Elasto-plasticity in Amorphous Solids

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With

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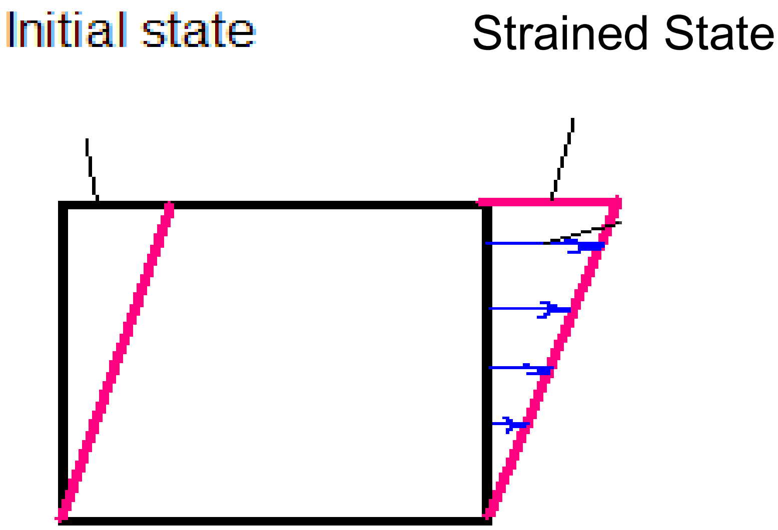
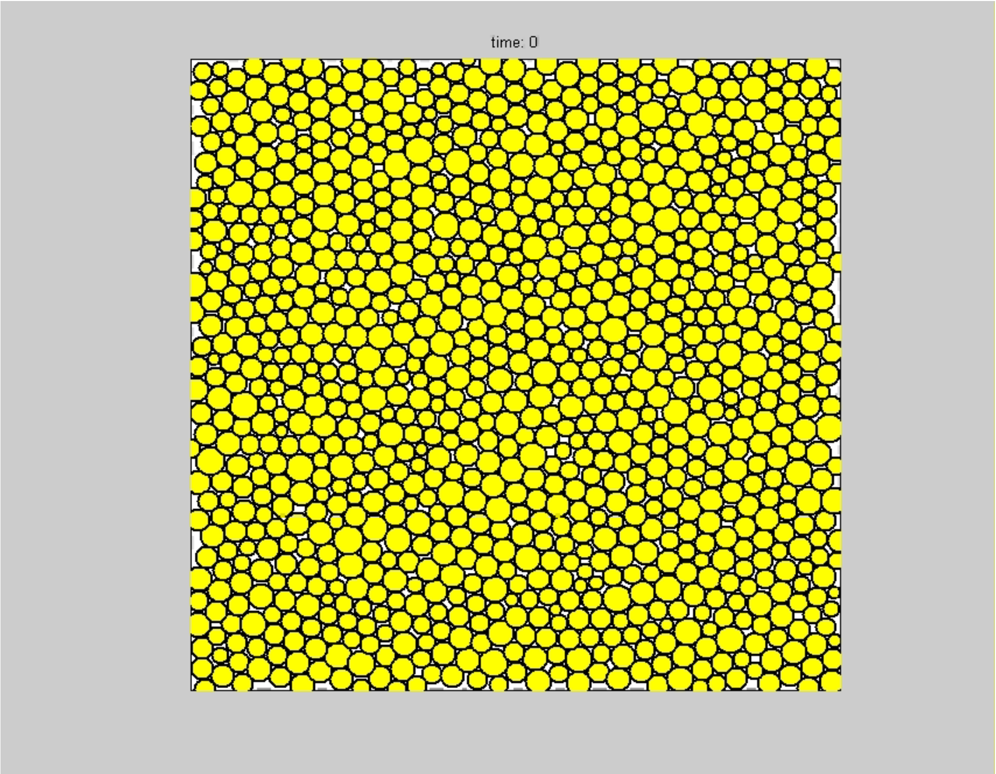
Computer Experiment of Simple Shear





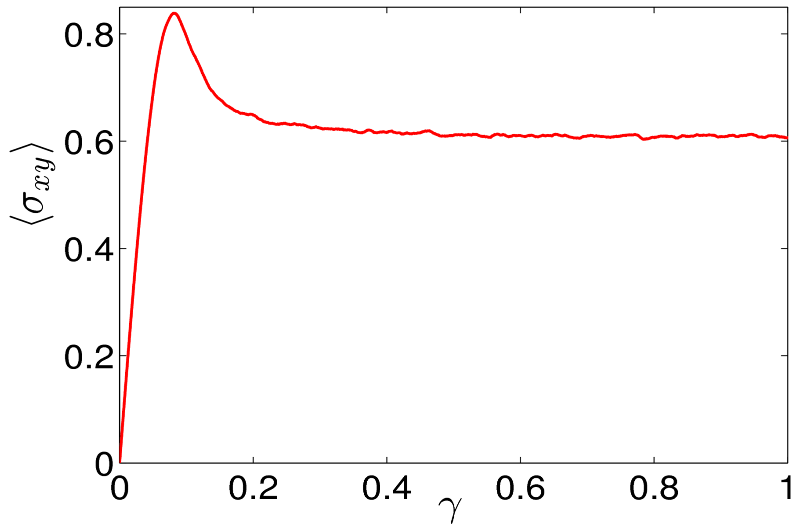
Simple Shear :

$$\mathbf{r}_{ix} = \mathbf{r}_{ix} + \gamma \mathbf{r}_{iy}$$

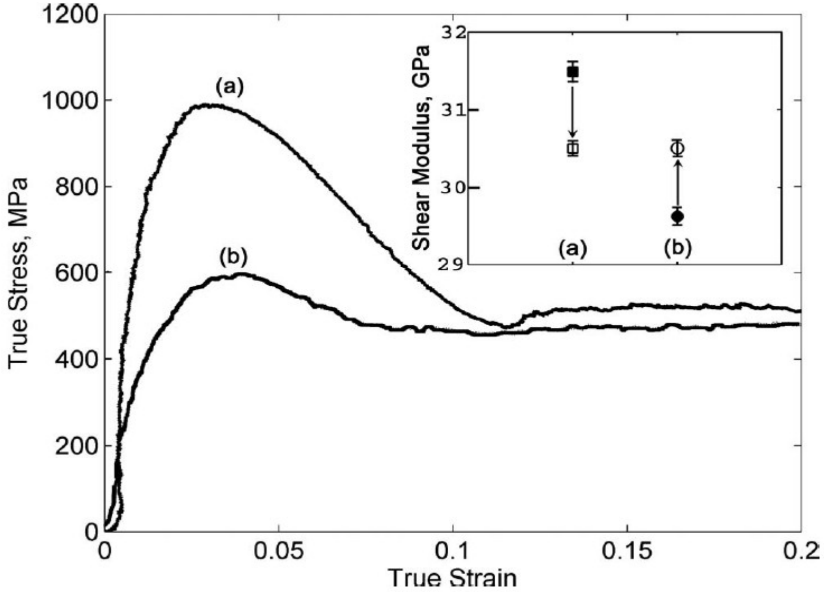
$$\mathbf{r}_{iy} = \mathbf{r}_{iy}$$

$$\mathbf{r}_{iz} = \mathbf{r}_{iz} \,(in\, 3D)$$

Response of the Amorphous System under Simple Shear

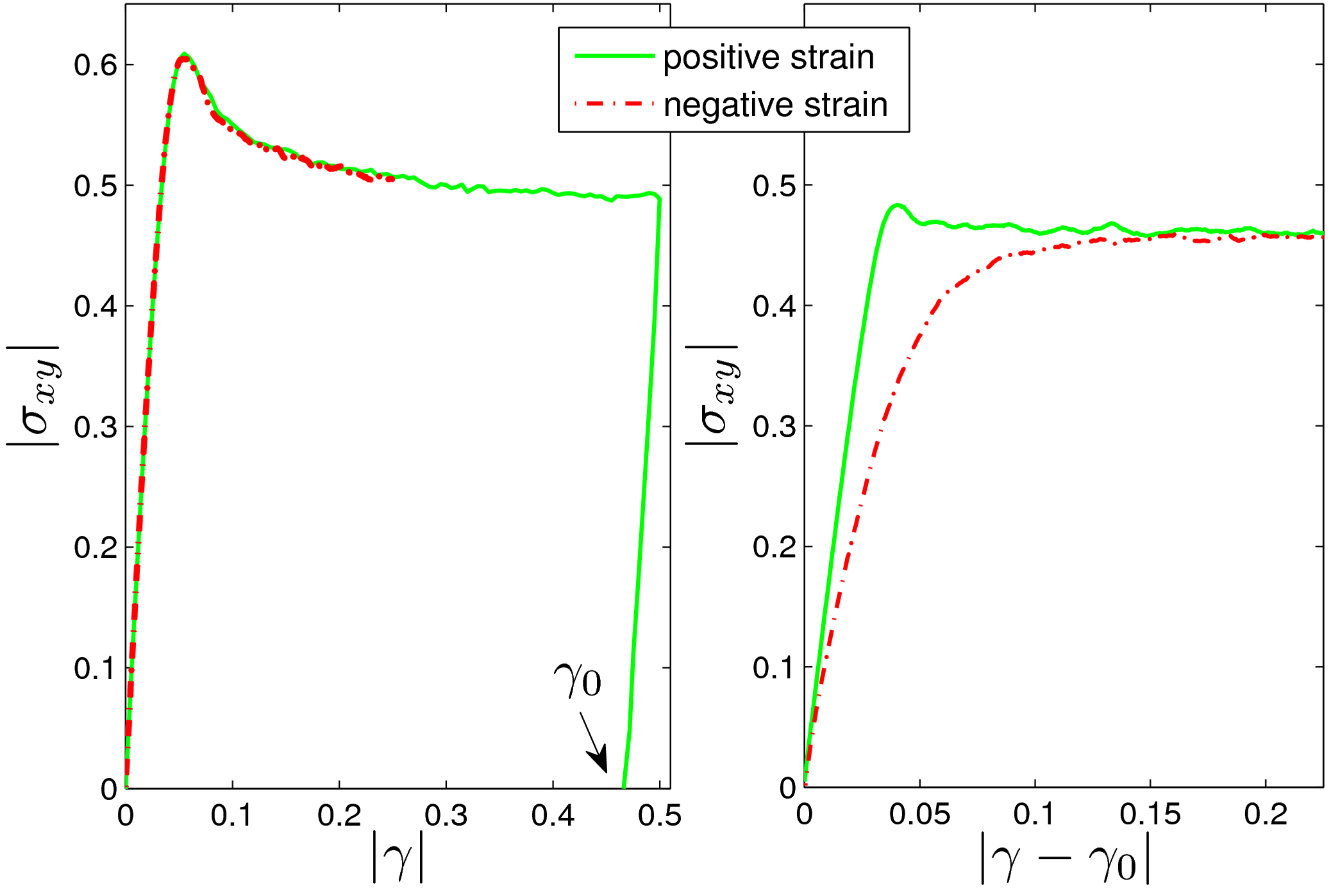


Simulation :: Binary soft disk with pure repulsive interaction



Experiment :: A four component metallic glass (Pd, Ni, Cu, P)
- W. Johnson et al. - APL, **90**, 131912 (2007)

Anisotropic Response :: Bauschinger Effect



- Response to +ve and -ve straining is identical in isotropic case
- Response is markedly anisotropic in the steady state

Order Parameter ?

- What is the order parameter which controls the jamming (solid) to unjamming (steady flowing state) transition of an amorphous solids under external shear?
- What is the order parameter which encodes the system's past life in steady flowing state and gives rise to anisotropic response ?
- STZ order parameter ⟹ But its difficult to calculate

$$m = \frac{n_+ - n_-}{n_+ + n_-}$$

Lets do Computer Simulations to gain some insights

Simulation Details

- Thermal Simulation ::

Sllod Equation ::

$$\dot{\mathbf{r}}_{ix} = \frac{\mathbf{p}_{ix}}{m} + \dot{\gamma}$$

$$\dot{\mathbf{r}}_{iy} = \frac{\mathbf{p}_{iy}}{m}$$

$$\dot{\mathbf{r}}_{iz} = \frac{\mathbf{p}_{iz}}{m} \; [in \, 3D]$$

$$\dot{\mathbf{p}}_{ix} = \mathbf{f}_{ix} - \dot{\gamma}\mathbf{p}_{iy}$$

$$\dot{\mathbf{p}}_{iy} = \mathbf{f}_{iy}$$

$$\dot{\mathbf{p}}_{iz} = \mathbf{f}_{iz} \; [in \, 3D]$$

- Athermal Simulation ::

$$\mathbf{r}_{ix} = \mathbf{r}_{ix} + \gamma \mathbf{r}_{iy}$$

$$\mathbf{r}_{iy} = \mathbf{r}_{iy}$$

$$\mathbf{r}_{iz} = \mathbf{r}_{iz} \; (in \, 3D)$$

Minimize the strained state using Conjugate gradient minimizer and Repeat the procedure to desired Straining amount

Simulation Model

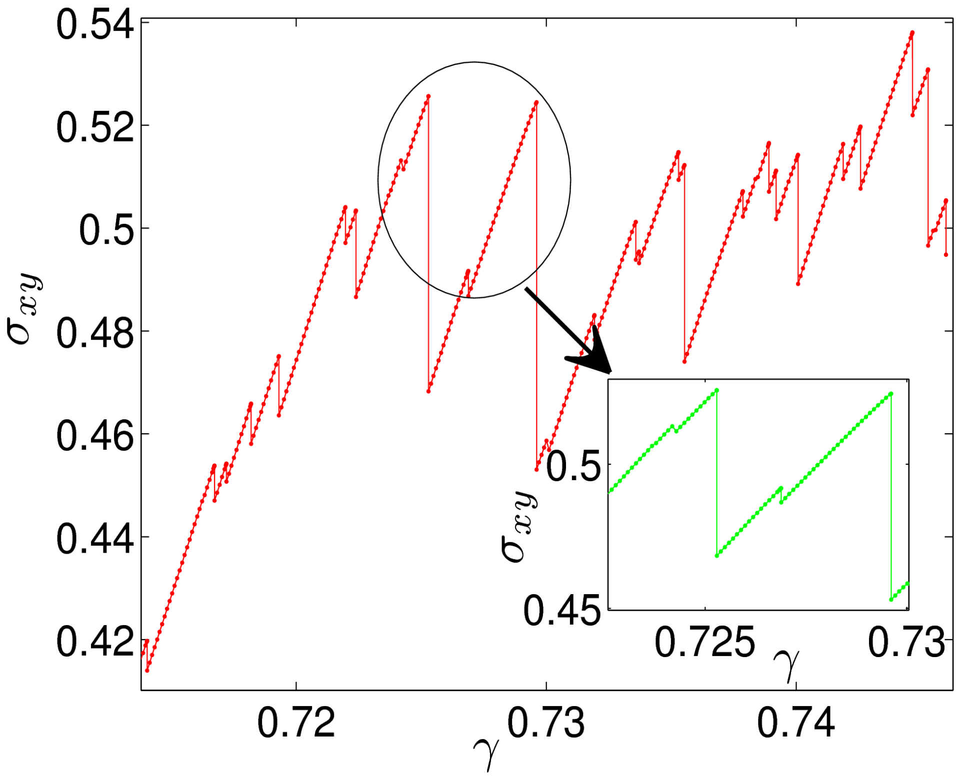
$$\phi\left(\frac{r_{ij}}{\lambda_{ij}}\right) = \begin{cases} \varepsilon\left[\left(\frac{\lambda_{ij}}{r_{ij}}\right)^k + \sum_{\ell=0}^{q} c_{2\ell}\left(\frac{r_{ij}}{\lambda_{ij}}\right)^{2\ell}\right] & , \ \frac{r_{ij}}{\lambda_{ij}} \leq x_c \\ 0 & , \ \frac{r_{ij}}{\lambda_{ij}} > x_c \end{cases}$$

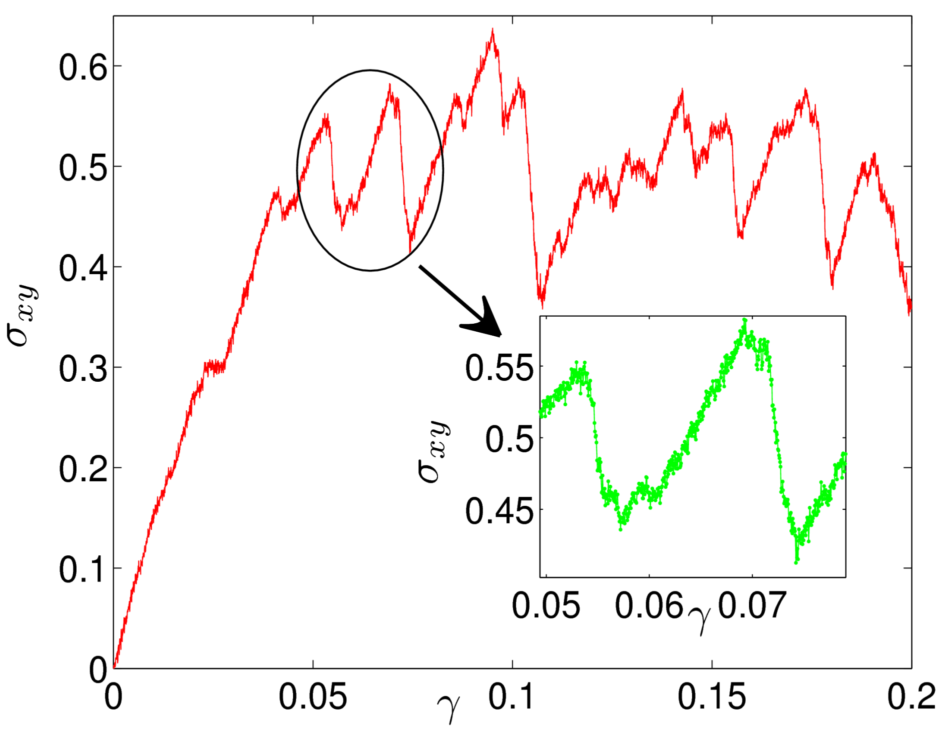
$$c_{2\ell} = \frac{(-1)^{\ell+1}}{(2q-2\ell)!!(2\ell)!!}\frac{(k+2q)!!}{(k-2)!!(k+2\ell)}x_c^{-(k+2\ell)}$$

This special form of the potential is to ensure the smoothness of the higher order derivatives of the potential at cut off

Close look at Stress-Strain Curve

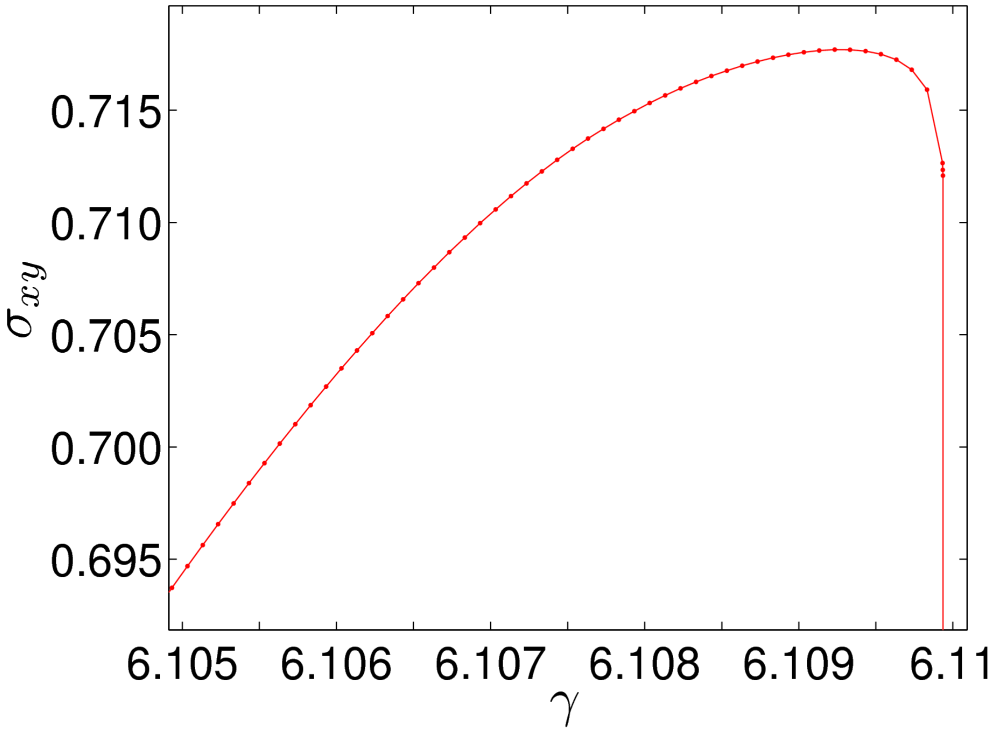
- Athermal condition ::
- Thermal condition ::

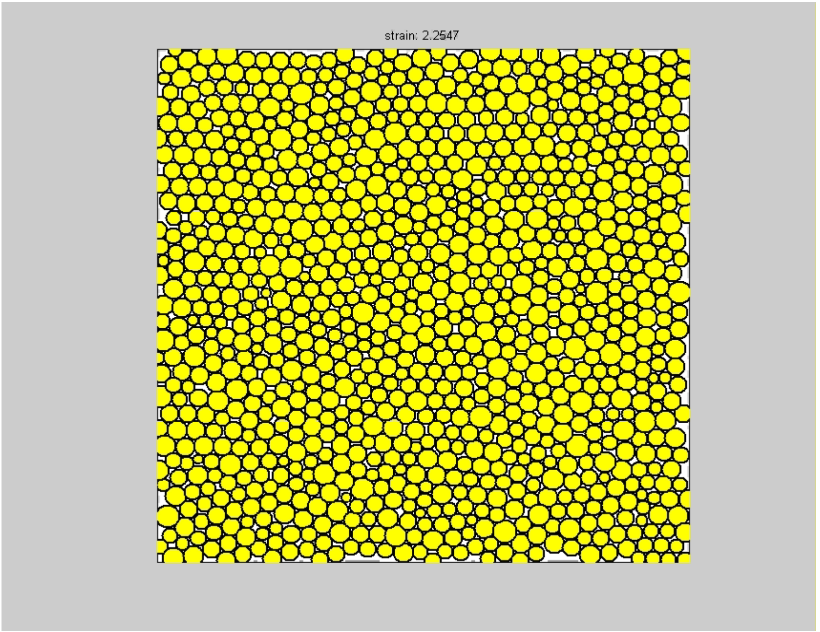




Notice the effect of finite temperature which smears out the sharpness the plastic failures

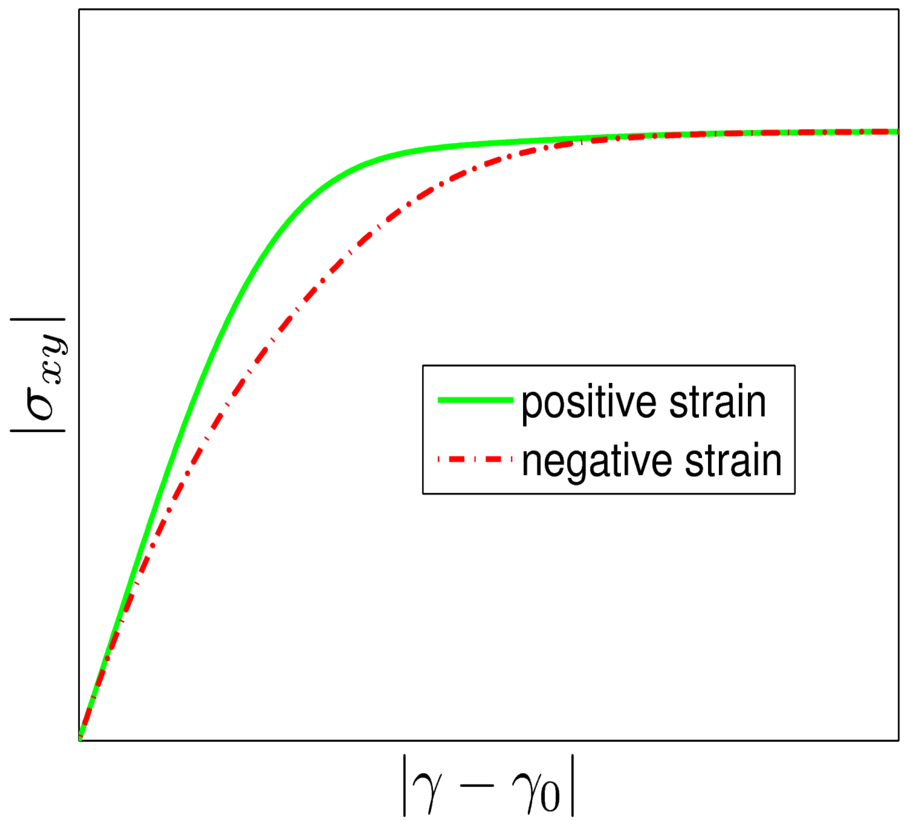
Need non-Linear Elasticity ?





- Marked deviation from linear elasticity near the plastic drop
- Shear Modulus μ diverges at the failure point

Order Parameter B_2



$$\sigma \sim tanh\left(\frac{\mu|\gamma-\gamma_0|}{\sigma_\infty}\right)$$
$$+\beta|\gamma-\gamma_0|^2 e^{-|\gamma-\gamma_0|^2}$$

Model stress-strain curve :

The remarkable similarity with the previous stress-strain curve in the steady state implies that the sought after order parameter can be the

$$\sigma \simeq \sigma_0 + \mu\gamma + \frac{1}{2}B_2\gamma^2 \ldots$$

stress with strain

Relation between B_2 and non-linear elastic coefficients

Strain Tensor:

$$\epsilon_{\alpha\beta} \equiv \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\nu}{\partial x_\alpha}\frac{\partial u_\nu}{\partial x_\beta}\right)$$

Expand the free energy density up to 3rd order in strain

$$\frac{\mathcal{F}}{V} = C_1^{\alpha\beta}\epsilon_{\alpha\beta} + \tfrac{1}{2}C_2^{\alpha\beta\nu\eta}\epsilon_{\alpha\beta}\epsilon_{\nu\eta} + \tfrac{1}{6}C_3^{\alpha\beta\nu\eta\kappa\chi}\epsilon_{\alpha\beta}\epsilon_{\nu\eta}\epsilon_{\kappa\chi}$$

Stress is defined as: $\sigma_{\alpha\beta} \equiv \frac{1}{V}\frac{\partial\mathcal{F}}{\partial\epsilon_{\alpha\beta}}$

$$\sigma_{\alpha\beta} = C_1^{\alpha\beta} + C_2^{\alpha\beta\nu\eta}\epsilon_{\nu\eta} + \frac{1}{2}C_3^{\alpha\beta\nu\eta\kappa\chi}\epsilon_{\nu\eta}\epsilon_{\kappa\chi}$$

For simple shear :

$$\epsilon = \frac{1}{2}\begin{pmatrix} 0 & \delta\gamma \\ \delta\gamma & \delta\gamma^2 \end{pmatrix}$$

$$\begin{aligned}\sigma_{xy} =& C_1^{xy} + C_2^{xyxy}\delta\gamma \\ &+ \tfrac{1}{2}(C_2^{xyyy} + C_3^{xyxyxy})\delta\gamma^2 + \mathcal{O}(\delta\gamma^3)\end{aligned}$$

Relation between B_2 and non-linear elastic coefficients

So B_2 in the athermal limit is given by :

$$B_2(\gamma_0) \equiv \lim_{T\to 0}[C_2^{xyyy} + C_3^{xyxyxy}] = \lim_{T\to 0} \left.\frac{\partial^2 \sigma_{xy}}{\partial \gamma^2}\right|_{\gamma=\gamma_0}$$

We have calculated the derivative by finite difference scheme

$$\frac{\partial^2 \sigma_{xy}}{\partial \gamma^2} \approx \frac{\sigma_{xy}(\delta\gamma)+\sigma_{xy}(-\delta\gamma)-2\sigma_{xy}(0)}{\delta\gamma^2}$$

We measure this in a athermal quasi-static scheme which consists of affine transformation of each particle coordinates and then potential energy minimization under Lees-Edwards boundary condition. We choose the stopping criterion for $|\nabla_i U| < 10^{-9}\frac{\varepsilon}{\lambda}$ nization to be for each particle coordinates

Calculation of B_2 analytically

$$\mu = \mu_B - \boldsymbol{\Xi} \boldsymbol{H}^{-1} \boldsymbol{\Xi} \, , \quad \boldsymbol{\Xi}_i \equiv \frac{\partial^2 U}{\partial \gamma \partial \boldsymbol{r}_i} \, , \quad \boldsymbol{H}_{ij} \equiv \frac{\partial^2 U}{\partial \boldsymbol{r}_j \partial \boldsymbol{r}_i}$$

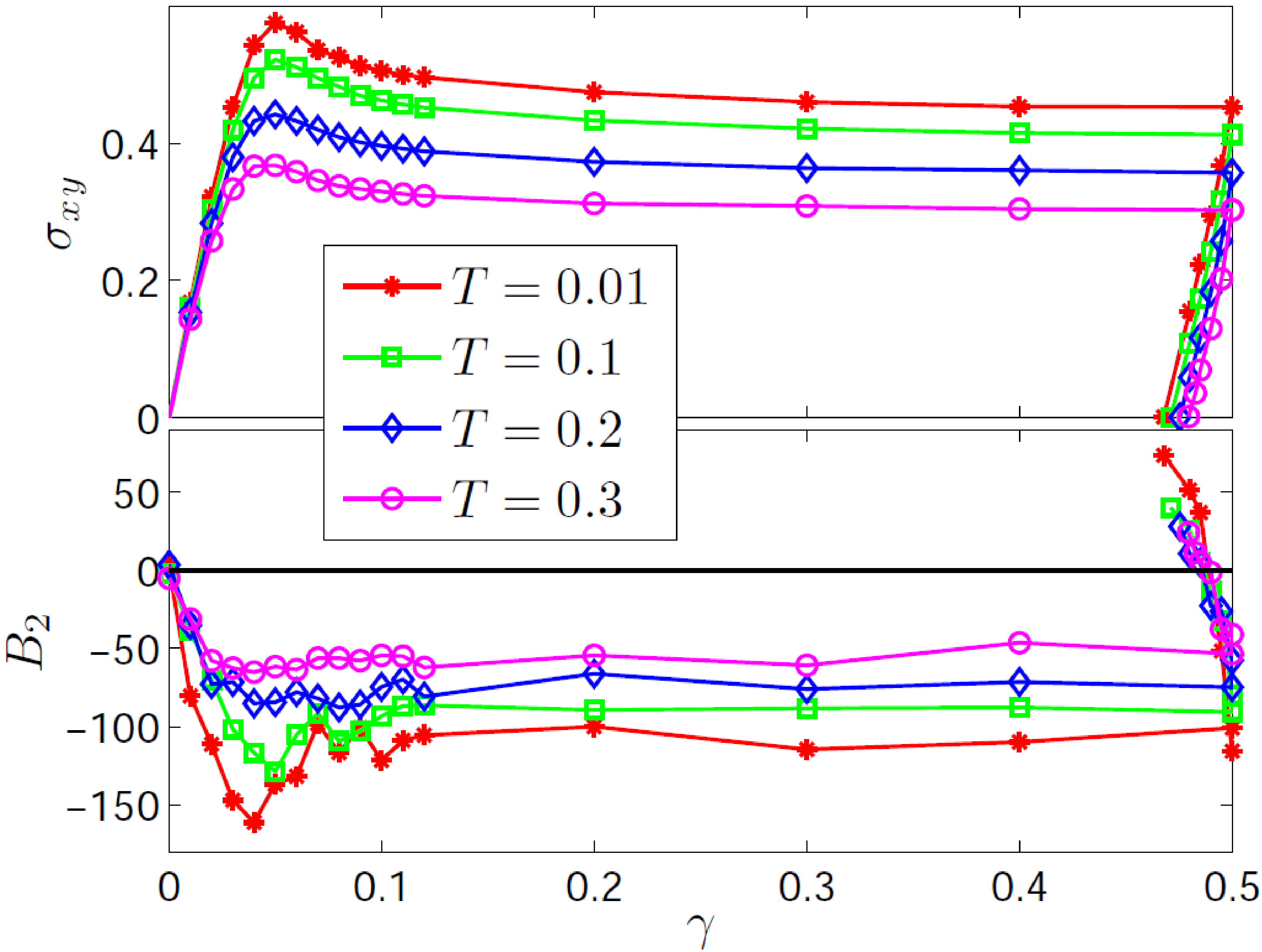
$$\mathcal{V}^i_{\kappa\alpha\beta} = \left. \frac{\partial X^i_\kappa}{\partial \epsilon_{\alpha\beta}} \right|_{\boldsymbol{f}} = - \sum_j (\mathcal{H}^{-1})^{ij}_{\kappa\nu} \Xi^j_{\nu\alpha\beta}$$

$$\left. \frac{\partial^3 U}{\partial \epsilon_{\kappa\chi} \partial \epsilon_{\iota\upsilon} \partial \epsilon_{\alpha\beta}} \right|_{\boldsymbol{f},\boldsymbol{f},\boldsymbol{f}} = \left. \frac{\partial^3 U}{\partial \epsilon_{\kappa\chi} \partial \epsilon_{\iota\upsilon} \partial \epsilon_{\alpha\beta}} \right|_{\boldsymbol{X}} + \sum_j \left. \frac{\partial \mathcal{V}^j_{\eta\iota\upsilon}}{\partial \epsilon_{\kappa\chi}} \right|_{\boldsymbol{f}} \Xi^j_{\eta\alpha\beta} + \sum_j \mathcal{V}^j_{\eta\iota\upsilon} \left. \frac{\partial \Xi^j_{\eta\alpha\beta}}{\partial \epsilon_{\kappa\chi}} \right|_{\boldsymbol{X}}$$

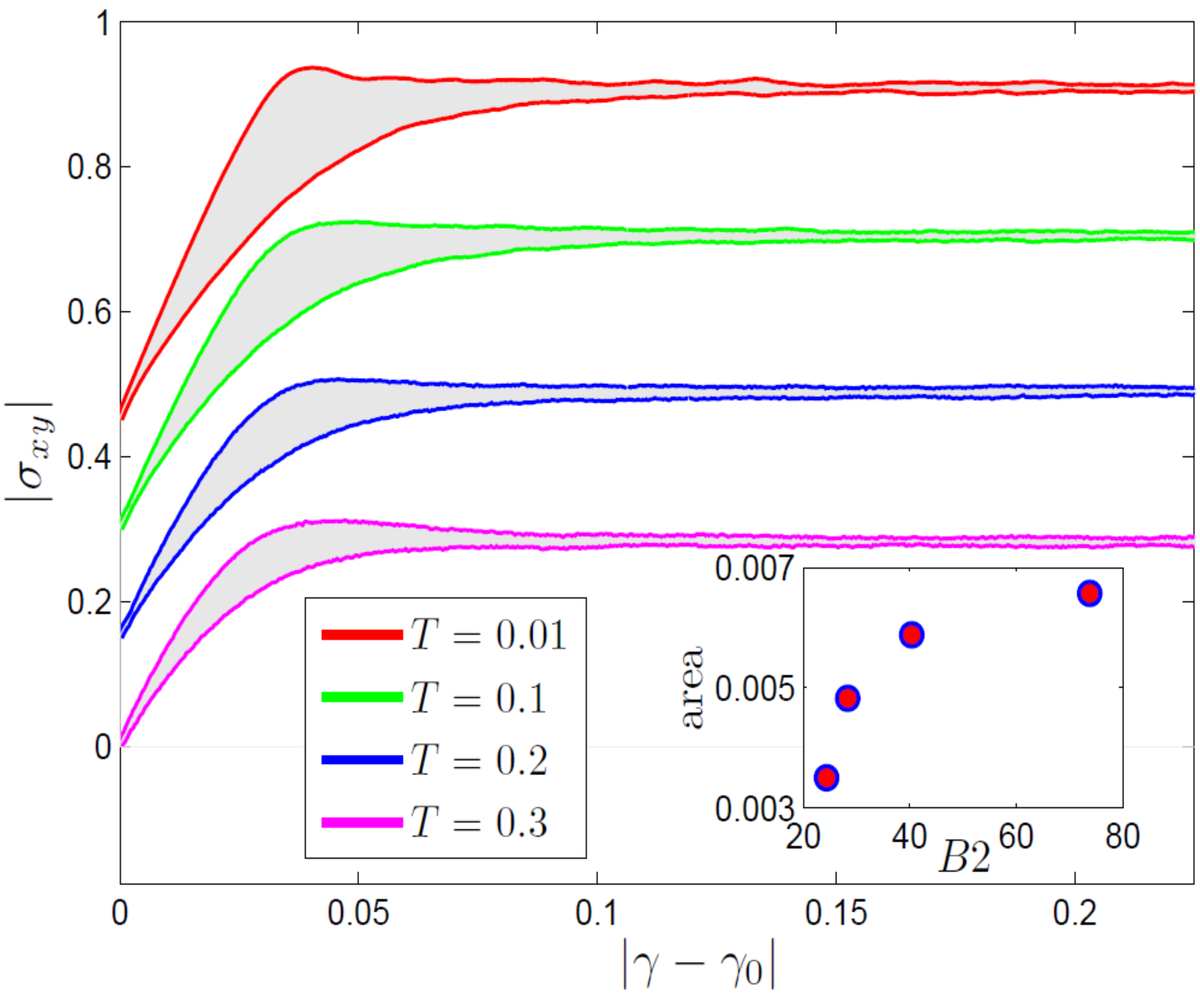
$$+ \sum_i \mathcal{V}^i_{\nu\kappa\chi} \left. \frac{\partial^3 U}{\partial X^i_\nu \partial \epsilon_{\iota\upsilon} \partial \epsilon_{\alpha\beta}} \right|_{\boldsymbol{X}\epsilon} + \sum_{i,j} \mathcal{V}^i_{\nu\kappa\chi} \mathcal{V}^j_{\eta\iota\upsilon} \left. \frac{\partial \Xi^j_{\eta\alpha\beta}}{\partial X^i_\nu} \right|_{\epsilon} .$$

$$\left. \frac{\partial \Xi^\ell_{\nu\alpha\beta}}{\partial \epsilon_{\kappa\chi}} \right|_{\boldsymbol{X}} + \sum_i \mathcal{V}^i_{\vartheta\kappa\chi} \left. \frac{\partial \Xi^\ell_{\nu\alpha\beta}}{\partial X^i_\vartheta} \right|_{\epsilon} + \sum_j \left. \frac{\partial \mathcal{H}^{\ell j}_{\nu\eta}}{\partial \epsilon_{\kappa\chi}} \right|_{\boldsymbol{X}} \mathcal{V}^j_{\eta\alpha\beta} + \sum_j \sum_i \mathcal{V}^i_{\vartheta\kappa\chi} \left. \frac{\partial \mathcal{H}^{\ell j}_{\nu\eta}}{\partial X^i_\vartheta} \right|_{\epsilon} \mathcal{V}^j_{\eta\alpha\beta} + \sum_j \mathcal{H}^{\ell j}_{\nu\eta} \left. \frac{\partial \mathcal{V}^j_{\eta\alpha\beta}}{\partial \epsilon_{\kappa\chi}} \right|_{\boldsymbol{f}} = 0 \, ,$$

Evolution of : B_2



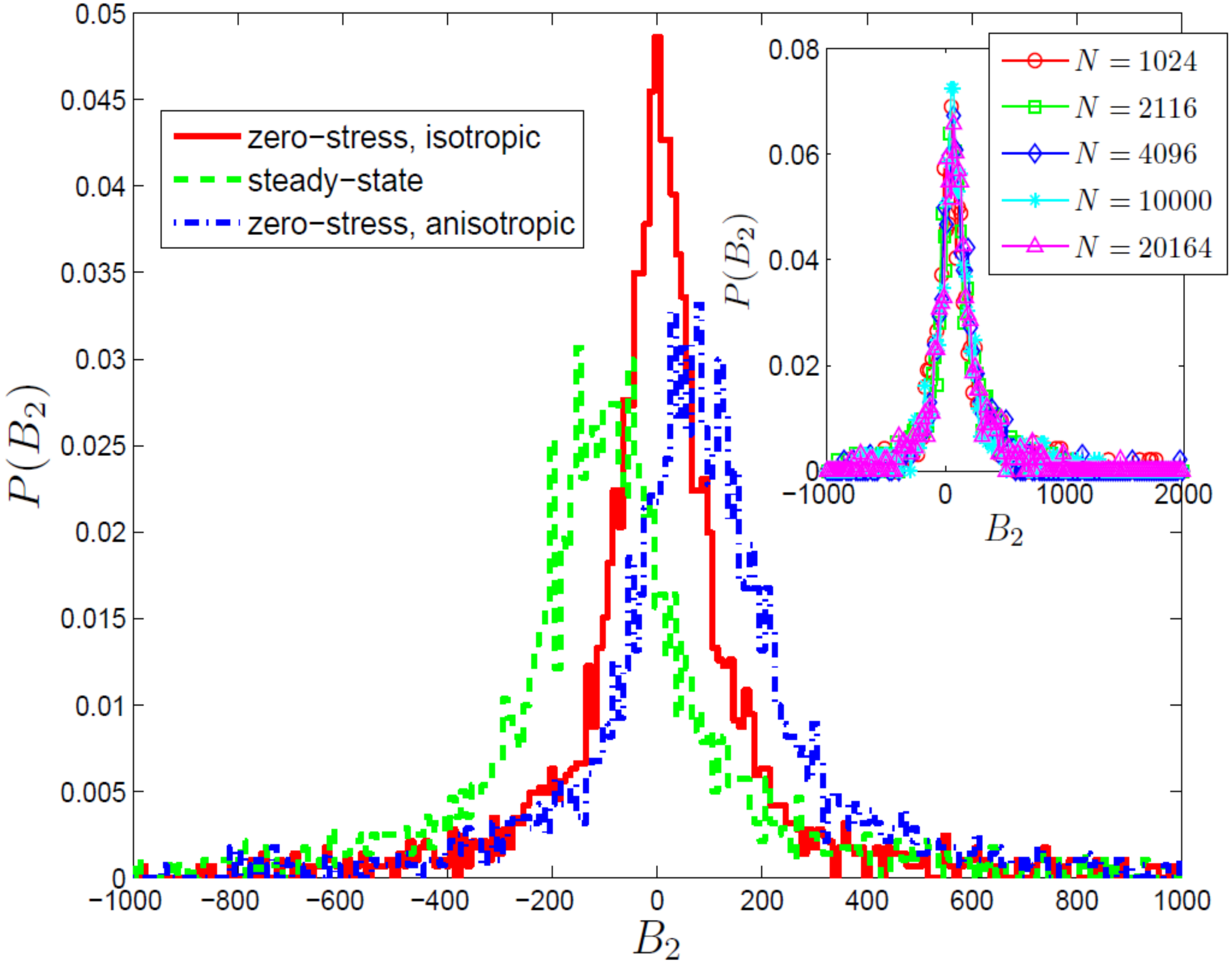
Temperature Dependence of Bauschinger Effect



- Notice the decrease of Bauschinger Effect with increasing Temperature.The Shaded area indicates the difference between The forward and Backward trajectory.

- Inset shows the variation of area as a function of B_2

Probability Distribution of B_2

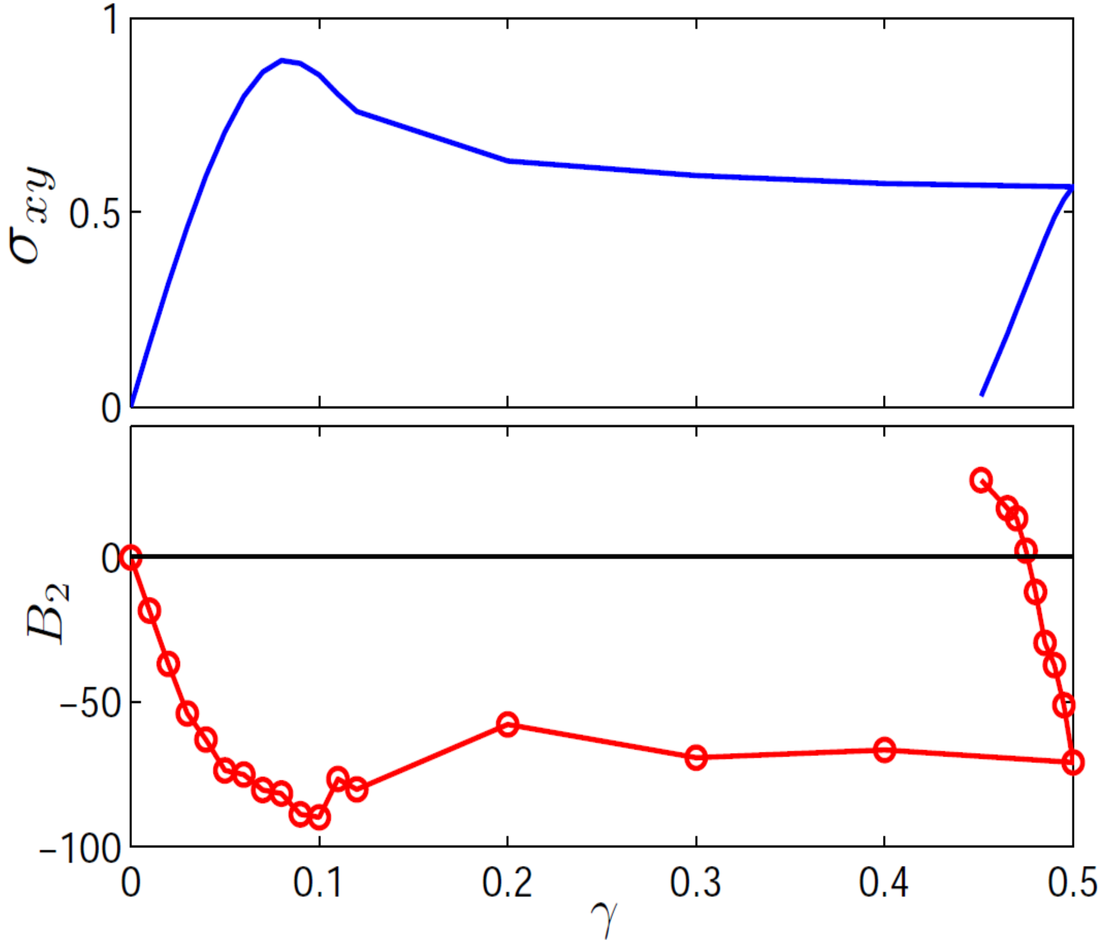


Isotropic :
pdf is symmetric around zero

Steady State :
pdf has a -ve mean and more weight in the -ve tail.

Bauschinger Point :
pdf has a +ve mean and more weight in the +ve tail.

3D Case & Conclusion - I



- Proposed Order Parameter is generic and is valid in any dimension.

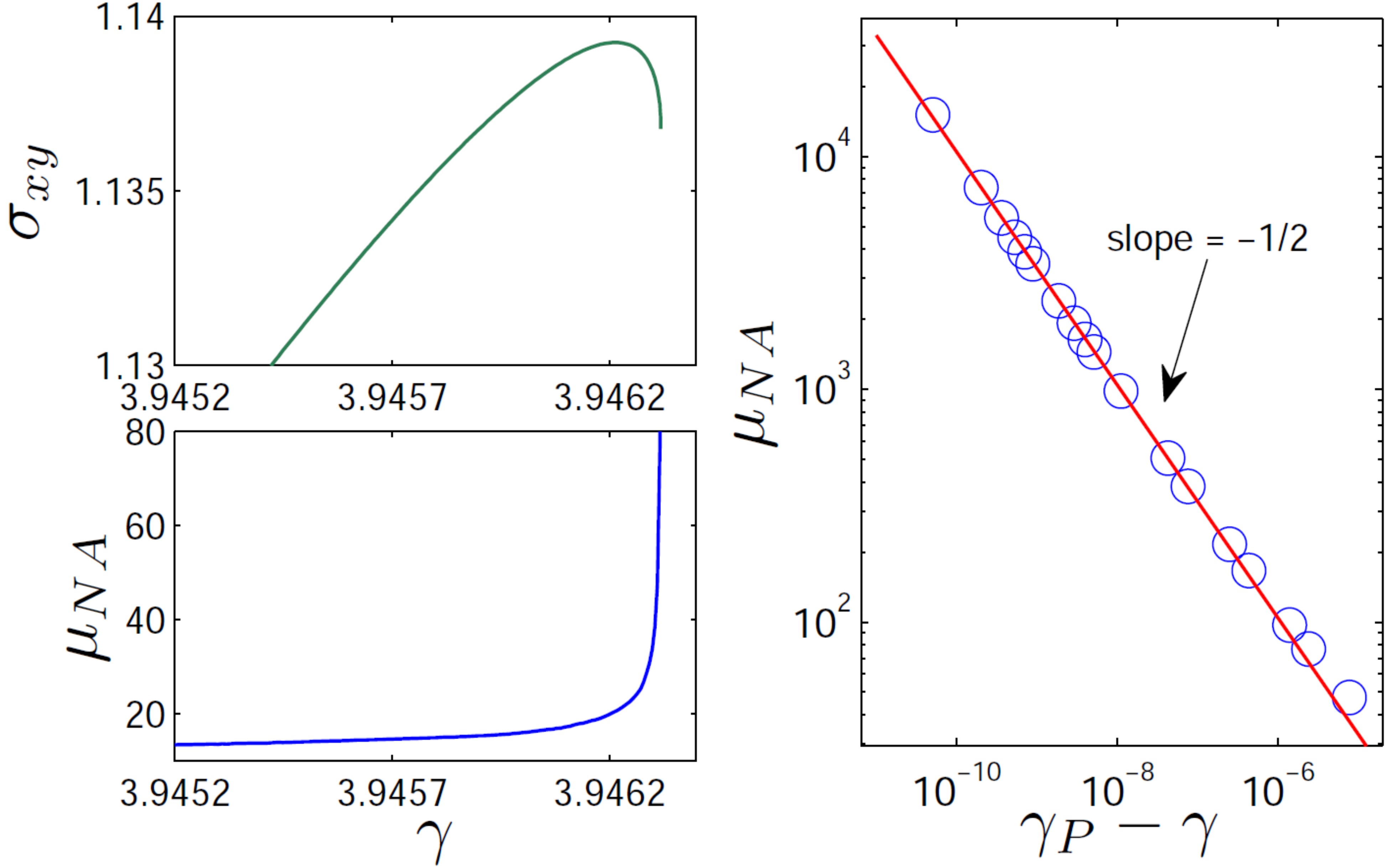
- A possible analog of the STZ order parameter '***m***', but with the obvious advantage of easily calculable in any system not only model systems but in real systems by calculating the higher order non-linear elastic coefficients.

- ***Further usefulness in predicting the plastic failure***

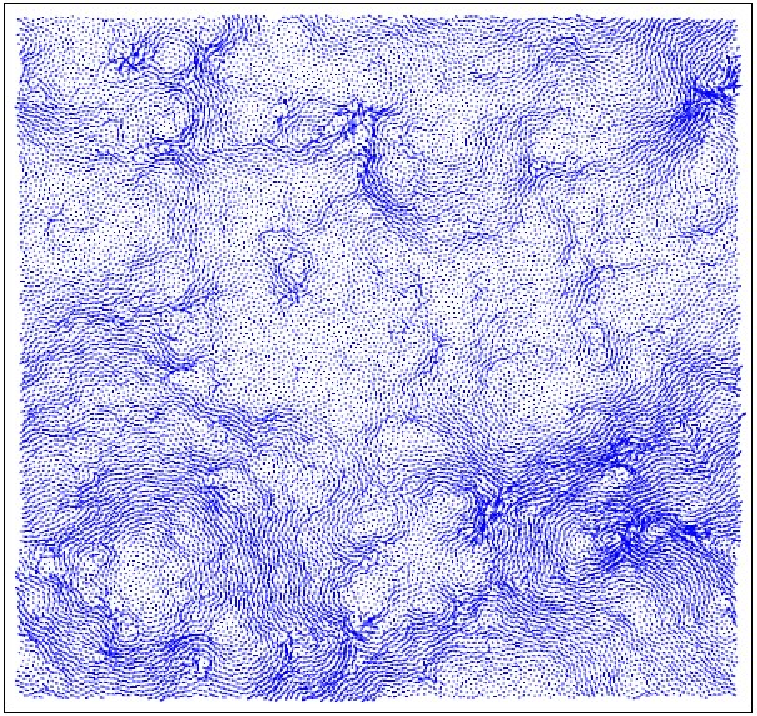
Can we predict the Plasticity ?

Lets look at one of the plastic failures once again and try to analyze its nature

Can we predict the Plasticity ?



Square Root Divergence of μ & Non Affine Field



Non Affine Field Definition

$$\mathbf{r}_{ix} = \mathbf{r}_{ix} + \gamma \mathbf{r}_{iy}$$

$$\mathbf{r}_{iy} = \mathbf{r}_{iy}$$

$$\mathbf{r}_{iz} = \mathbf{r}_{iz} \; (in \, 3D)$$

Minimized the strained state and the difference between the strained and the minimized state is the non affine field

Equivalently non affine field is the displacement of a configuration under external strain with the constraint that force on each particle is zero before and after the transformation

$$\frac{d\mathbf{f}_i}{d\gamma} = 0, \quad \forall i$$

Or

$$\frac{d\mathbf{f}_i}{d\gamma} = \frac{d}{d\gamma}\left(\frac{\partial U}{\partial \mathbf{r}_i}\right) = \mathbf{\Xi}_i + \mathcal{H}_{ij}\frac{d\mathbf{r}_j}{d\gamma} = 0$$

Thus

$$\frac{d\mathbf{r}_i}{d\gamma} = -\mathcal{H}_{ij}^{-1}\mathbf{\Xi}_j = -\sum_k \frac{\psi_j^{(k)} \cdot \mathbf{\Xi}_j}{\lambda_k}\psi_i^{(k)}$$

$$\approx \frac{\psi_j^{(P)} \cdot \mathbf{\Xi}_j}{\lambda_P}\psi_i^{(P)}, \quad \boldsymbol{H}_{ij}\boldsymbol{\psi}_j^{(k)} = \lambda_k \boldsymbol{\psi}_i^{(k)}$$

Integrating

$$\boldsymbol{r}_i(\gamma) - \boldsymbol{r}_i(\gamma_P) = X(\gamma)\boldsymbol{\psi}_i^{(P)}$$

Where

$$\frac{dX(\gamma)}{d\gamma} \approx -\frac{\boldsymbol{\psi}_j^{(P)} \cdot \mathbf{\Xi}_j}{\lambda_P}\boldsymbol{\psi}_i^{(P)}$$

Now use the crucial information that eigenvalue crosses zero with a finite slope which is reminiscent of the saddle node bifurcation or the ***Fold Catastrophe***, i.e.

$$\lambda_P \approx Ax + \mathcal{O}(x^2) \ ,$$

We get

$$X(\gamma) \propto \sqrt{\gamma_P - \gamma}$$

With this we conclude that

$$\mu \approx \mu_B - \frac{a/2}{\sqrt{\gamma_P - \gamma}} + \mathcal{O}(\sqrt{\gamma_P - \gamma})$$

*C. Maloney and A. Lemaitre - PRL **93**, 195501 (2004)*

Ansatz for the Approximate Series

Lets define

$$\sigma_{xy}(\gamma) = \sum_{n=0}^{\infty} \frac{B_n}{n!}(\gamma - \gamma_0)^n \ , \quad B_n = \lim_{T\to 0} \left. \frac{d^n \sigma_{xy}}{d\gamma^n} \right|_{\gamma=\gamma_0}$$

In the vicinity of the divergence we can write

$$\sigma_{xy} \sim \sigma_P + a\sqrt{\gamma_P - \gamma} + b(\gamma_P - \gamma)^{3/2} \ , \quad \gamma < \gamma_P$$

On the other hand near γ_0

$$\sigma_{xy} \sim \mu(\gamma - \gamma_0) + \ldots .$$

So together we can write

$$\sigma_{xy}(\gamma) = \sigma_0 + \mu(\gamma - \gamma_0) + a\sqrt{\gamma_P - \gamma} + b(\gamma_P - \gamma)^{3/2}$$

Higher Order Derivatives B_n

Lets calculate the higher order derivatives :

$$B_2 = \frac{1}{4\sqrt{\gamma_P - \gamma_0}}\left[3b - \frac{a}{\gamma_P - \gamma_0}\right],$$

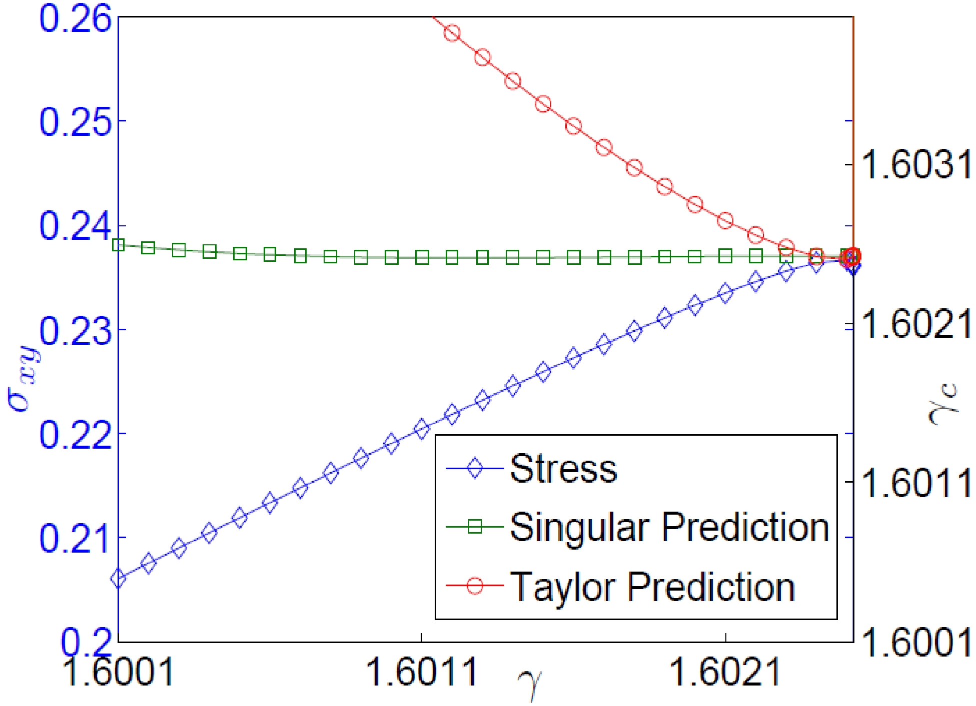
$$B_3 = \frac{3}{8(\gamma_P - \gamma_0)^{3/2}}\left[b - \frac{a}{\gamma_P - \gamma_0}\right],$$

$$B_4 = \frac{3}{16(\gamma_P - \gamma_0)^{5/2}}\left[3b - \frac{5a}{\gamma_P - \gamma_0}\right]$$

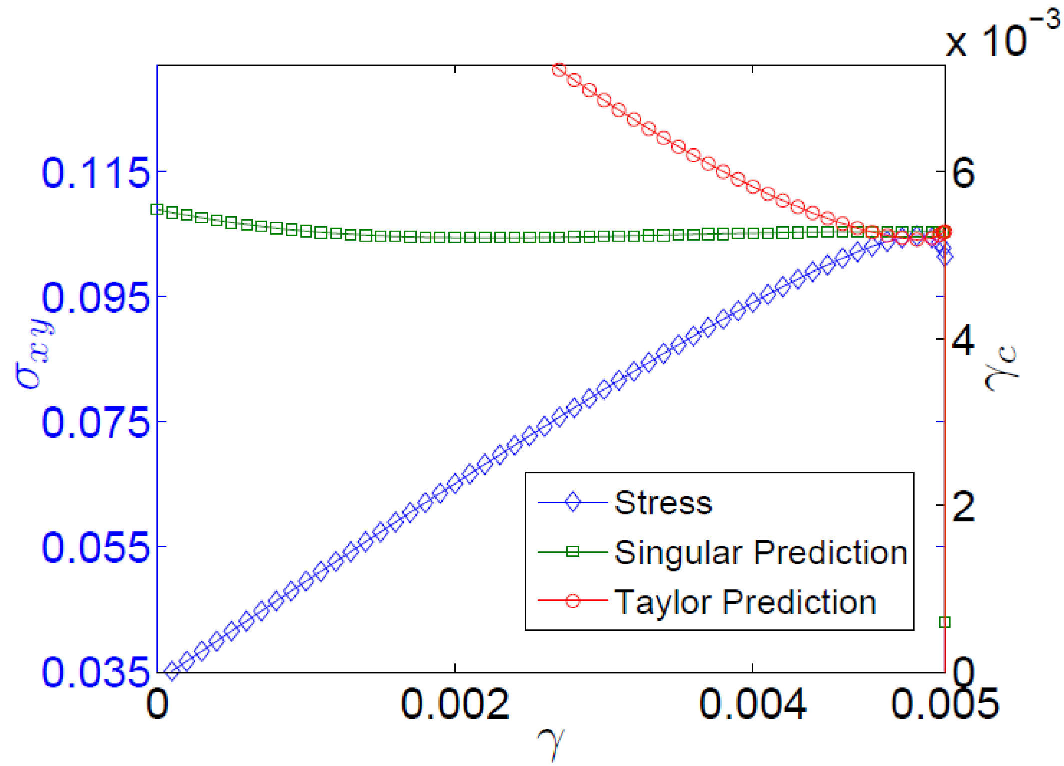
With these the prediction reads :

$$\gamma_P = \gamma_0 + \frac{3B_3 - \sqrt{9B_3^2 - 2B_2B_4}}{2B_4}$$

Verification of the Ansatz



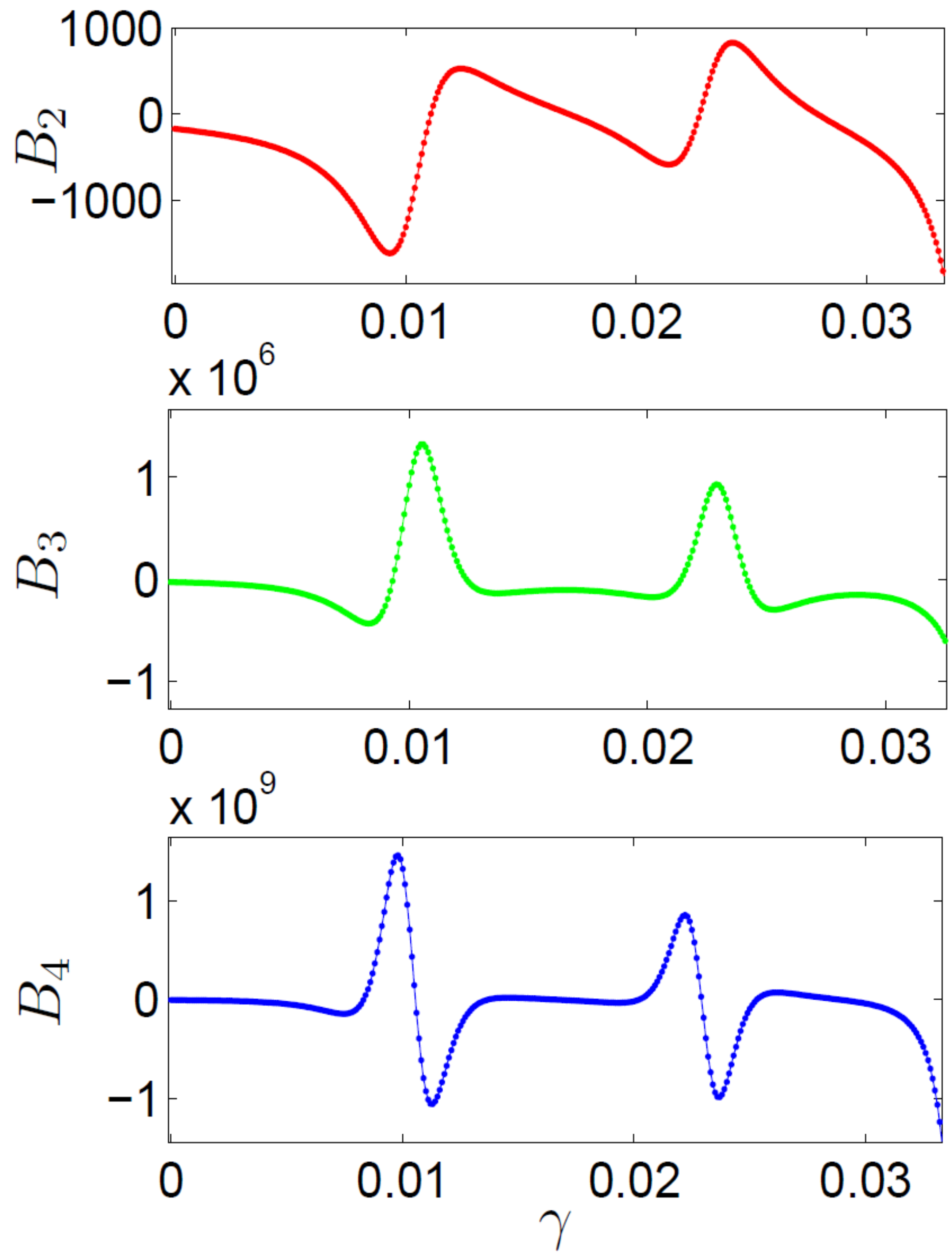
Steady State



Isotropic State

Notice the Failure of the Taylor series in predicting the divergence

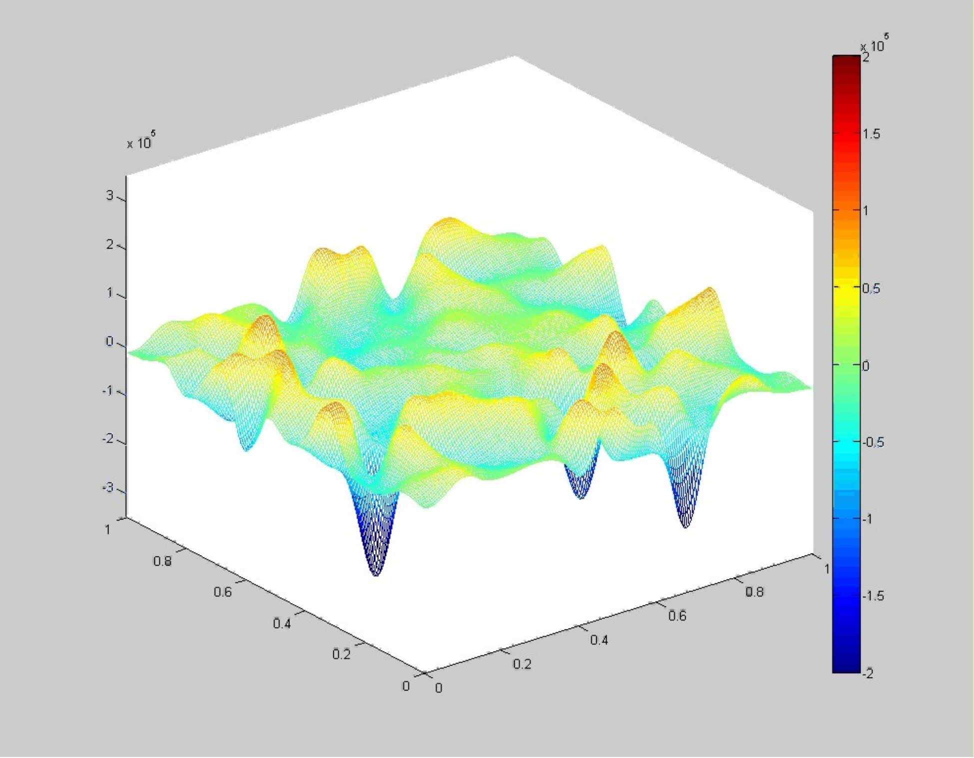
Weak Points ??



The elastic branch emanating from the isotropic equilibrium state may exhibit large non-affine elastic events which resemble a typical precursor to a plastic failure but avoids it by eventually stabilizing. Our derivatives will pick up these elastic events and will incorrectly predict a plastic failure before landing on the right prediction.

Evolution of B_2 Field

Spatial evolution of B_2 field as a function of strain. This shows the large non affine displacements which can happen in the system before the final catastrophe



This evolution makes the prediction more shuttle

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