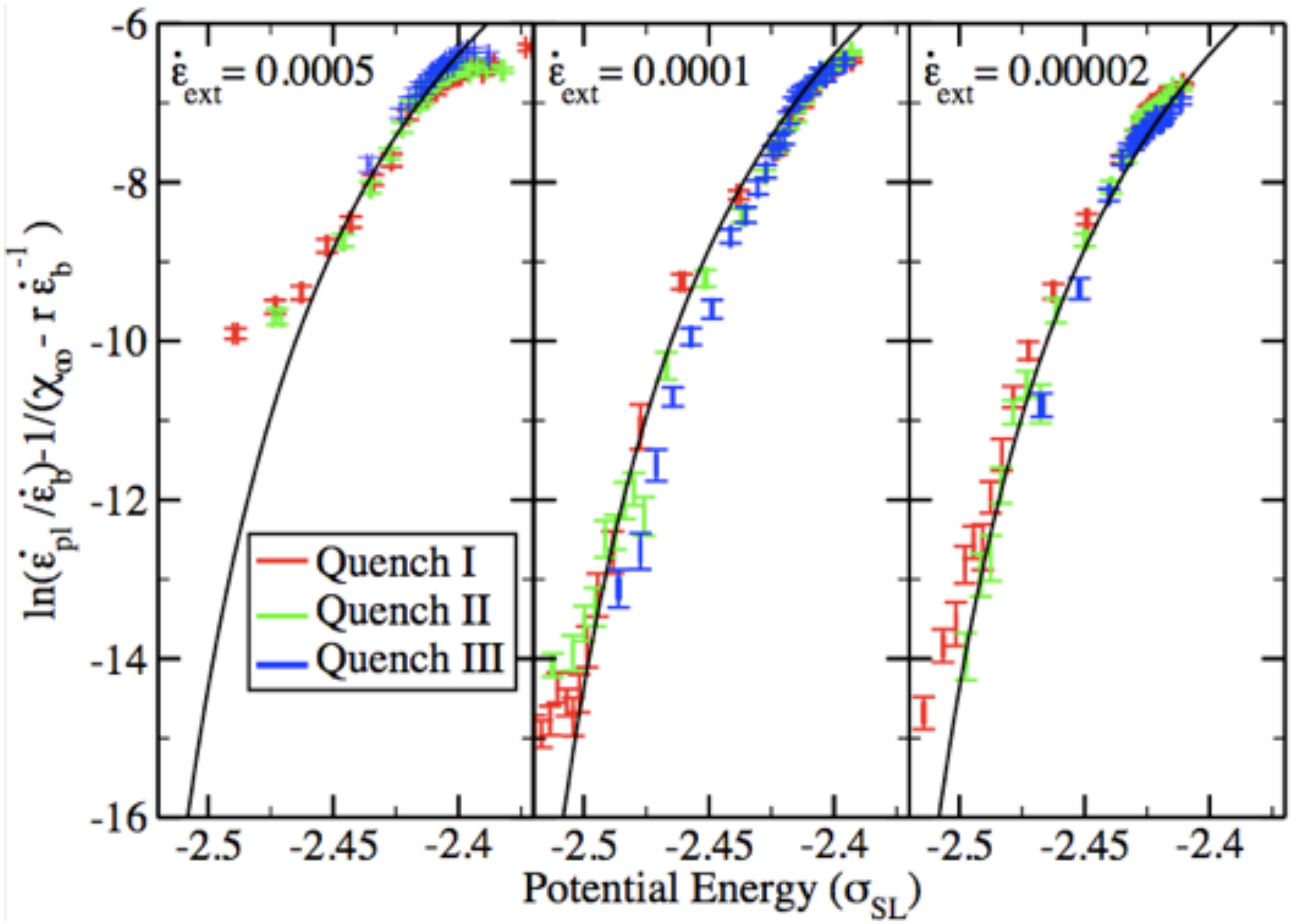
$$ln\left[\frac{\dot{\varepsilon}_{pl}(y)}{\dot{\varepsilon}_b}\right] = \frac{e_Z}{\chi_b} - \frac{C_1}{PE - PE_0}$$

$$2s\dot{\varepsilon}_b(\chi_\infty - \chi_b) = \kappa e^{-\beta/\chi_b}$$

$$ln\left[\frac{\dot{\varepsilon}_{pl}(y)}{\dot{\varepsilon}_b}\right] - \frac{e_Z}{\chi_\infty - r\dot{\varepsilon}_b^{-1}} = -\frac{C_1}{PE - PE_0}$$

Y. Shi, M.B. Katz, H. Li, MLF, Phys. Rev. Lett., 98, 185505 (2007)

Scaling verifies that varies as



- Assuming, $\chi_\infty = kT_g, e_Z = 1.9\varepsilon$

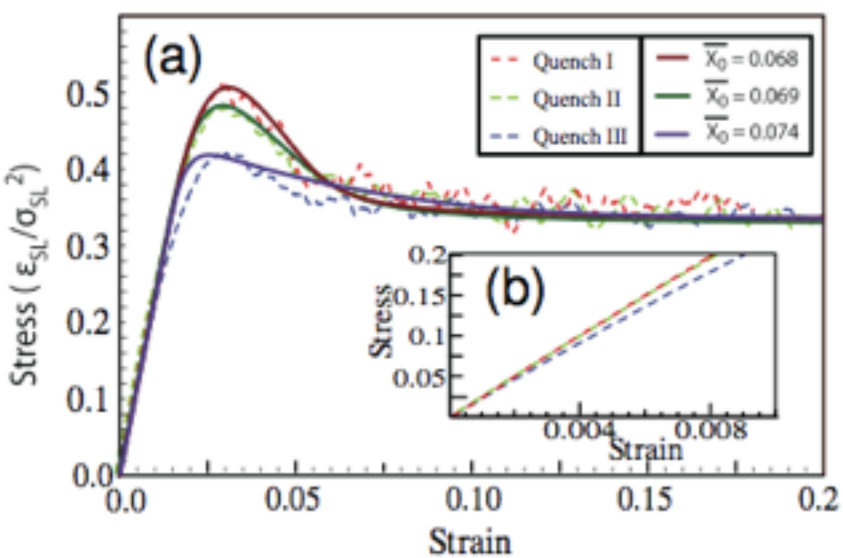
Y. Shi, M.B. Katz, H. Li, MLF, Phys. Rev. Lett., 98, 185505 (2007)

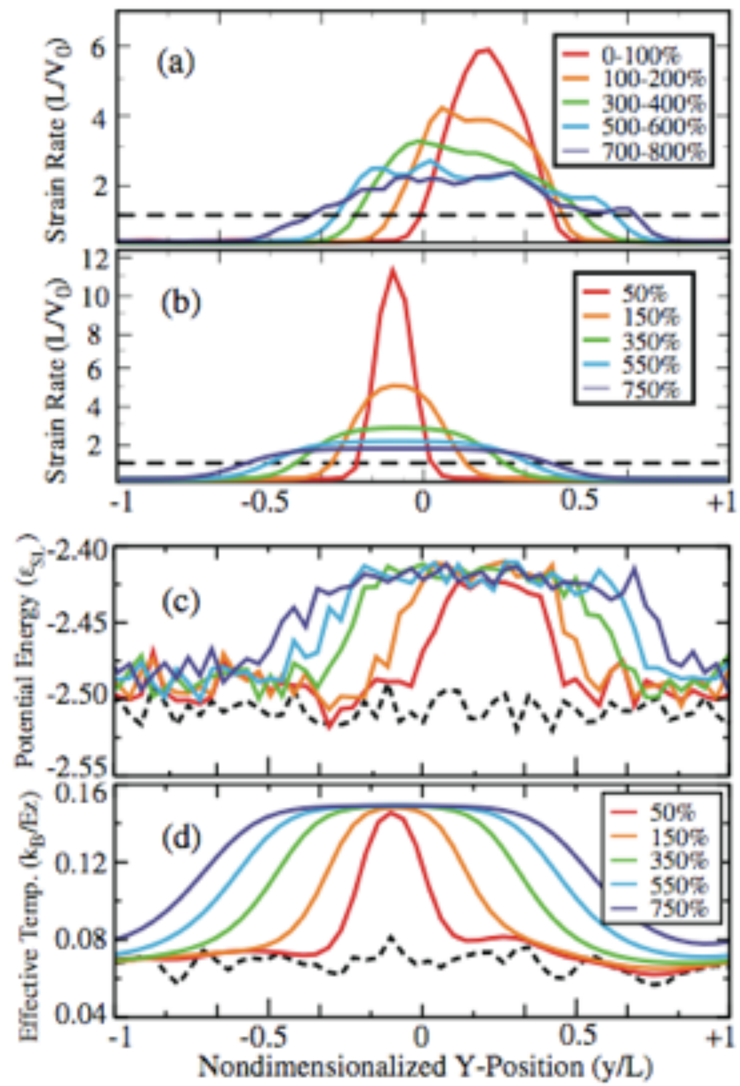
Numerical Results

M. Lisa Manning and J.S. Langer, PRE, 76, 056106(2007)

- These equations closely reproduce the details of the strain rate and structural profiles during band formation

$$\partial_t \chi - D\partial_x^2 \chi = \frac{2s\dot{\varepsilon}_{pl}}{c_0}\left(\chi_\infty - \chi\right)$$

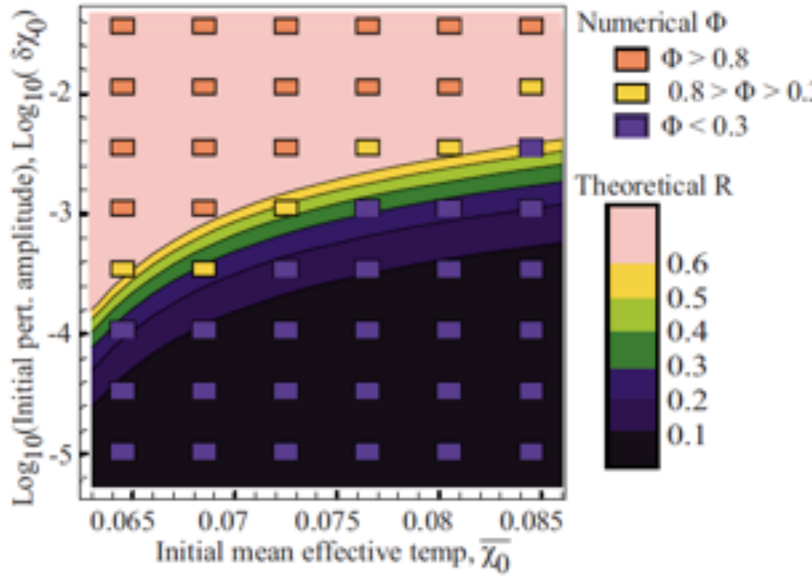


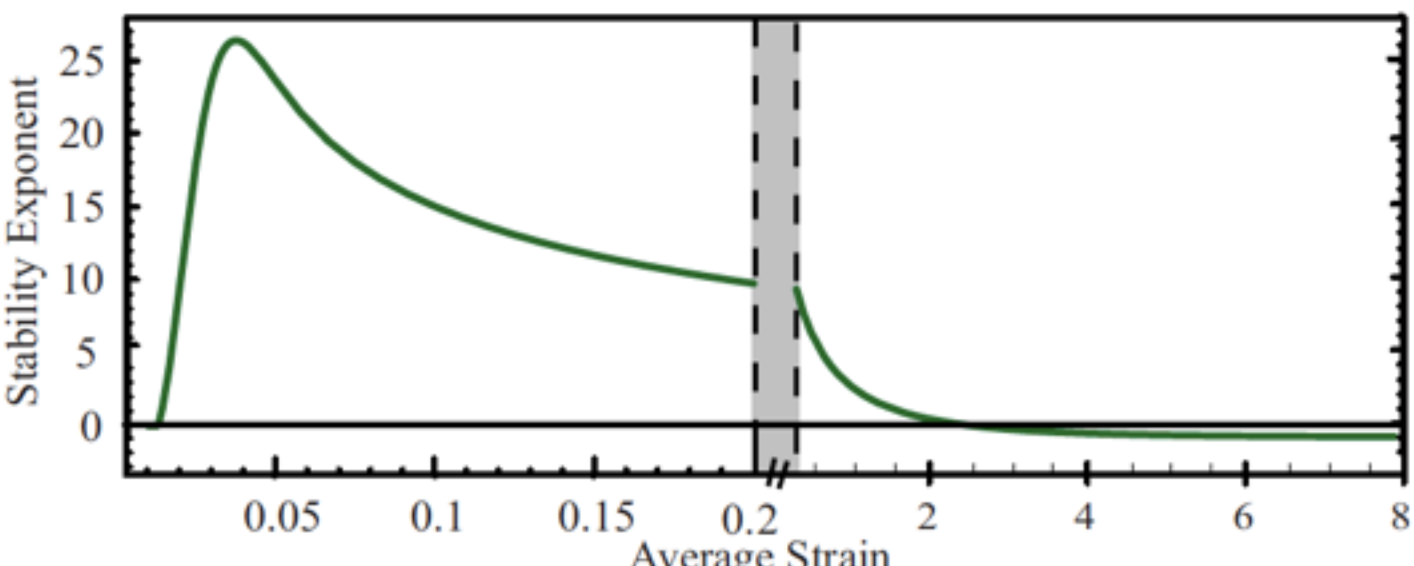


Stability Analysis

Manning, Langer and Carlson, PRE, 76, 056106(2007)

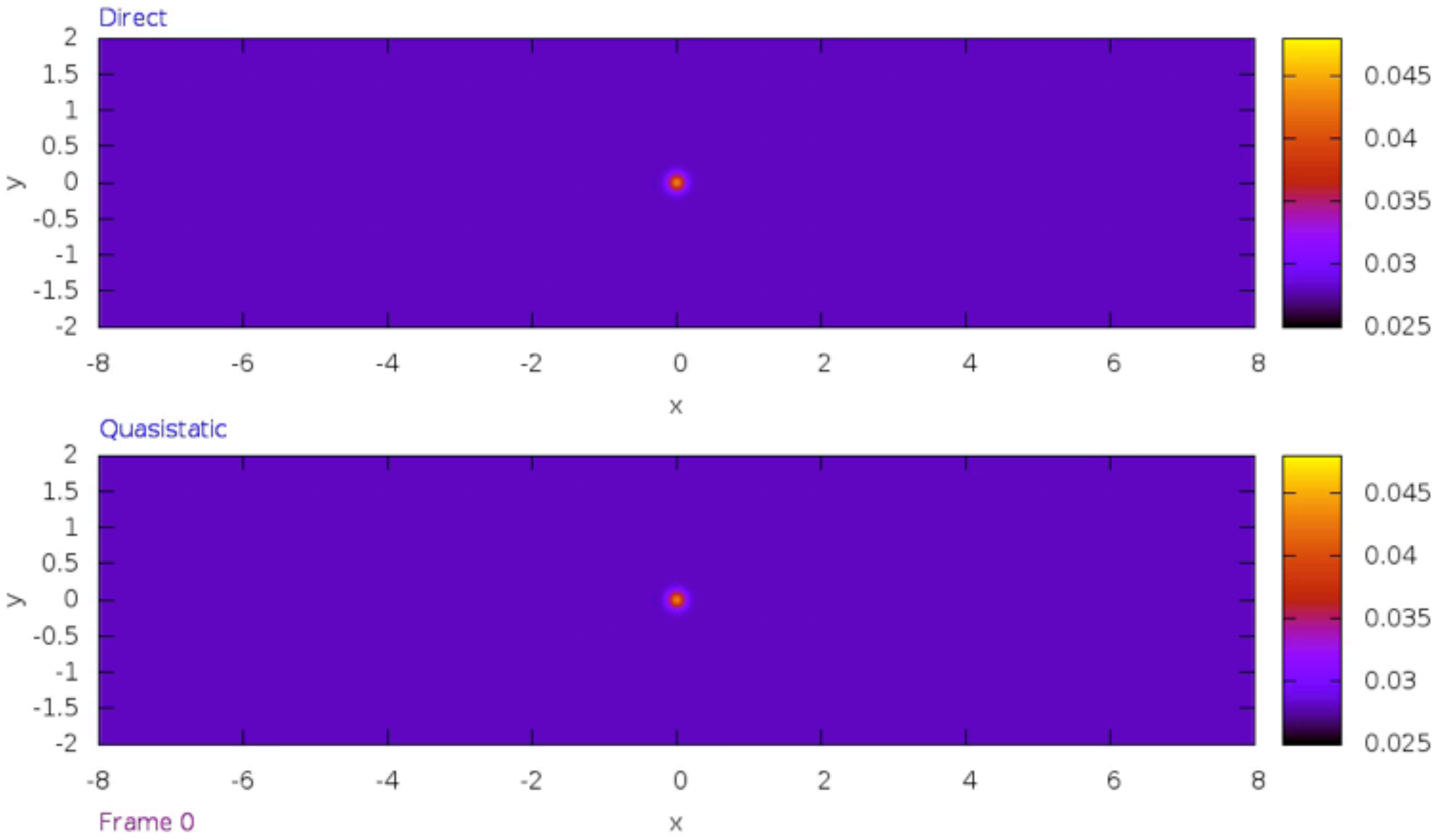
- Stability analysis of the equations indicates linear instability during **a portion** of the loading curve.
- Both the initial χ and the size of perturbations are important for determining strain localization.





2D Implementation

Chris Rycroft, Harvard Univ.



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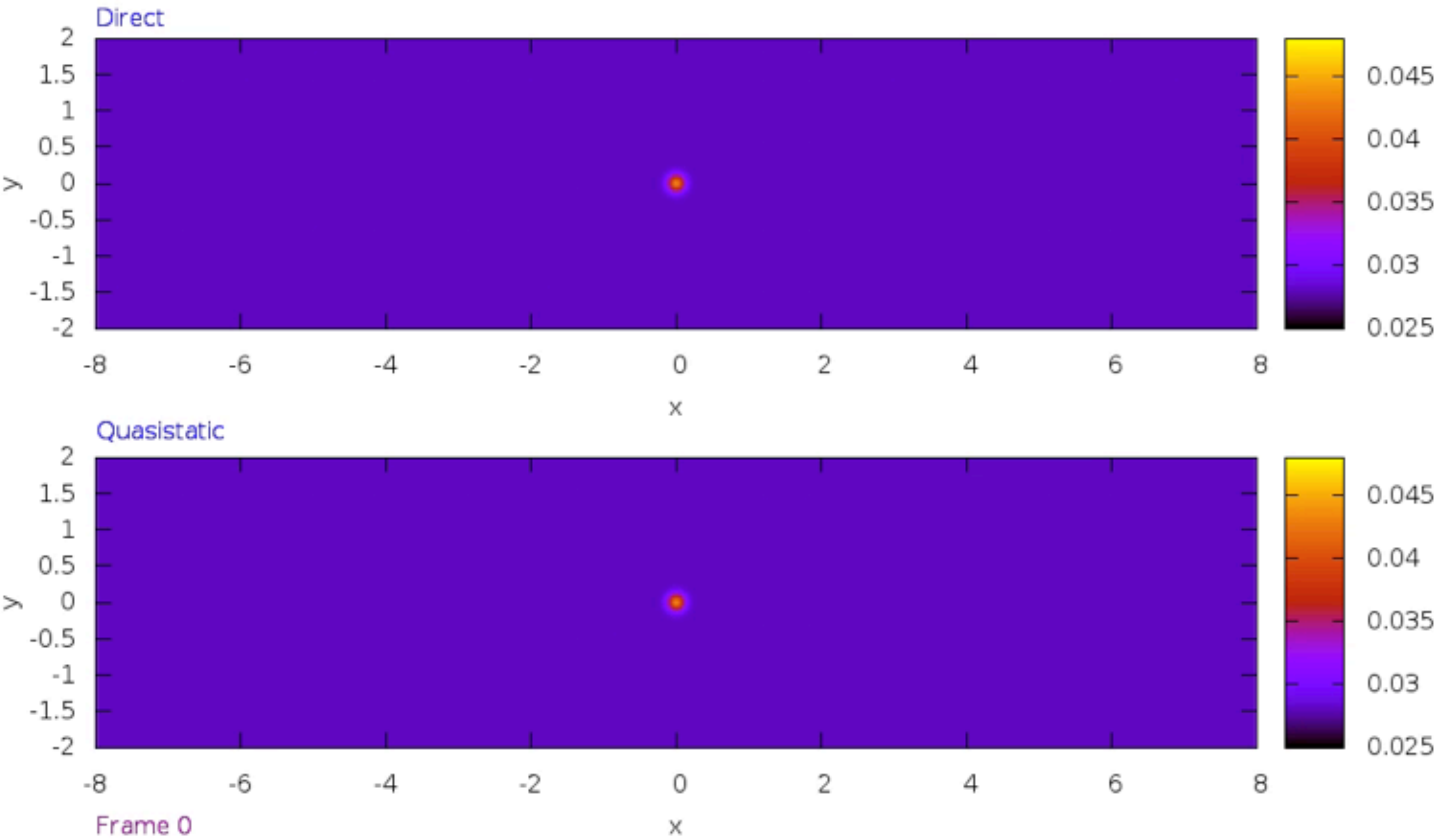
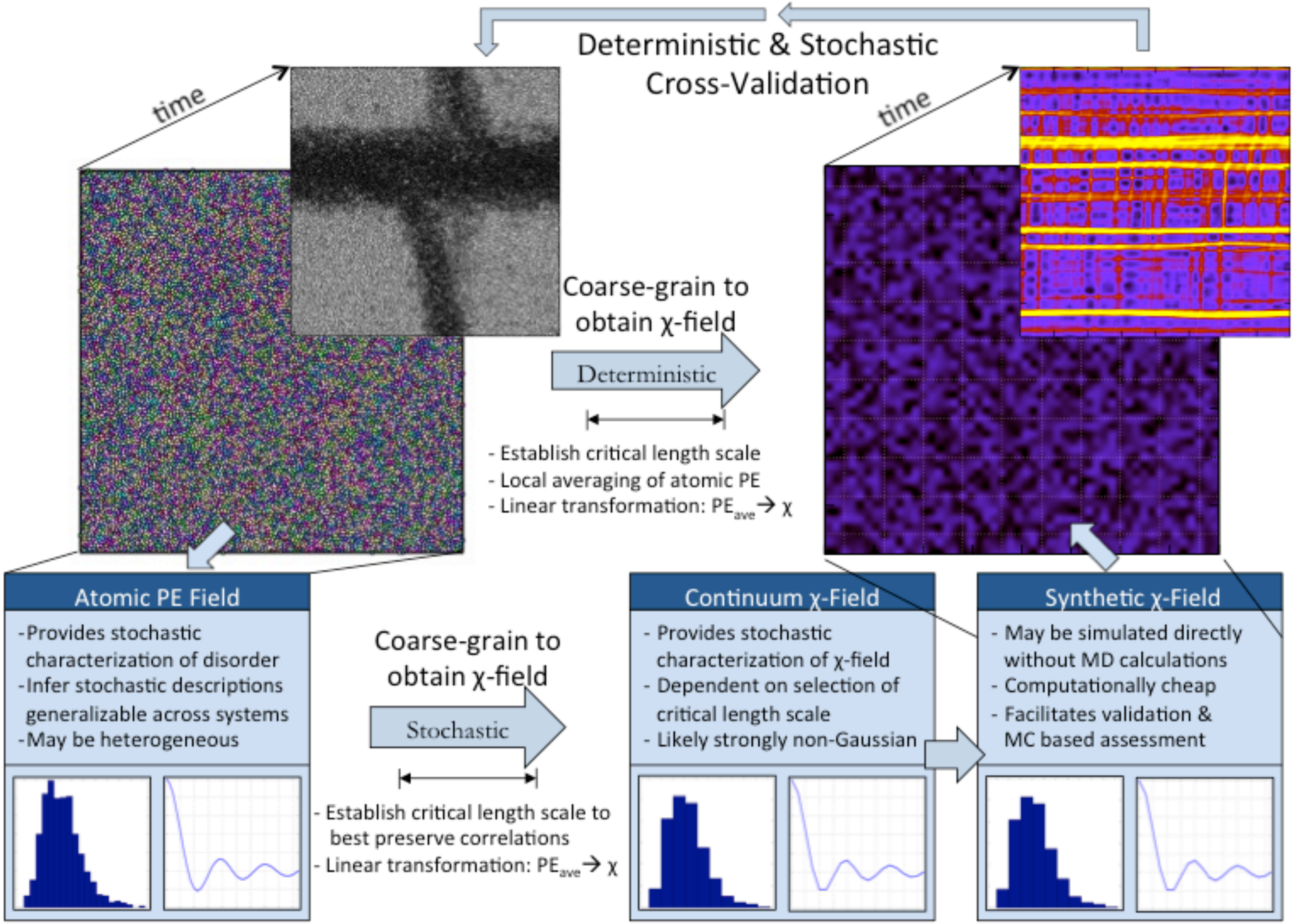


Cross Validation of MD and Stochastic Continuum Model

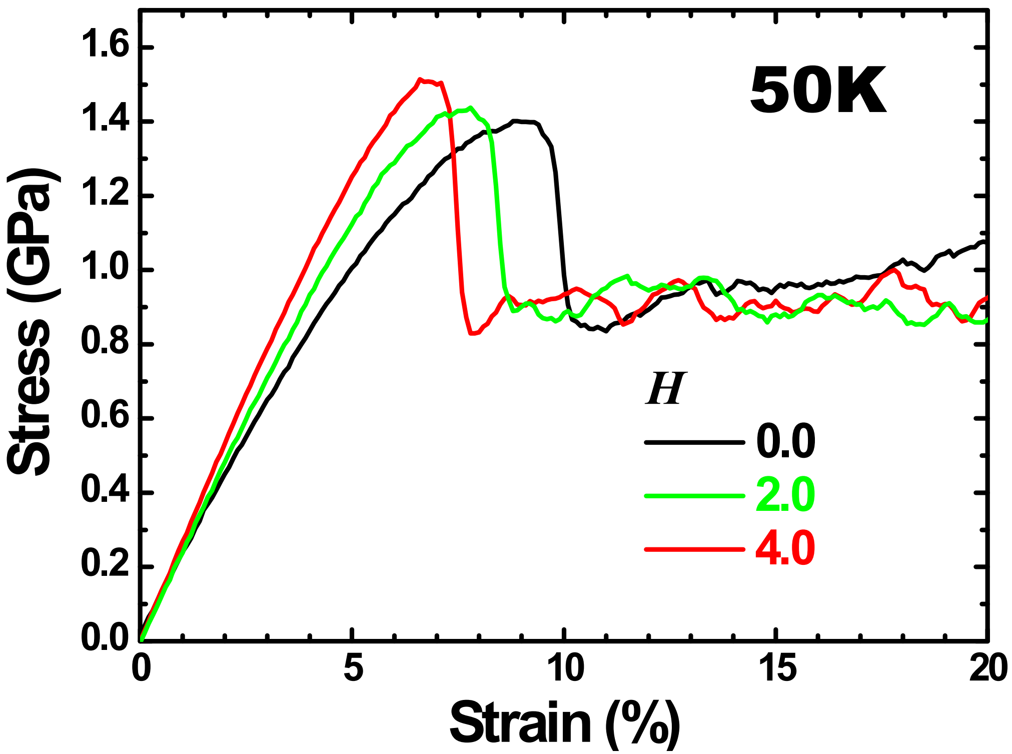


MD Simultion of Lamellar Composite

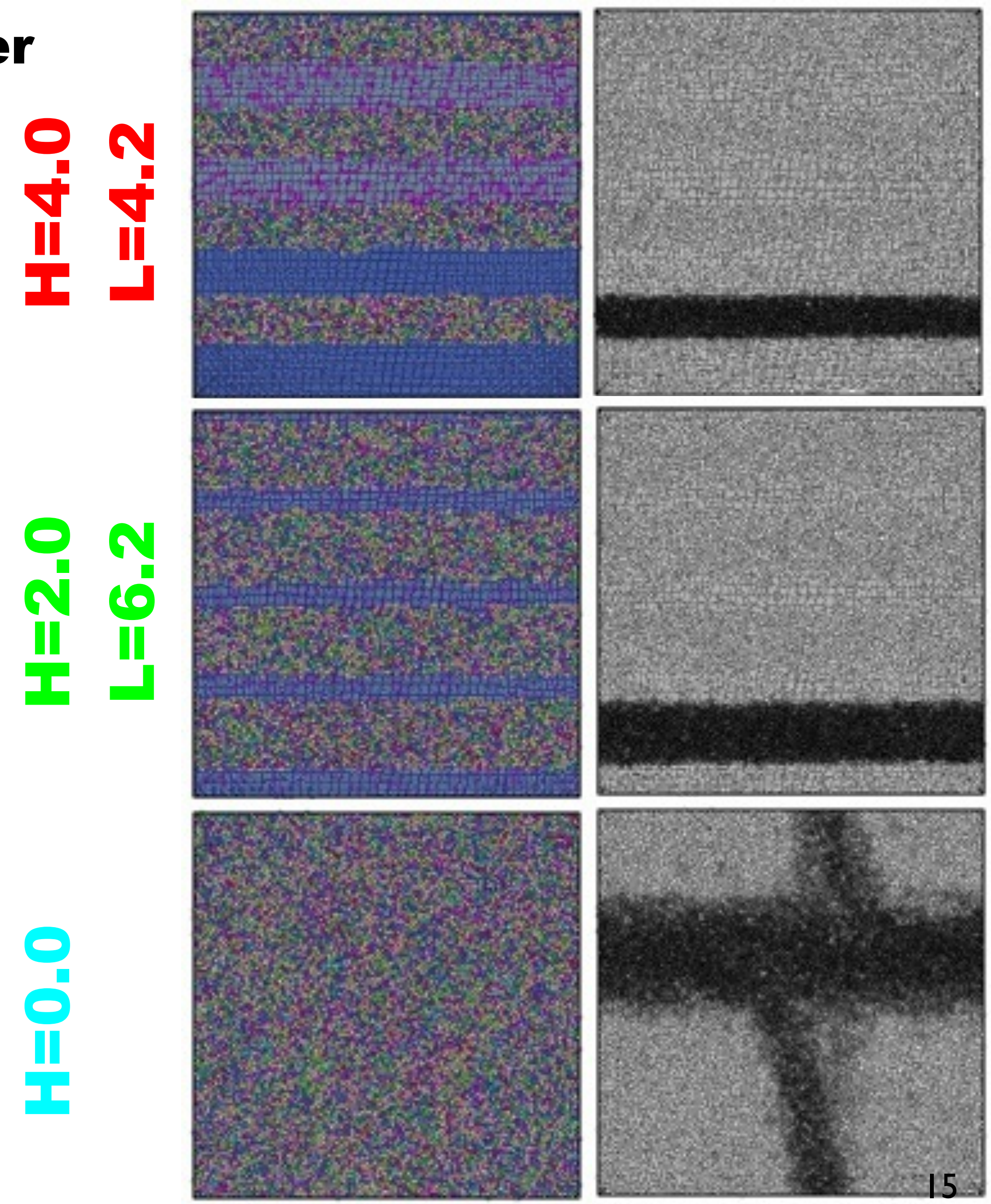
Pengfei Guan

H: thickness of the crystalline layer

L: thickness of glassy layer

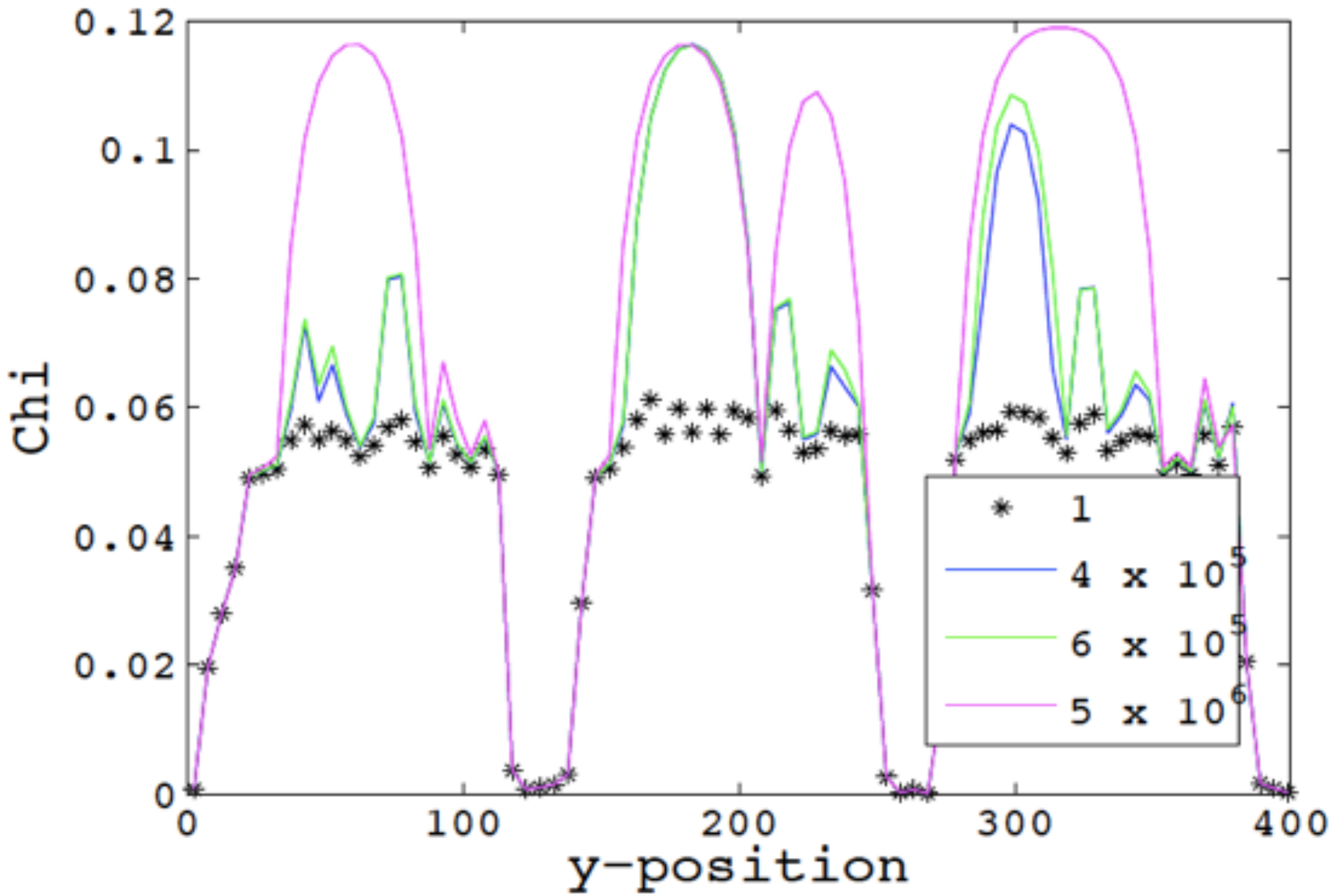


Zr_2Cu



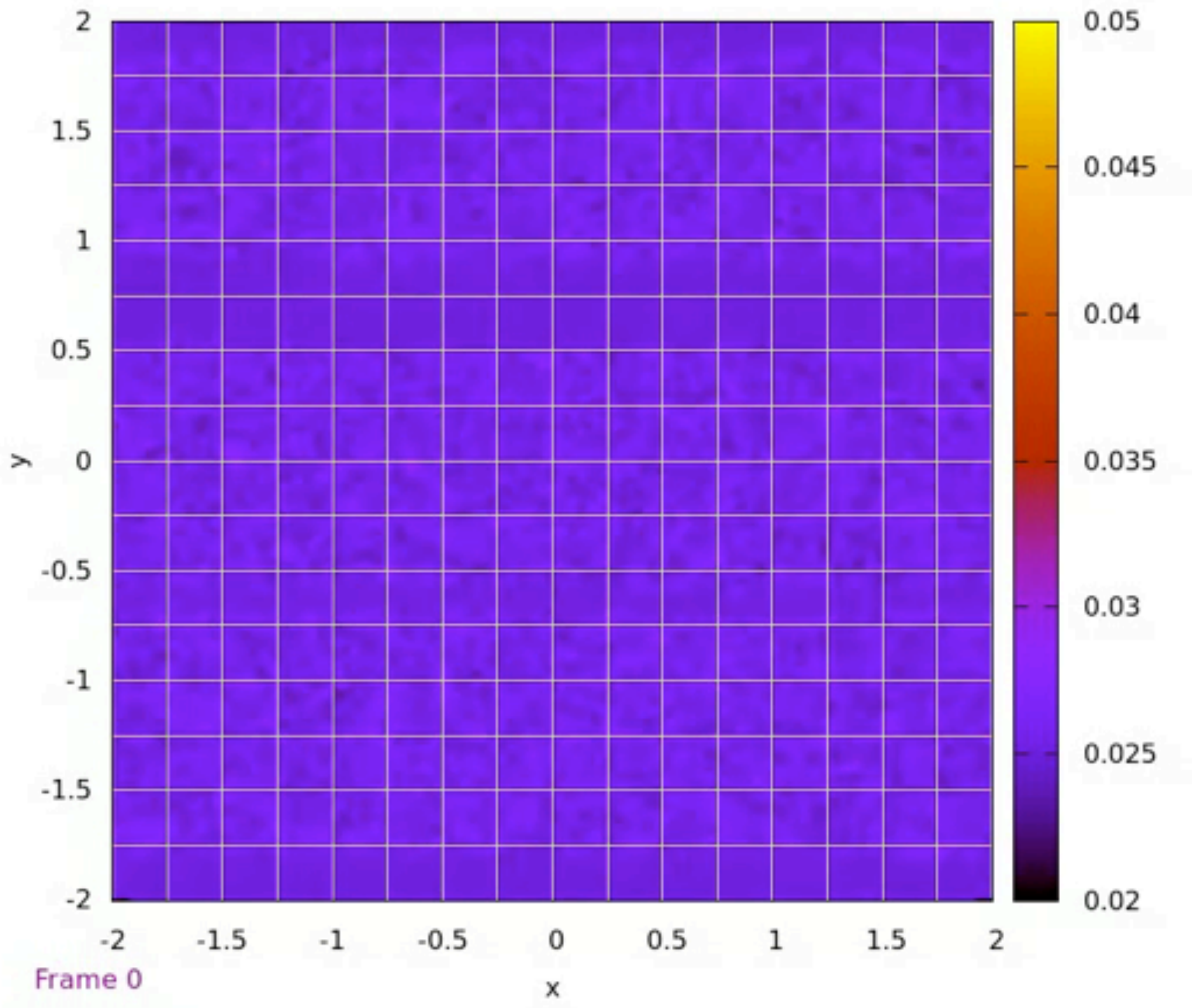
1D Modeling of Lamellar Composite

Adam Hinkle



2d Modeling of Lamellar Composite

Code: Chris Rycroft, Harvard; Sim: Adam Hinkle, JHU



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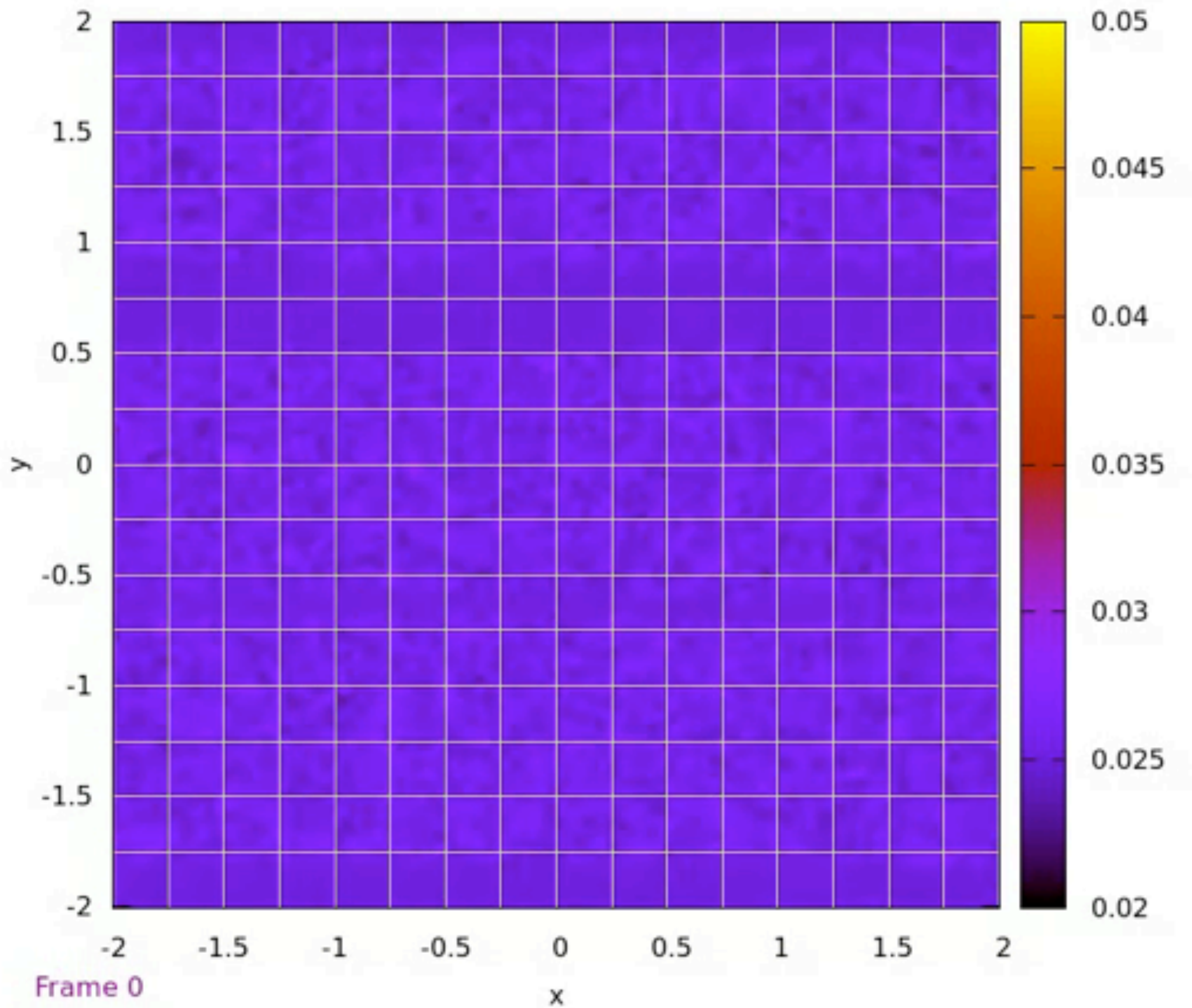
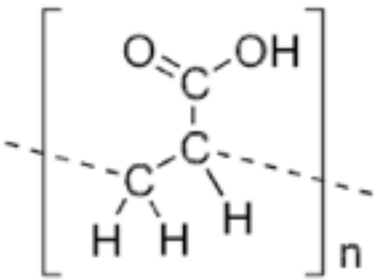


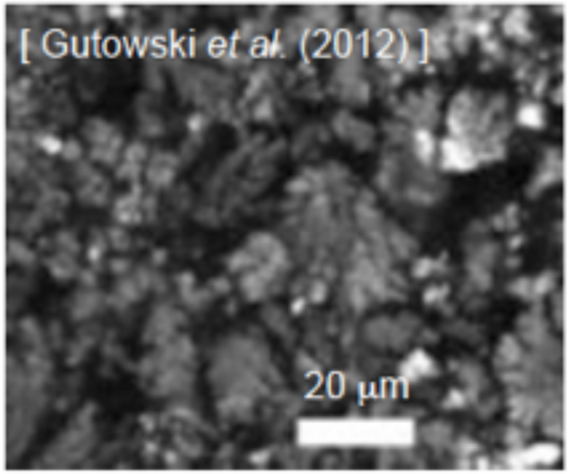
Transient Shear Banding in a Simple Yield Stress Fluid
Divoux, Tamarii, Barentin, Manneville
PRL 104, 208301 (2010)



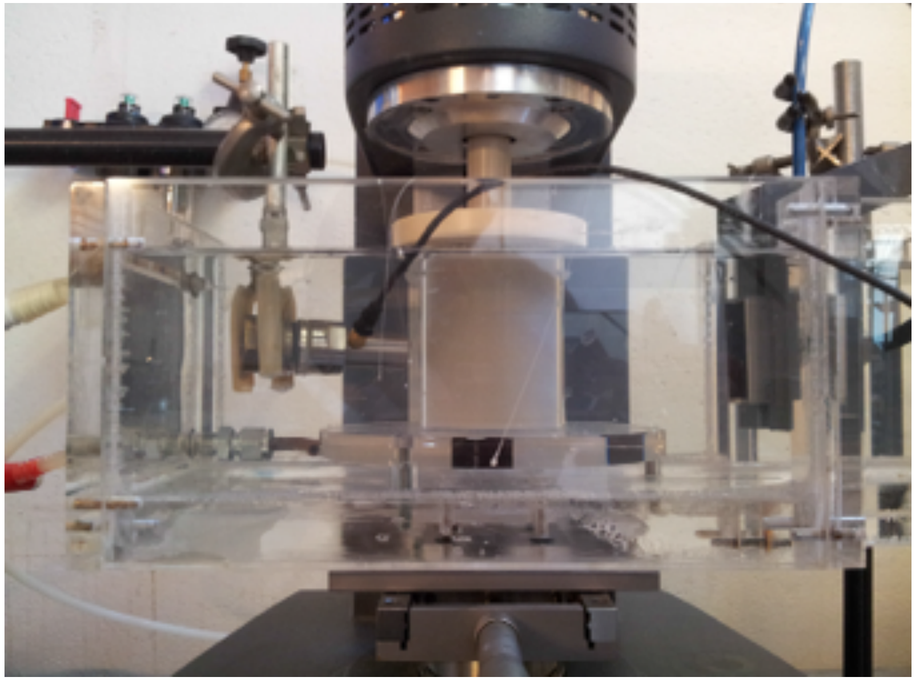
poly(acrylic acid) polymer

- 1% wt carbopol ETD 2050
- 0.5% wt hollow glass spheres

G' = 100 ± 10 Pa
G" = 12 ± 2 Pa



[Ketz *et al.* (1988), Baudonnet *et al.* (2004), Oppong *et al.* (2006), Lee (2011)]



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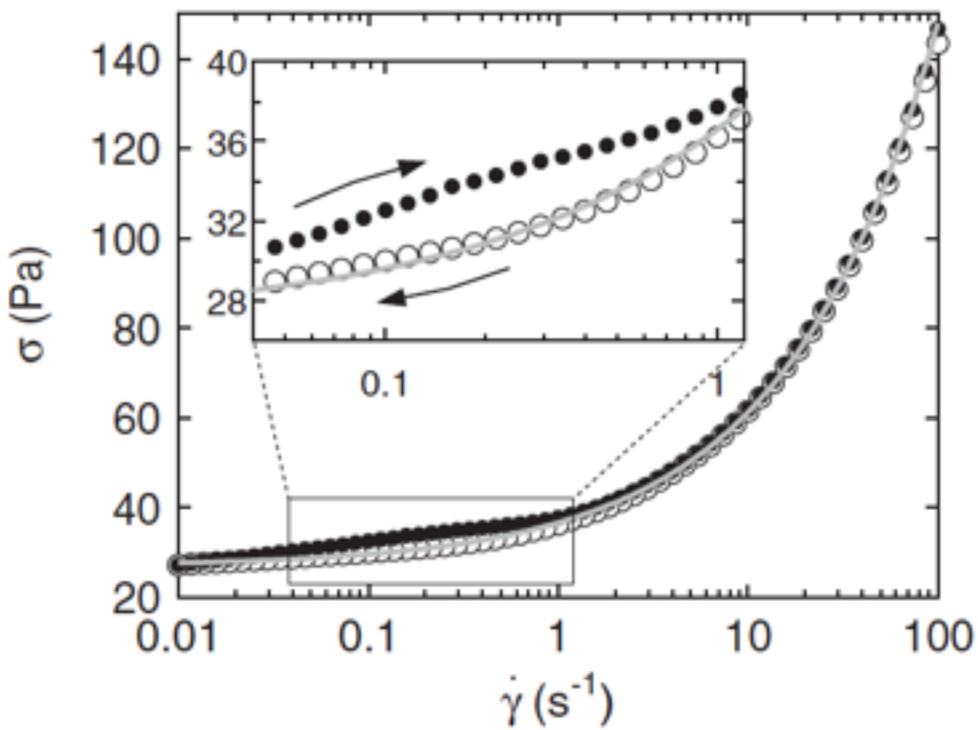

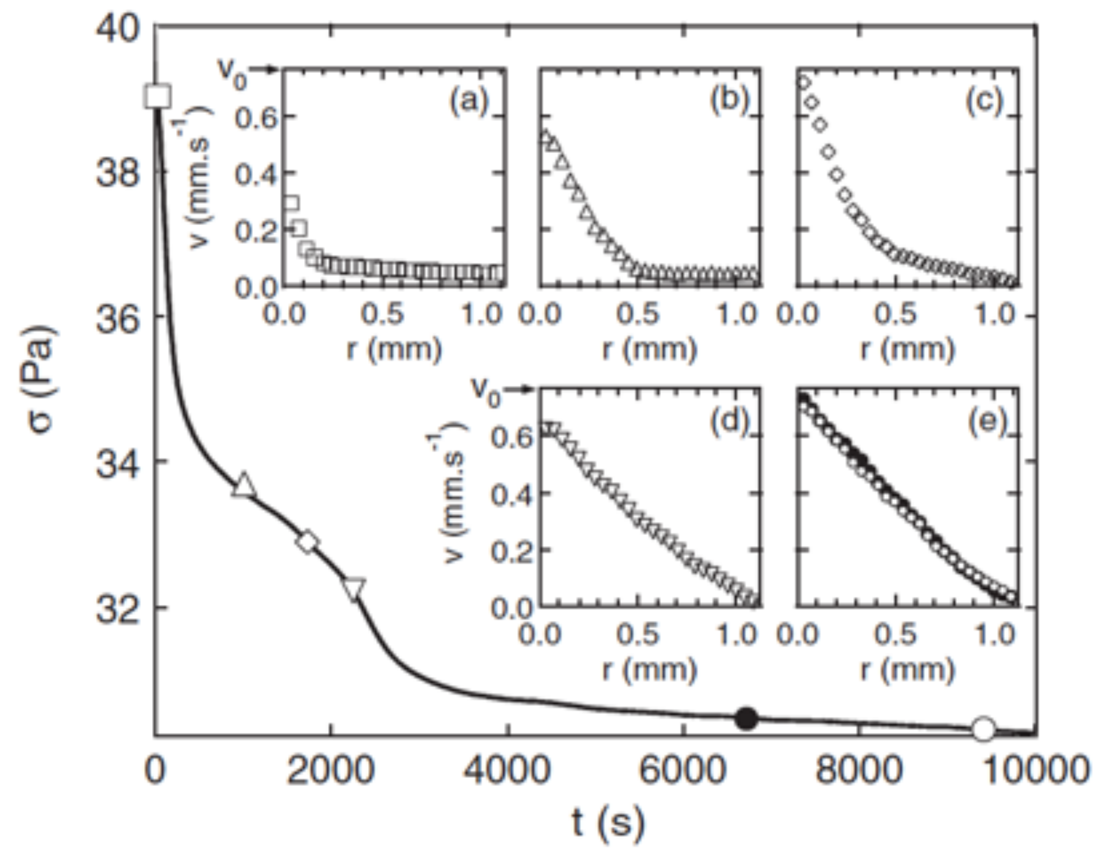

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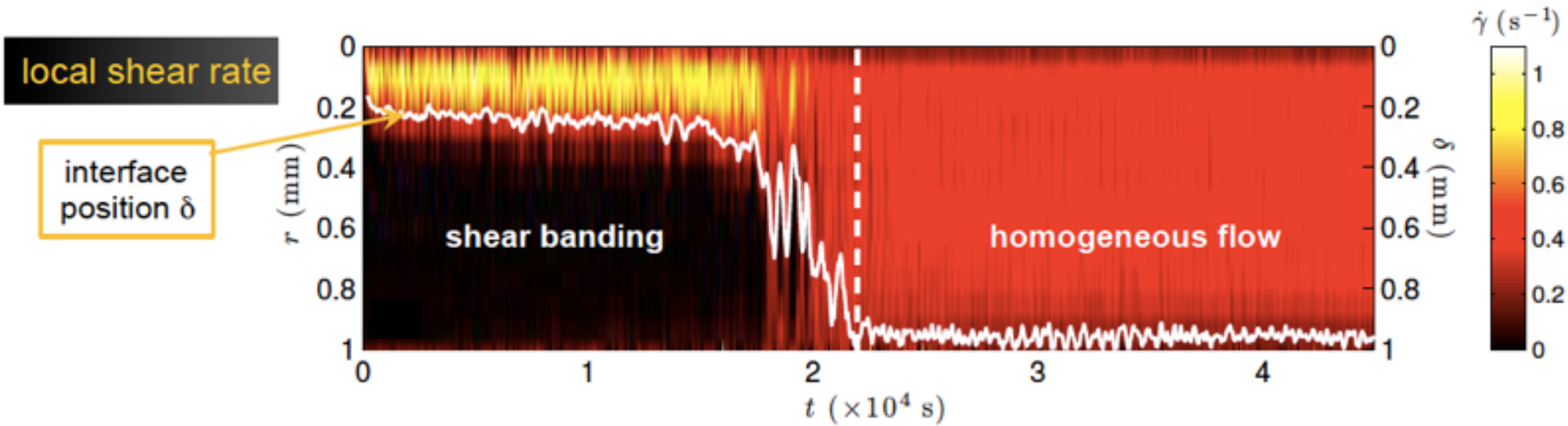

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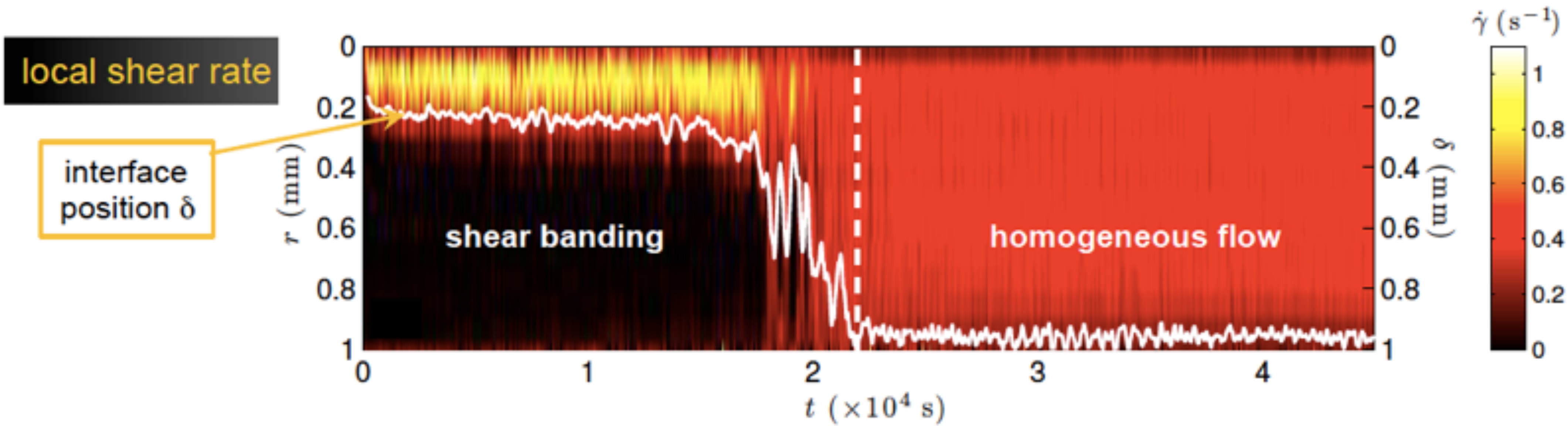

- Shear band nucleates at inner wall

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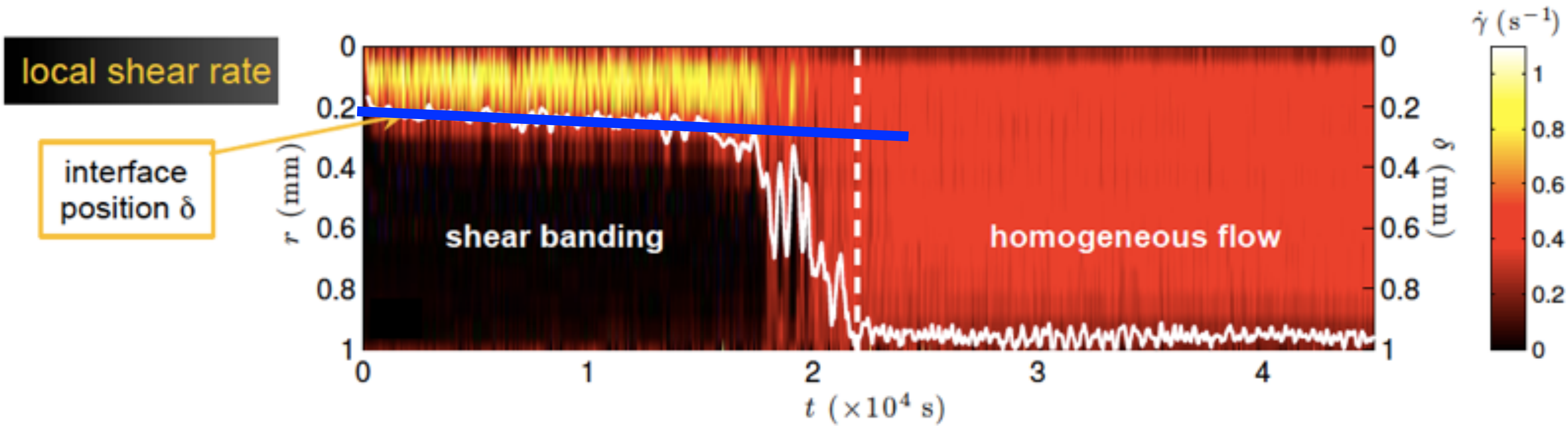

- Shear band nucleates at inner wall
- Shear band steadily broadens

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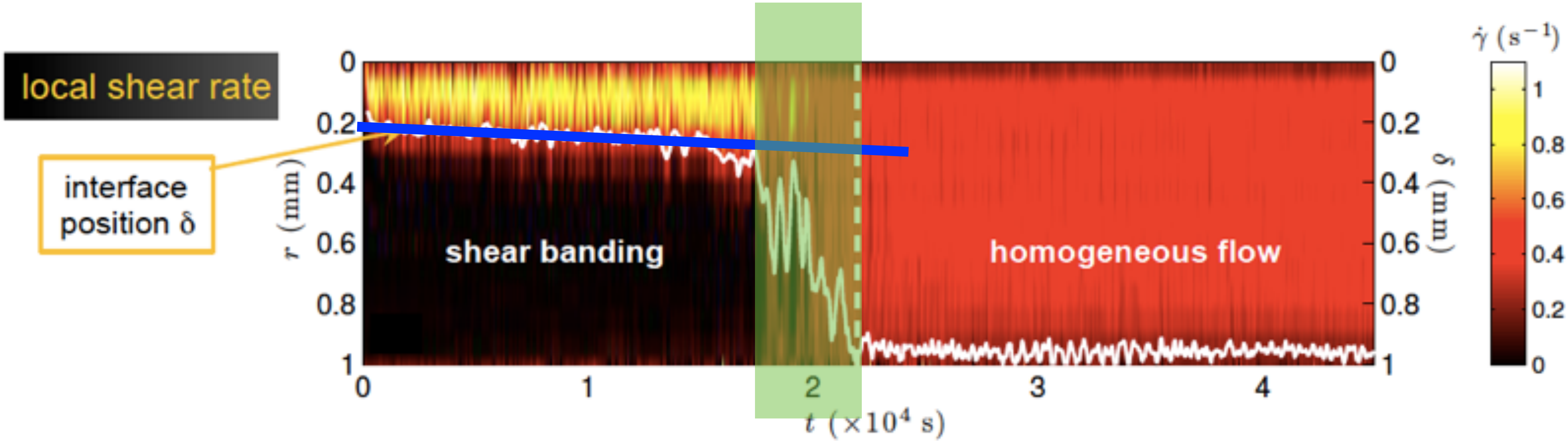


- Shear band nucleates at inner wall
- Shear band steadily broadens
- Before shear band propagates across entire cell, band destabilizes and homogeneous flow sets in.

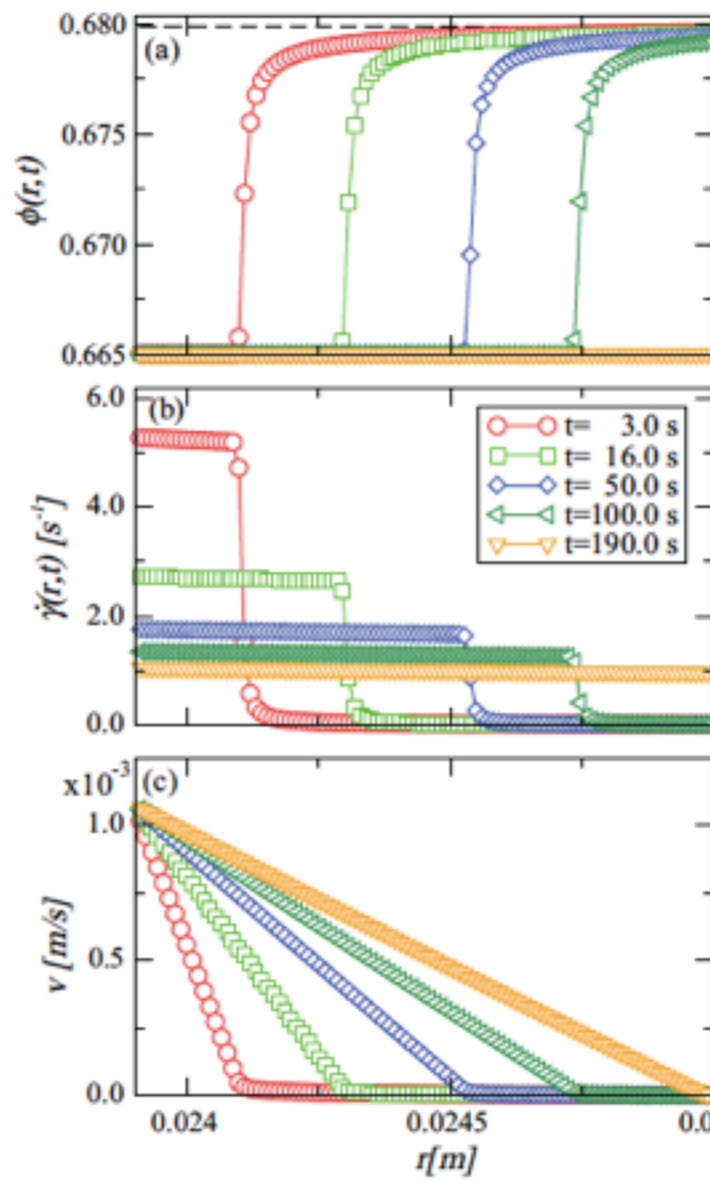
Transient shear banding in time-dependent fluids

Illa, Puisto, Lehtinen, Mohtaschemi, Alava, PRE 87, 022307 (2013)

$$\frac{d\phi}{dt} = \frac{A_b}{(\mu/\mu_o)^m} + (A_s - B_s\phi)\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^k,$$

$$\mu(\phi) = \mu_0\left(1 - \frac{\phi}{\phi_m}\right)^{-\eta},$$

- Develops transient shear band
- Fluidization time depends trivially on k
- No destabilization of band
- System once fluidized will not localize again on second sweep



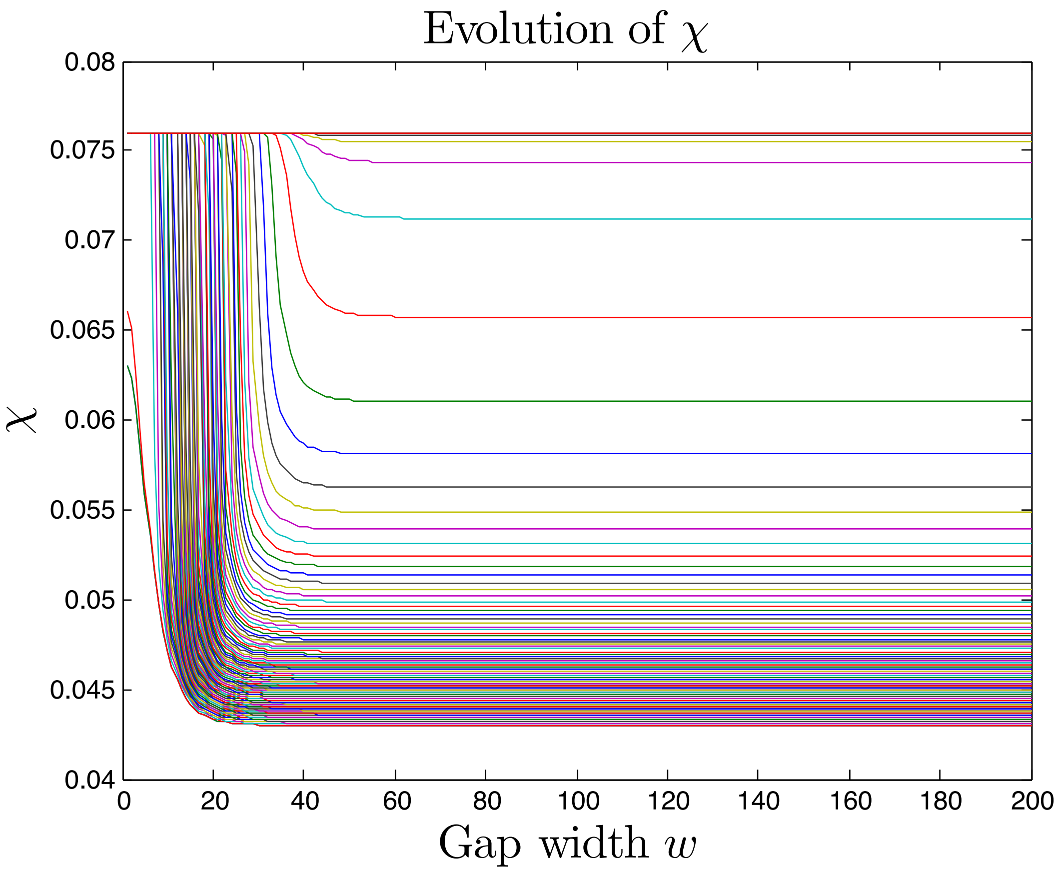
Effective Temperature Equations of Motion (Athermal Limit)

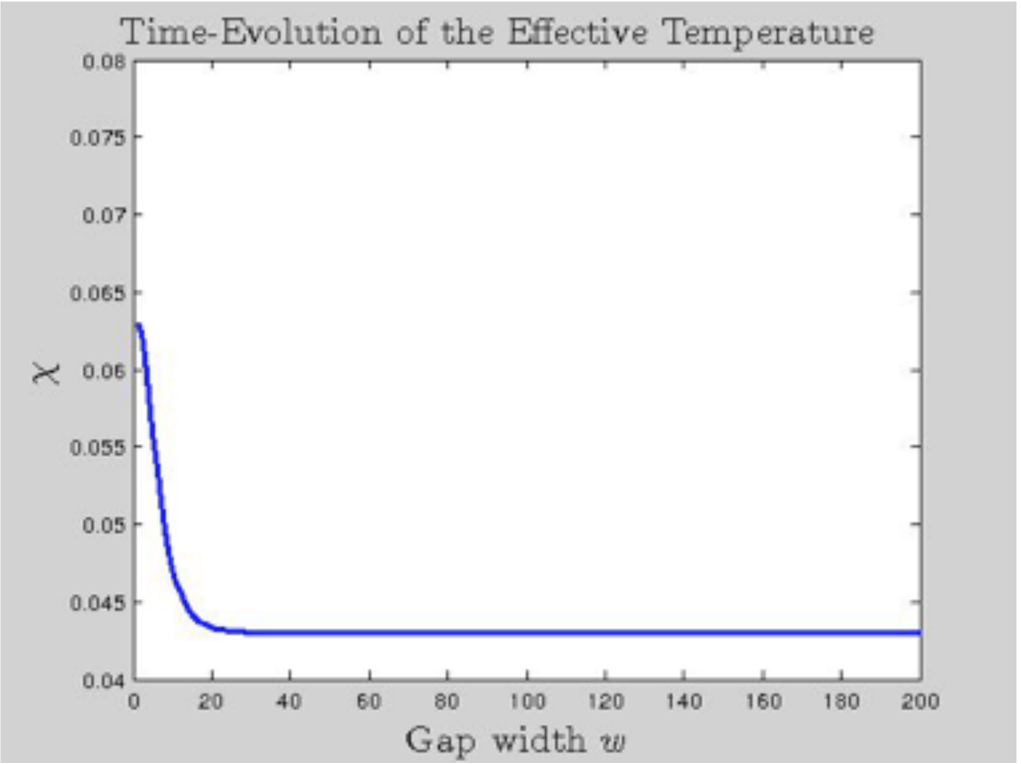
$$\dot{\epsilon}_{ij}^{pl} = e^{-e_Z/\chi} f_{ij}\left(s_{kl}\right)$$

$$c_0\dot{\chi} = 2s_{ij}\dot{\epsilon}_{ij}^{pl}\left(\chi_\infty - \chi\right) + l^2\left|\dot{\epsilon}_{ij}^{pl}\right|\nabla^2\chi$$

- Recall that in the STZ formulation the function ***f*(*s*)** is derived from the microscopic equations for the STZ flips.
- Here we will choose ***f*(*s*)** to be consistent with the steady state rheology, such that we recover the Herschel-Bulkley behavior.

Results of Simple Model





- Shear band quickly reaches steady state in center and begins to broaden.
- Before shear band sweeps across system the entire system fluidizes.

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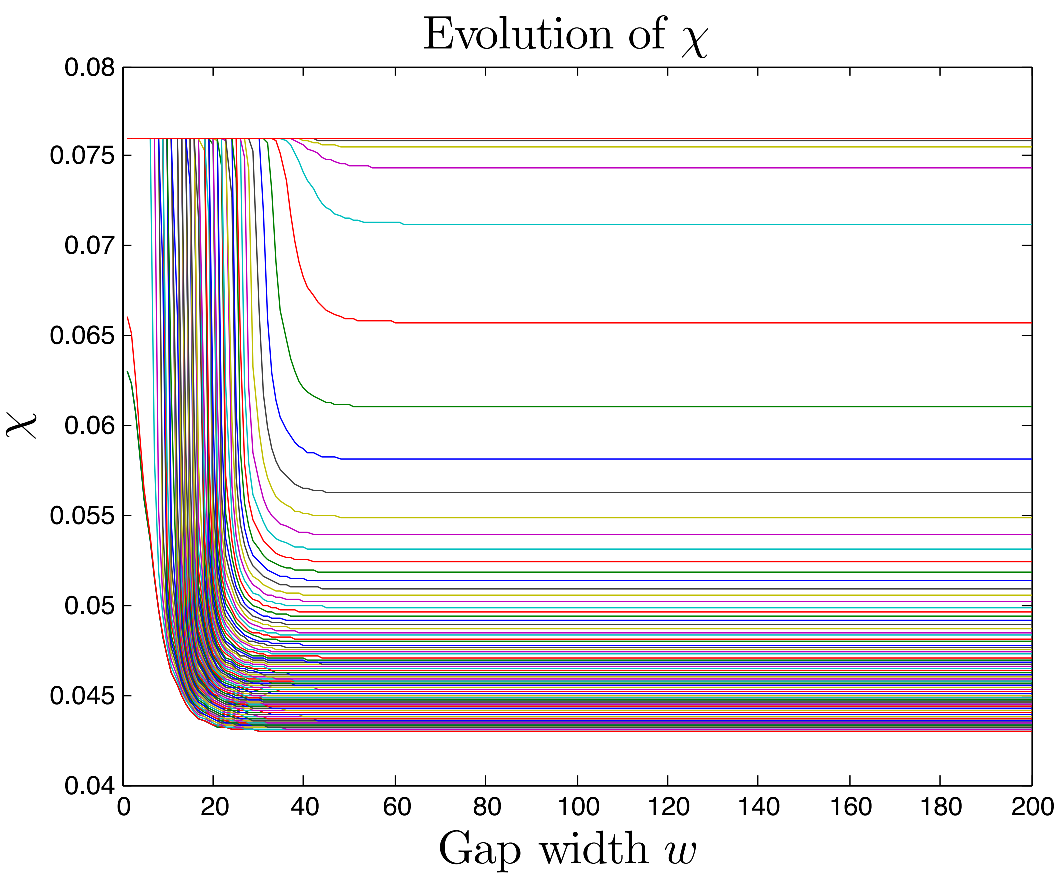

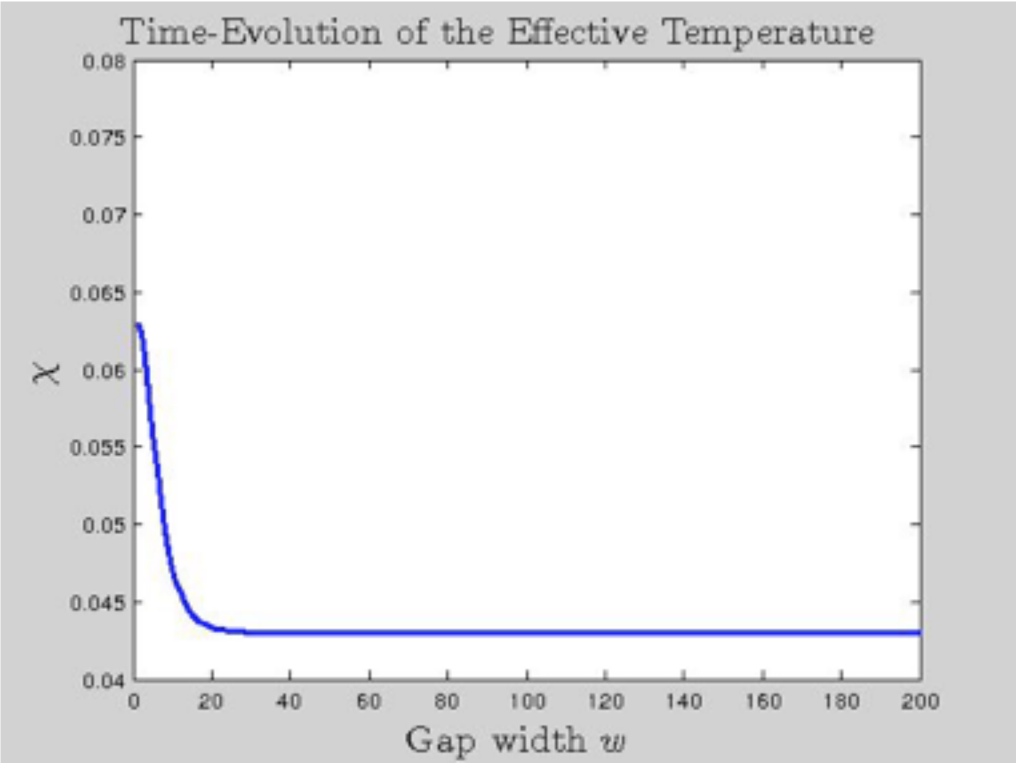

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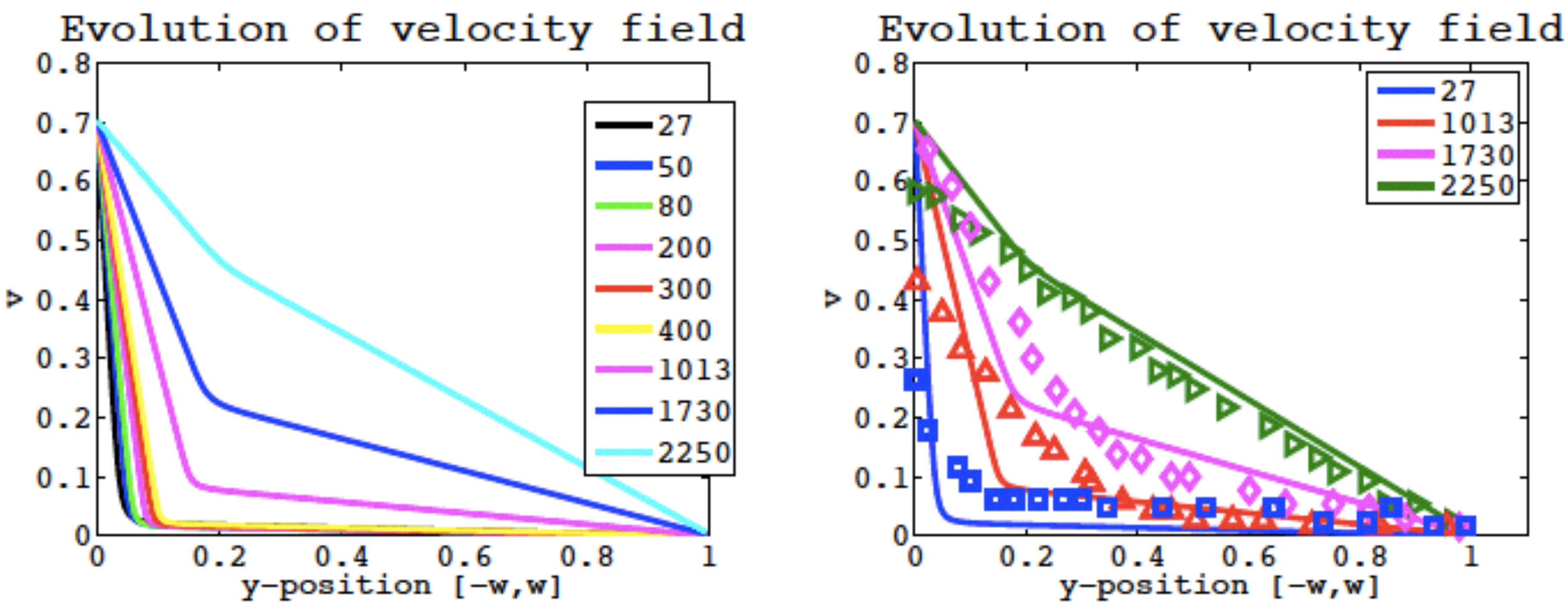

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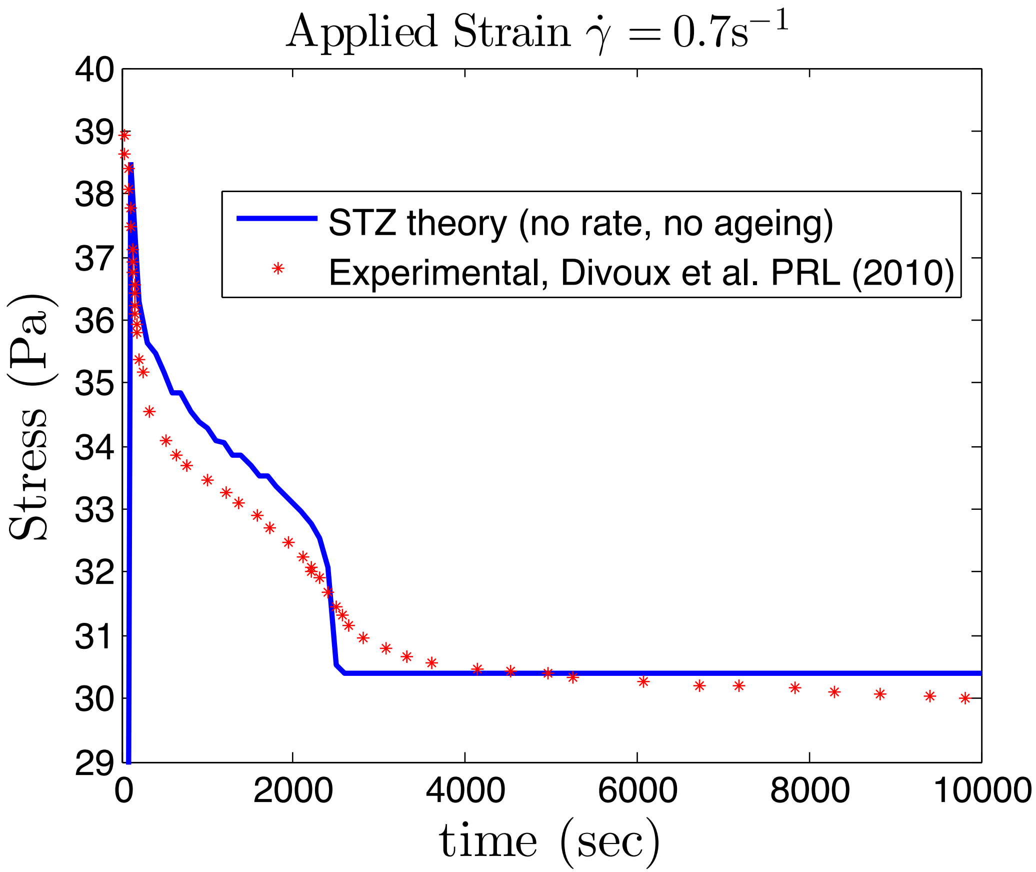

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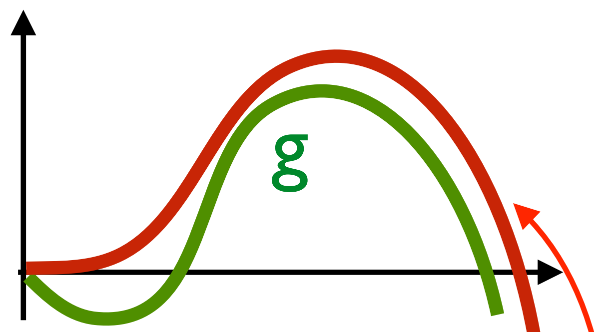
Analogy to F-KPP Equations

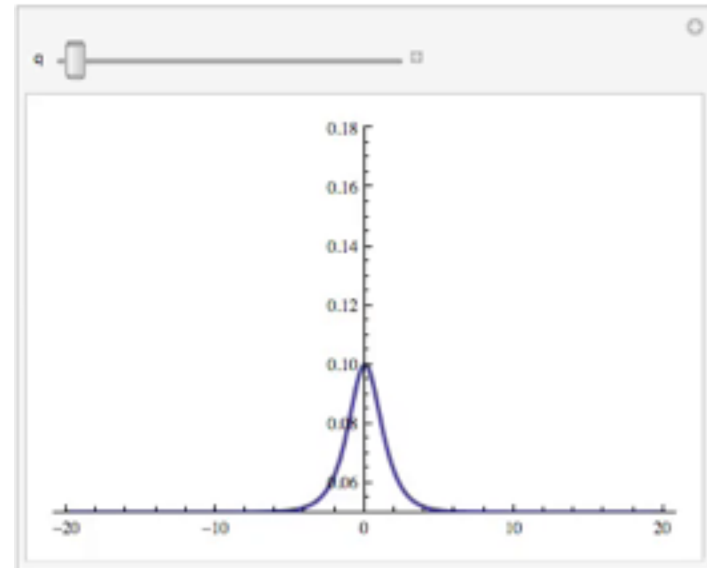
- This is a variant of the Fisher-Kolmogorov, Petrovsky, Piscouno (F-KPP) equation used in models of solidification.

$$\partial_t u - \partial_x^2 u = g(u)$$

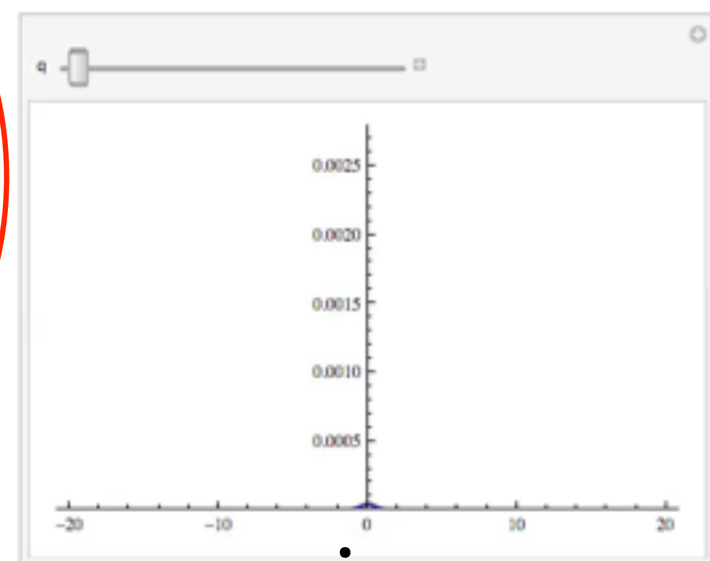


- In our case we have a strongly non-linear function on the RHS

$$\partial_t \chi - D\partial_x^2 \chi = \frac{2sf(s)}{c_0} e^{-1/\chi}(\chi_\infty - \chi)$$



χ



$\dot{\varepsilon}_{pl}$

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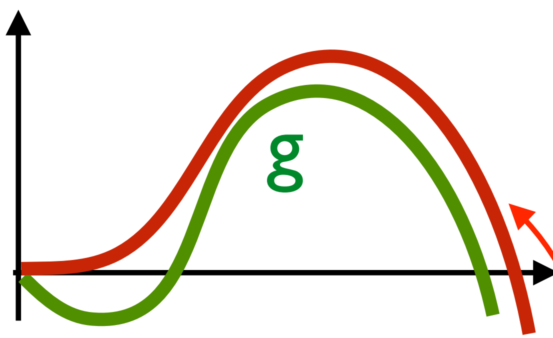

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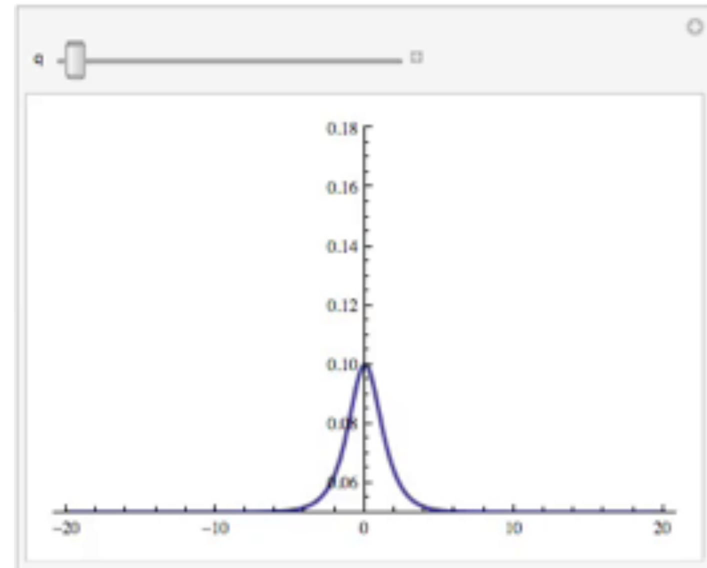
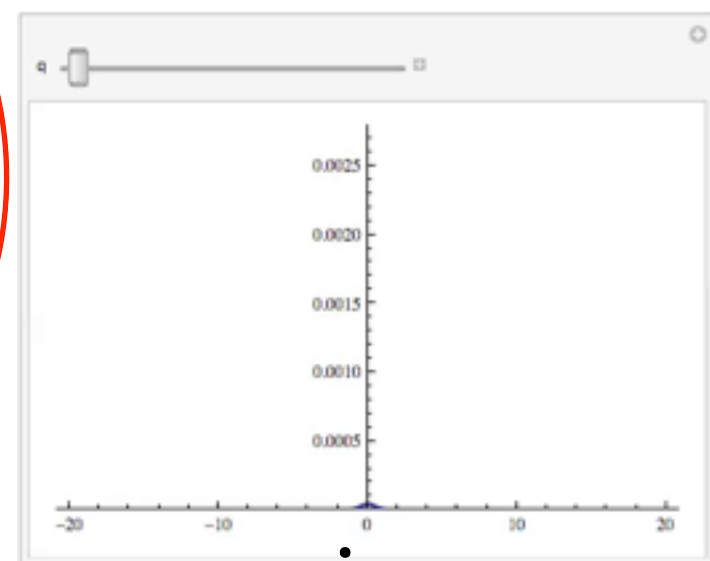


χ



$\dot{\varepsilon}_{pl}$

Initial Model

Successes

- Shear band growth and destabilization are both observed.
- The stress vs. time curve is reasonably close.

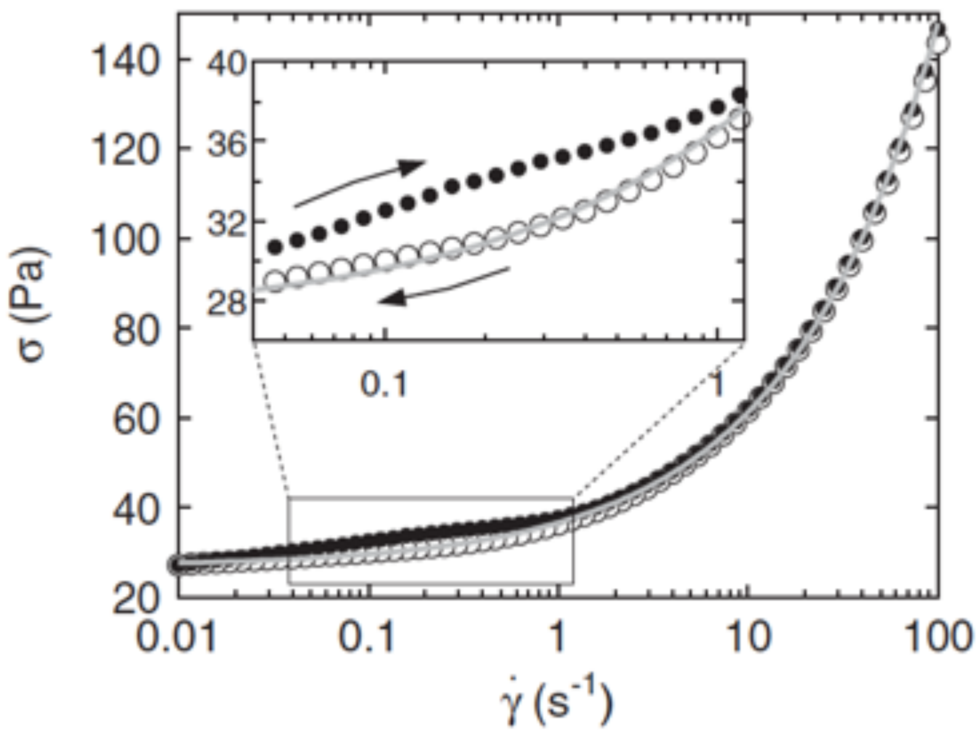
Deficiencies

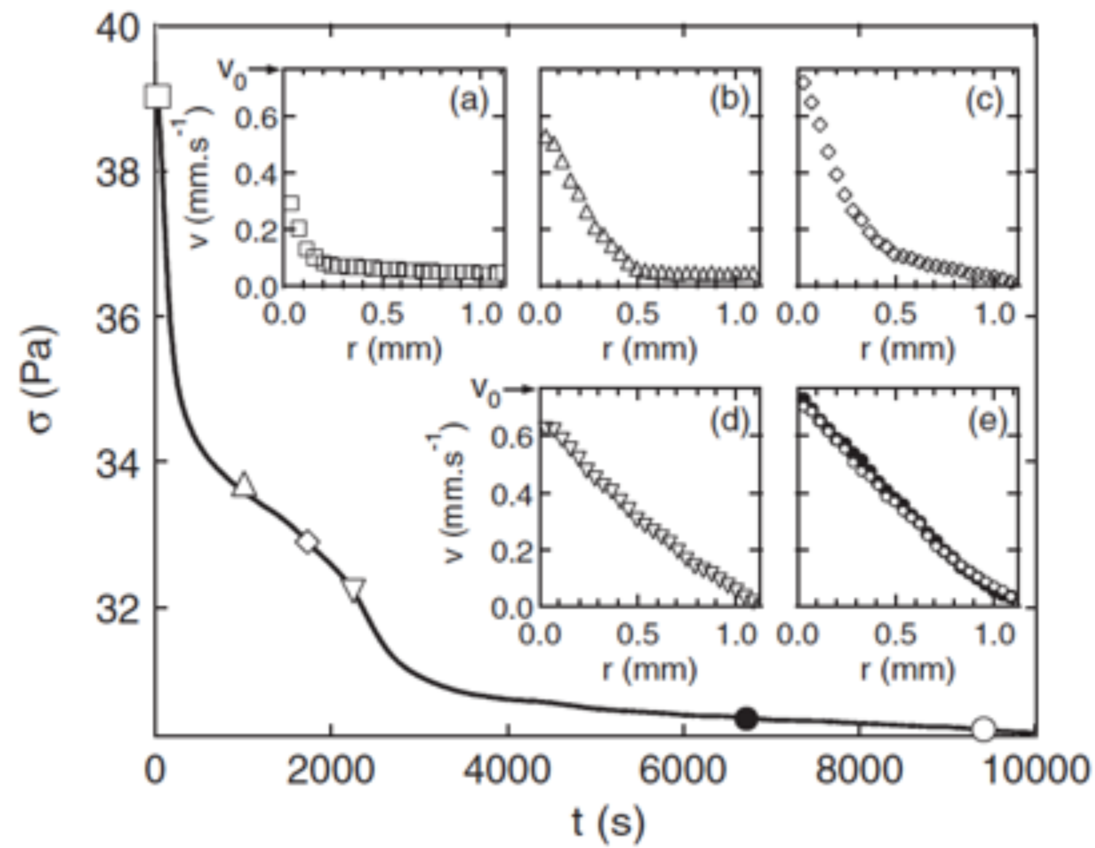
- Like IIIa, once fluidized the system is in a structural steady state and cannot band again.
- The scaling of fluidization time is trivial ($\tau_f \sim \dot{\gamma}^{-1}$)

Transient Shear Banding in a Simple Yield Stress Fluid

Divoux, Tamarii, Barentin, Manneville

PRL **104**, 208301 (2010)





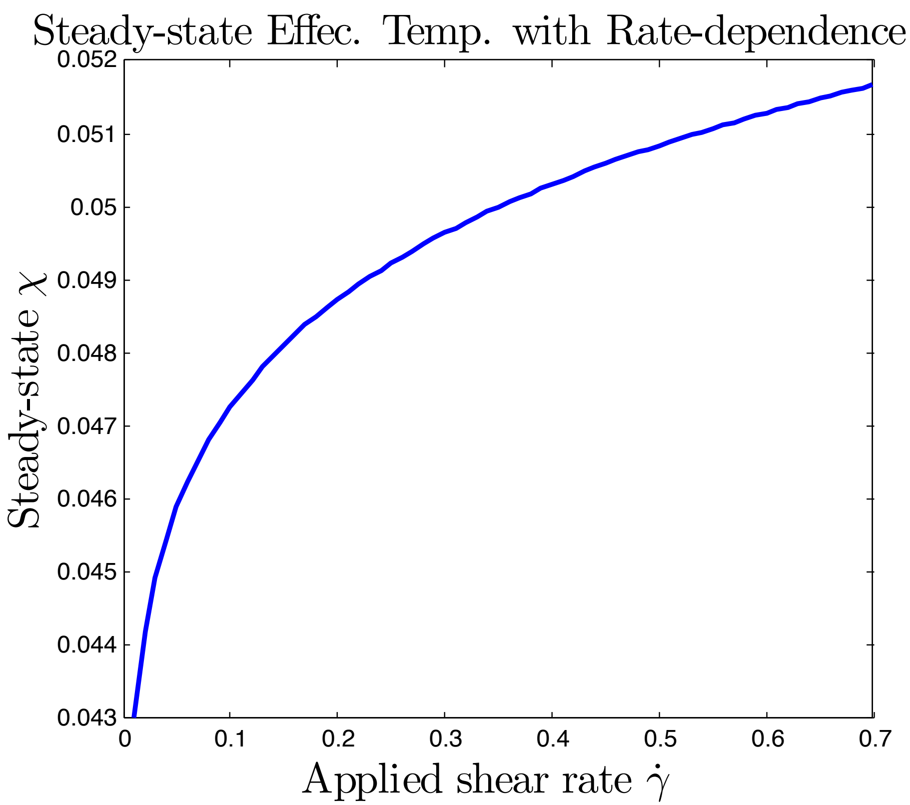
Effective Temperature Equations of Motion (Rate Dependent Disorder)

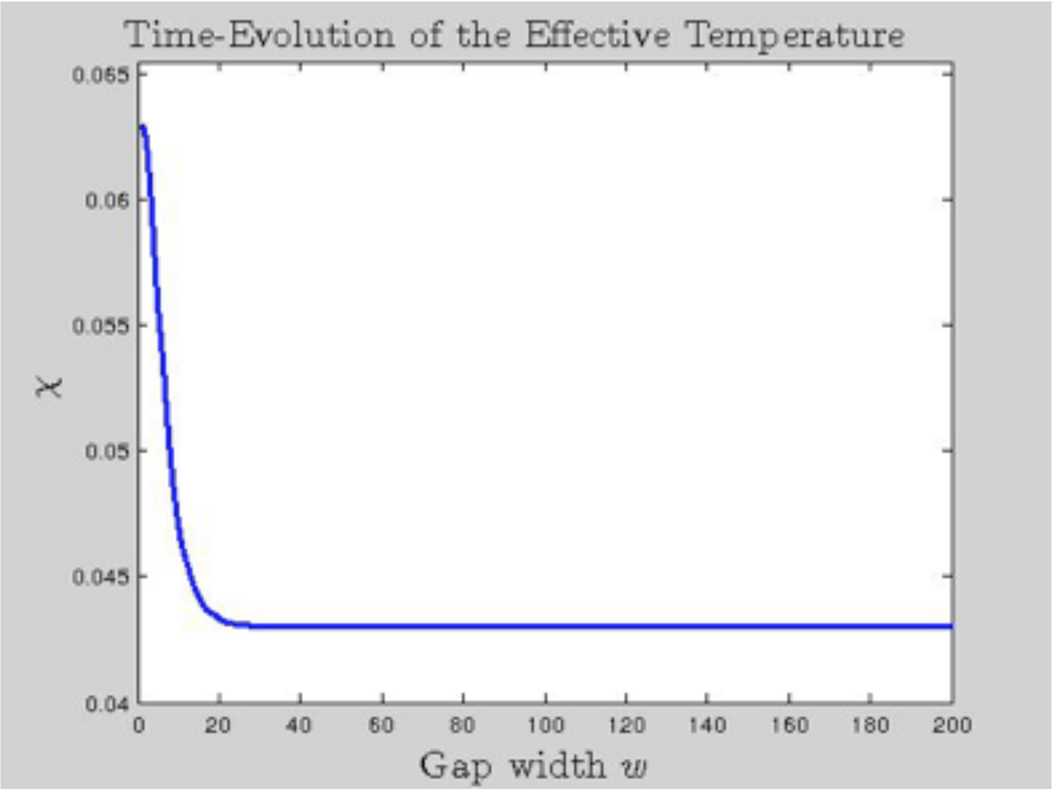
$$\dot{\epsilon}_{ij}^{pl} = e^{-e_Z/\chi} f_{ij}\left(s_{kl}\right)$$

$$c_0\dot{\chi} = 2s_{ij}\dot{\epsilon}_{ij}^{pl}\left[\chi_\infty(|\dot{\epsilon}^{pl}|) - \chi\right] + l^2\left|\dot{\epsilon}_{ij}^{pl}\right|\nabla^2\chi$$

- We make the degree of disorder explicitly dependent on the steady state shear rate. This permits low χ solutions at low rates of shear.
- Again we will choose $f(s)$ to be consistent with the steady state rheology, such that we recover the Herschel-Bulkley behavior.
- Form for χ_∞ taken from Manning, Daub, Langer and Carlson, PRE 79, 016110 (2009).

Effective Temperature Equations of Motion (Rate Dependent Disorder)





- Simultaneous broadening of band and fluidization outside.
- Can initialize the material at a value of χ corresponding to the low rate steady state, and induce shear band by driving at higher rates

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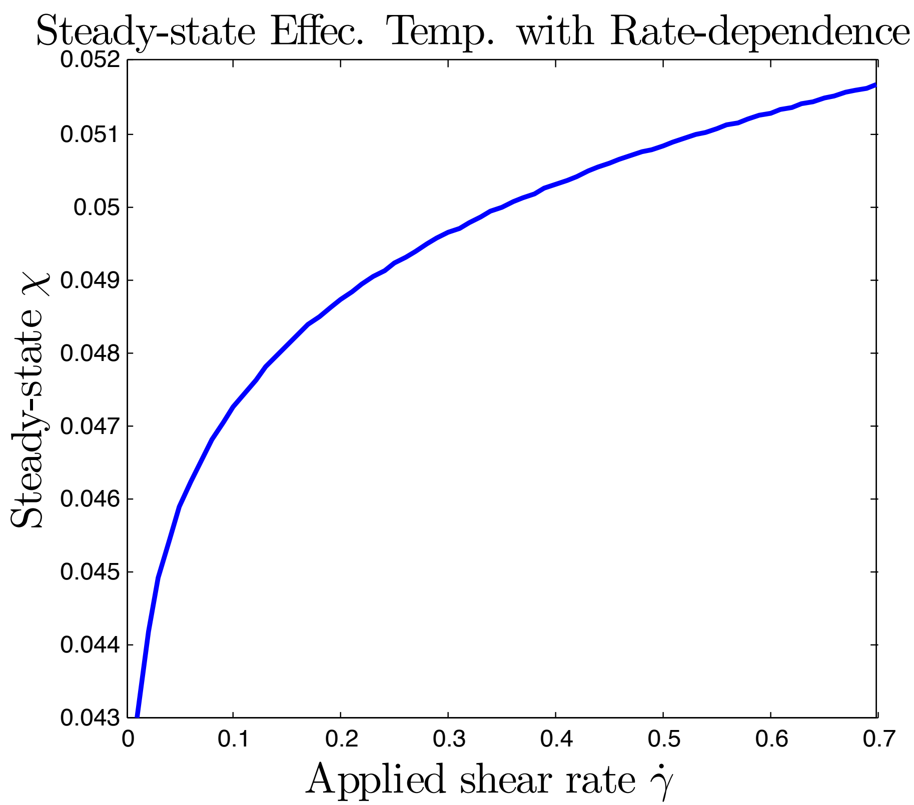

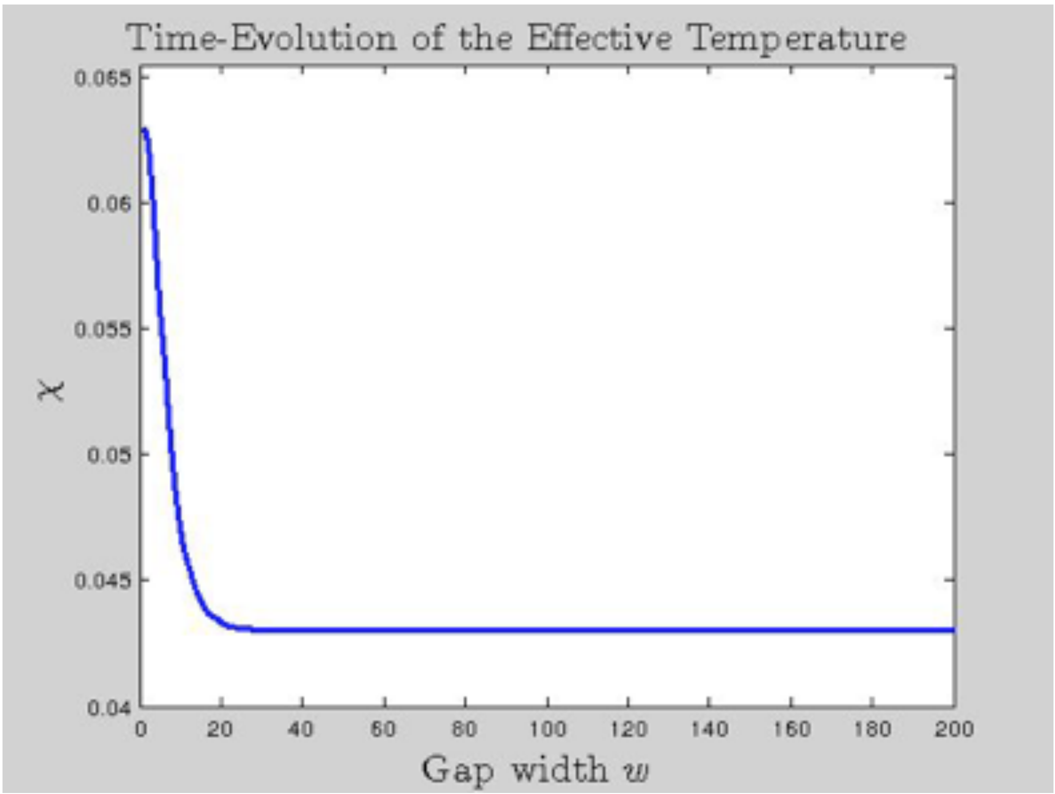

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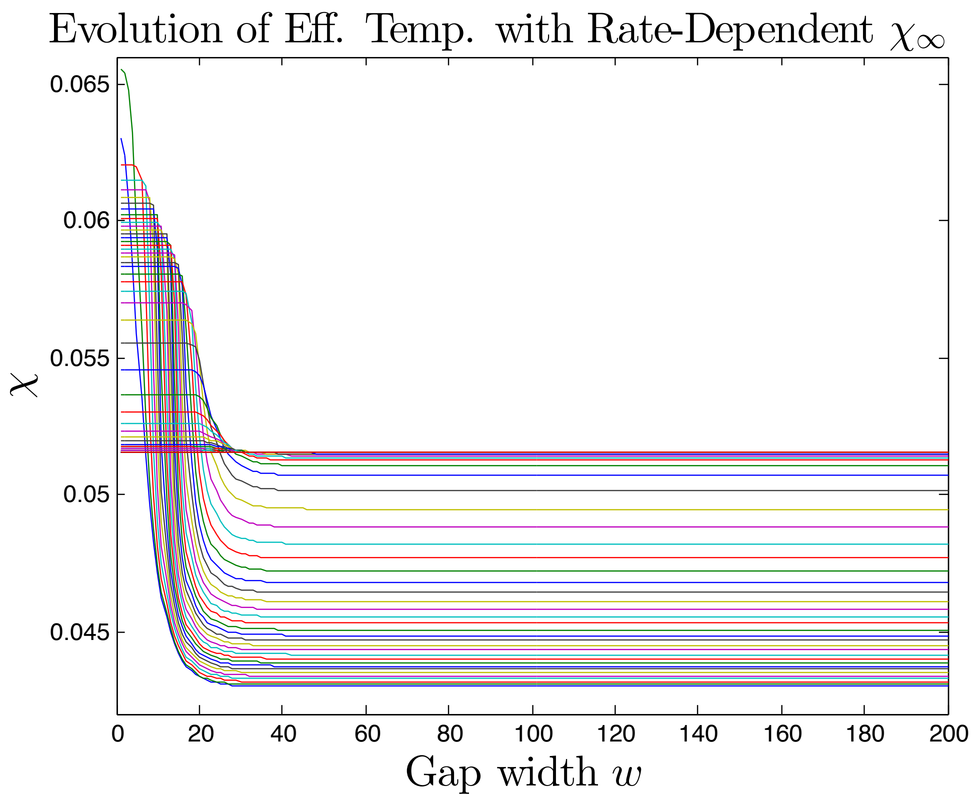
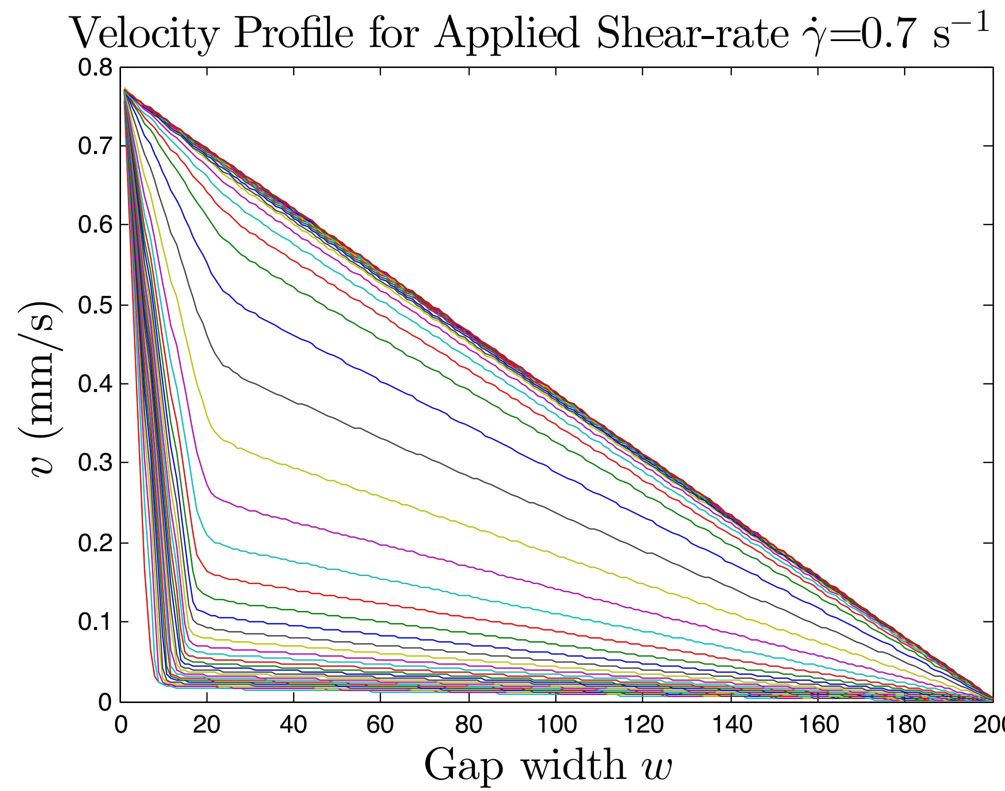
Effective Temperature Equations of Motion (Rate Dependent Disorder)





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- Can initialize the material at a value of χ corresponding to the low rate steady state and induce shear band by driving at higher rates

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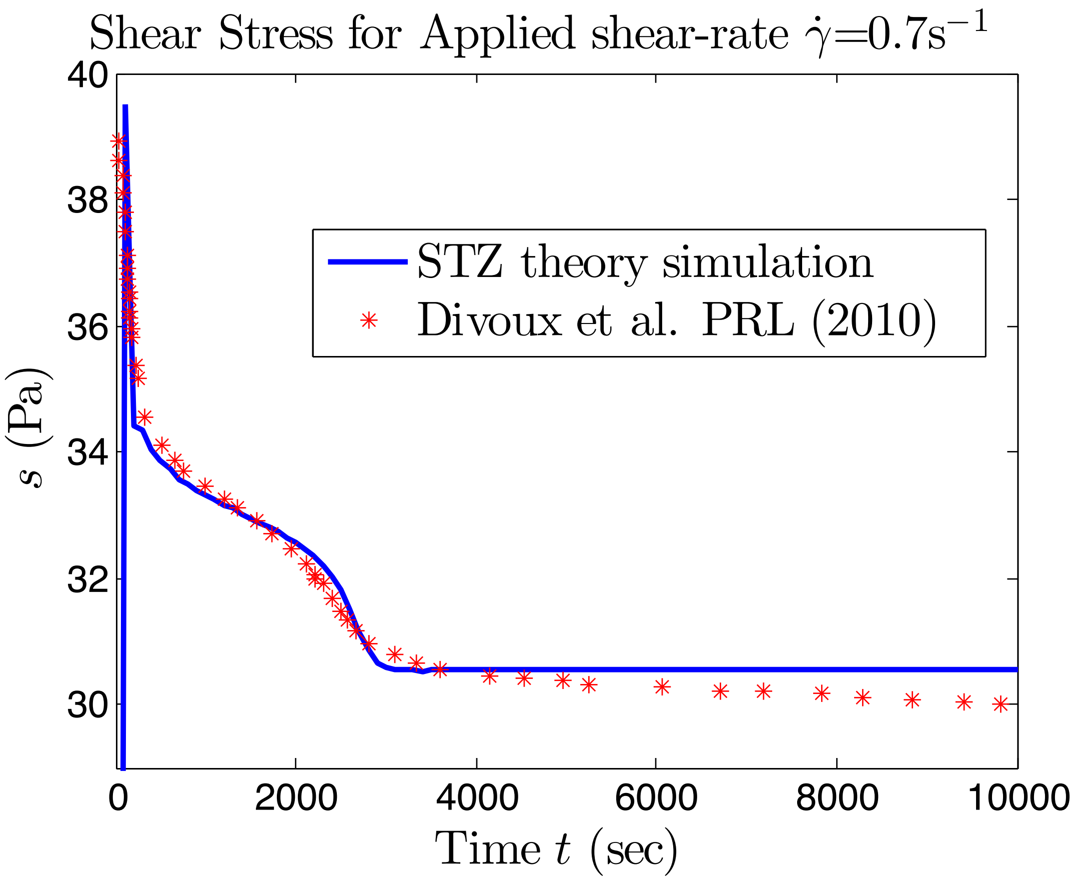

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Rate Dependent Disorder Model

Successes

- Shear band growth and destabilization are both observed.
- The stress vs. time curve is reasonably close.
- Can initialize the system at low rate and shear band at high rate.

Deficiencies

- Fluidization time varies like shear rate to the **-0.5**. This reflects more strain needed to reach higher disorder at higher rates.
- More complex functional form of the structural dependence of the yield stress?

Conclusions

- Modeling shear banding provides a challenge for constitutive theories.
- MD simulation indicates that predicting nucleation of shear bands in metallic glasses requires correctly characterizing fluctuations in the structure and that the nucleation process is sensitive to the dimensionality of the mechanics problem.
- The STZ effective temperature phenomenology produces a transition from shear band broadening to fluidization that matches the phenomenology in yield stress fluids.
- Introducing a rate dependent steady state χ permits shear banding on repeated loadings.
- Missing ingredient relating rate of fluidization to shear rate requires further study. Perhaps this arises due to structure dependence of yield stress.