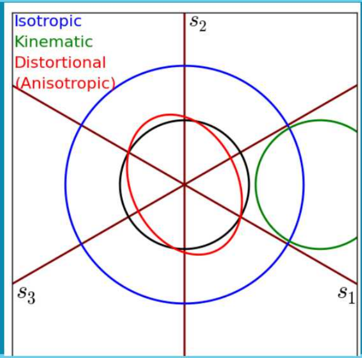
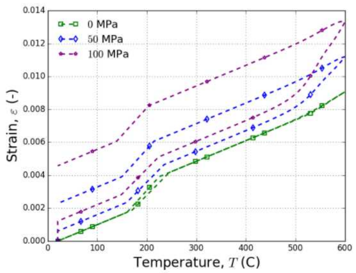
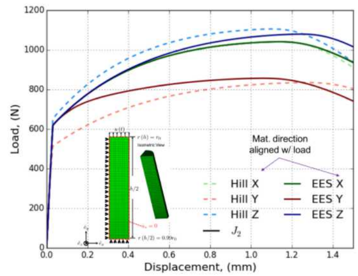
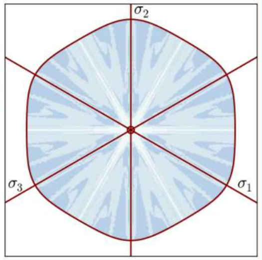
SAND2019-11653PE

Continuum Constitutive Modeling of Complex Responses: Development and Implementation









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Texas A&M University
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Acknowledgements

- Many people formally (and informally) contributed in various fashions to this this work

- Key contributors include
  - W. M. Scherzinger
  - J. Ostien
  - K. Long
  - S. Dai

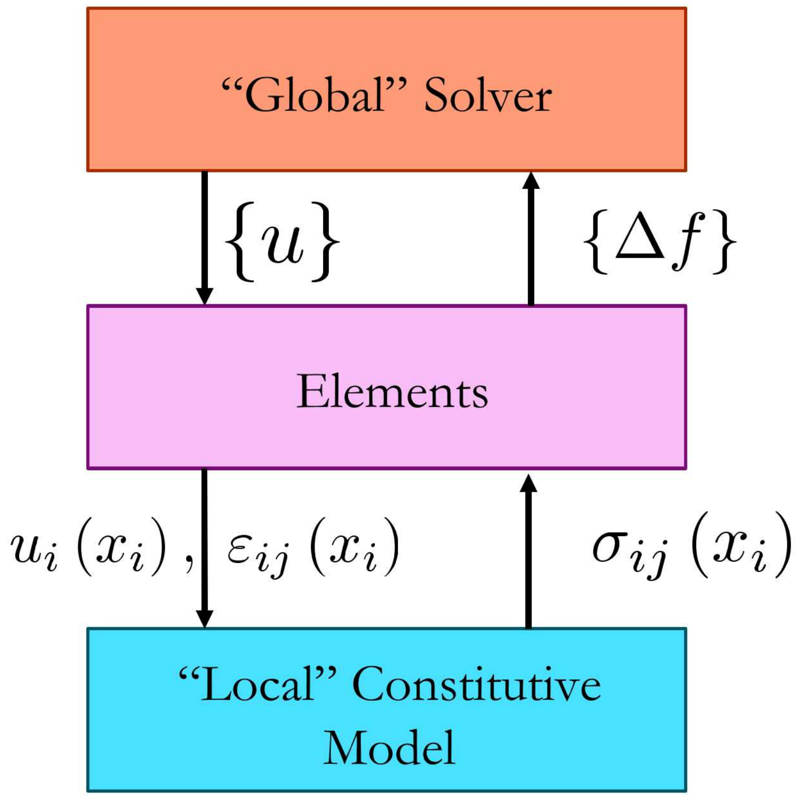
- Others have/continue to provide valuable insight, feedback, and collaboration

Constitutive Modeling

- "A constitutive equation demonstrates a relation between two physical quantities that is specific to a material or substance and does not follow directly from physical laws" (J. Fish, 2014, *Practical Multiscaling*, Wiley)

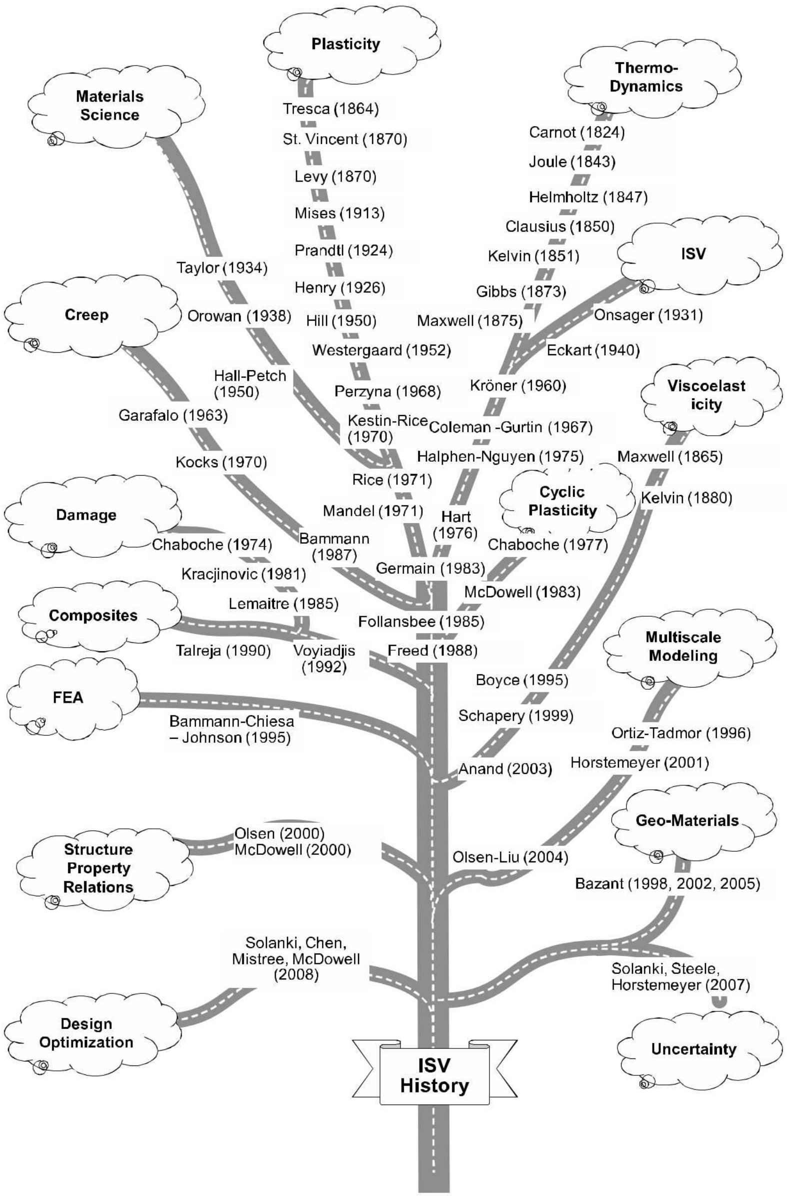
- Essential for the solution of structural boundary value problems
  - Provide mathematical closure
  - Introduce material physics

$$[K]\{u\} = \{\Delta f\}$$



$$\sigma_{ij} = f(\varepsilon_{ij})$$

Constitutive Modeling Utilization



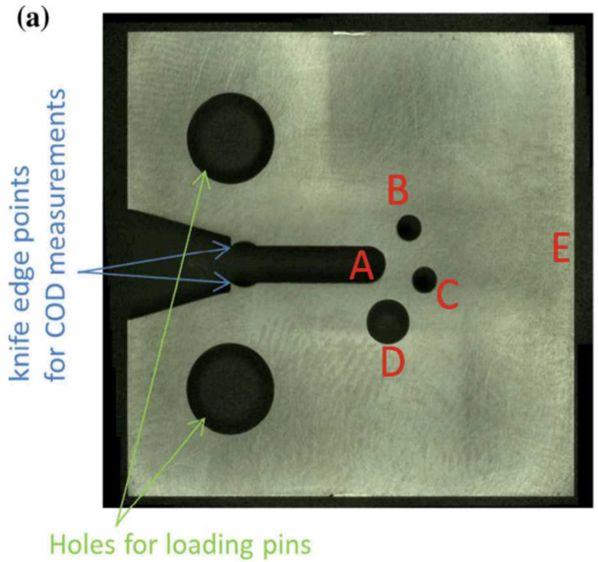
- Structural analyses require vastly different responses
  - Large range of deformation mechanisms
  - Dynamic and quasistatic
- Addressing needs requires
  - Flexible descriptions
  - Appropriate implementations
- "Library of Advanced Materials for Engineering" (LAMÉ)
  - Constitutive modeling library
  - Used w/ Sierra/SolidMechanics FE code

Horstmeyer and Bammann, 2010, *Int. Jrnl. Plas.*, 26: 1310--1334

Sandia Fracture Challenges

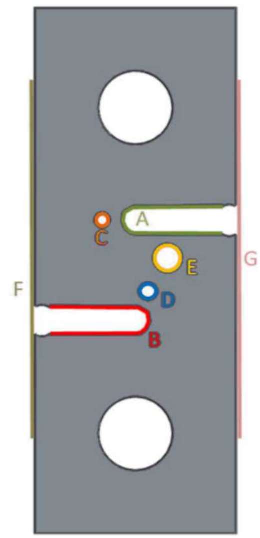
- Integration of constitutive and structural responses seen in Sandia Fracture Challenges (SFC)

1st Sandia Fracture Challenge



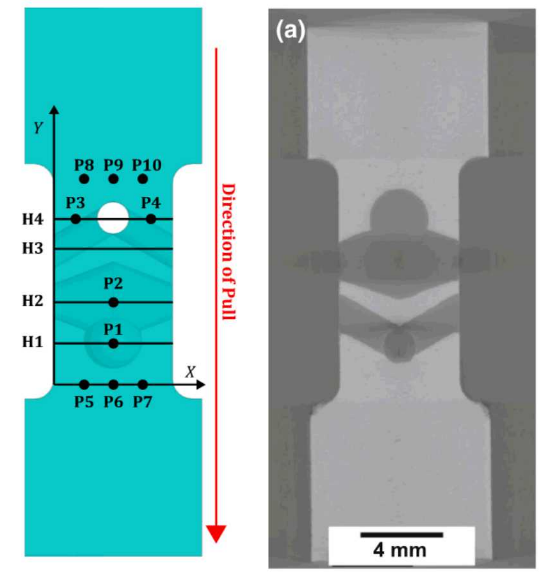
Boyce et al., 2014, *Int. Jrnl. Frac.*, 186: 5-68

2nd Sandia Fracture Challenge



Boyce et al., 2016, *Int. Jrnl. Frac.*, 198: 5-100

3rd Sandia Fracture Challenge

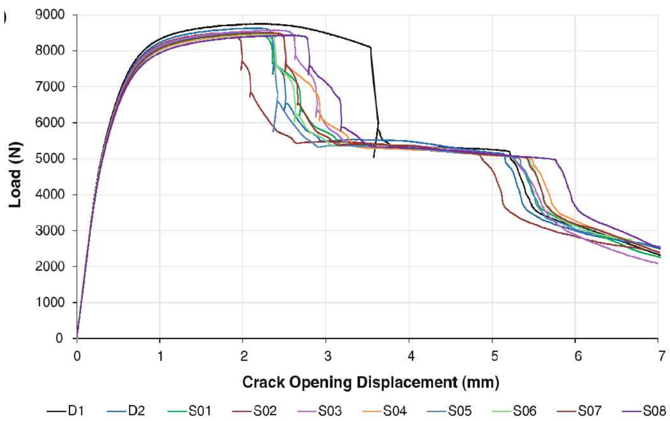


Kramer et al., 2019, *Int. Jrnl. Frac.*, 218, 5-61

- Various challenges asked for blind predictions of response with different complexities, e.g.:
  - Complex geometries; loading conditions
  - Material response characteristics (i.e. rate-dependence in SFC2)

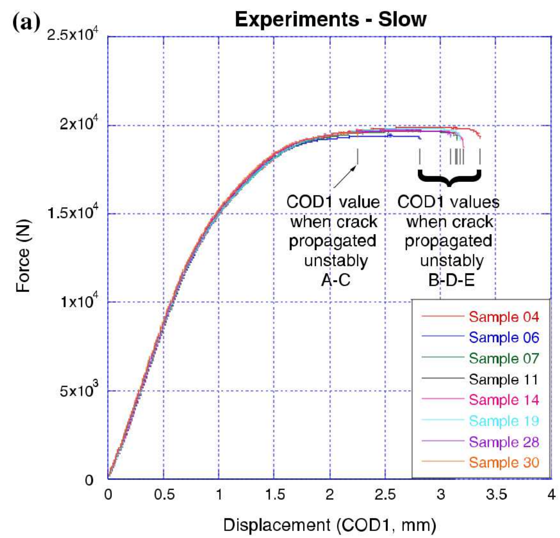
Sandia Fracture Challenges

1st Sandia Fracture Challenge



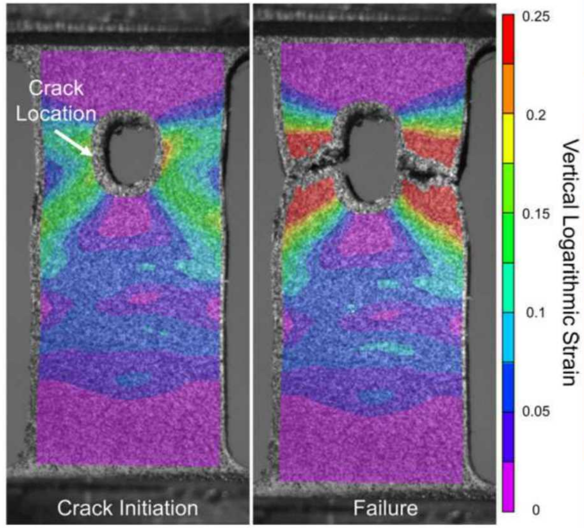
Boyce et al., 2014, *Int. Jrnl. Frac.*, 186: 5-68

2nd Sandia Fracture Challenge



Boyce et al., 2016, *Int. Jrnl. Frac.*, 198: 5-100

3rd Sandia Fracture Challenge



Kramer et al., 2019, *Int. Jrnl. Frac.*, 218, 5-61

- Results highlighted many important characteristics
  - Constitutive response through loading needed to predict failure
  - Some results (SFC2) highlighted importance of complex material responses (e.g. anisotropy, rate-dependent)

Objectives and Outline

- Improved constitutive capabilities represent enabling possibility for structural analysis
  - ***Create***: Development of new, refined material models
  - ***Code:*** Enhanced implementation and verification
  - ***Calibrate***: Methods to efficiently fit/determine parameters

- Focus on topics related to two model classes
  - Plasticity
    - Code: Trust-region based RMAs and verification
    - Create: Distortional hardening models
  - Glass-Ceramics
    - Create: Development of new material model

- Concluding thoughts and future perspectives

Plasticity – Implementation and Verification

Plasticity Modeling

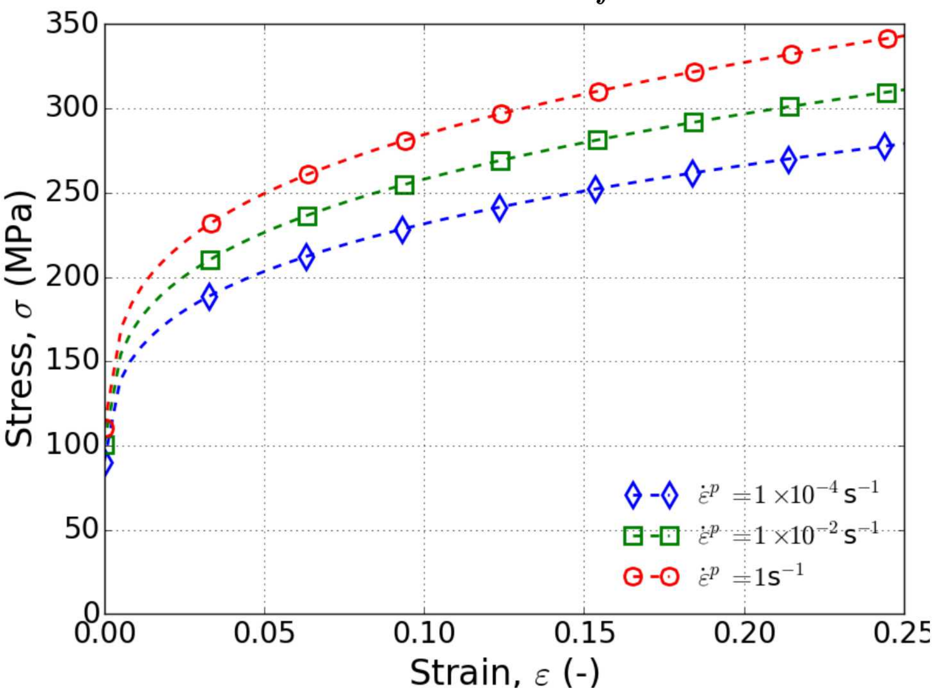
- Extensive (>century) of work has developed wealth of plasticity models

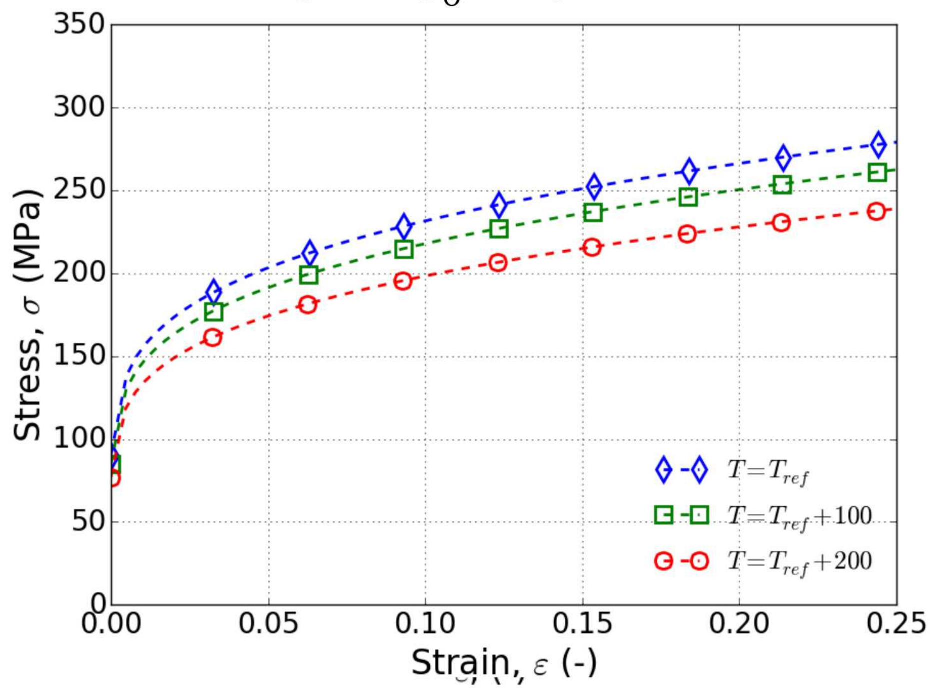
$$f(\sigma_{ij},\kappa,\dot{\kappa},T) = \phi(\sigma_{ij}) - \left(A + B(\kappa)^n\right)(1 + C\ln\dot{\varepsilon}^*)(1-(T^*)^m)$$

$$f(\sigma_{ij},\kappa) = \phi(\sigma_{ij}) - K(\kappa) \qquad \sigma_y^0$$

$T = T_{ref}$

$\dot{\varepsilon}^{\mathrm{p}} = \dot{\varepsilon}_0 \rightarrow \dot{\varepsilon}^* = 1$

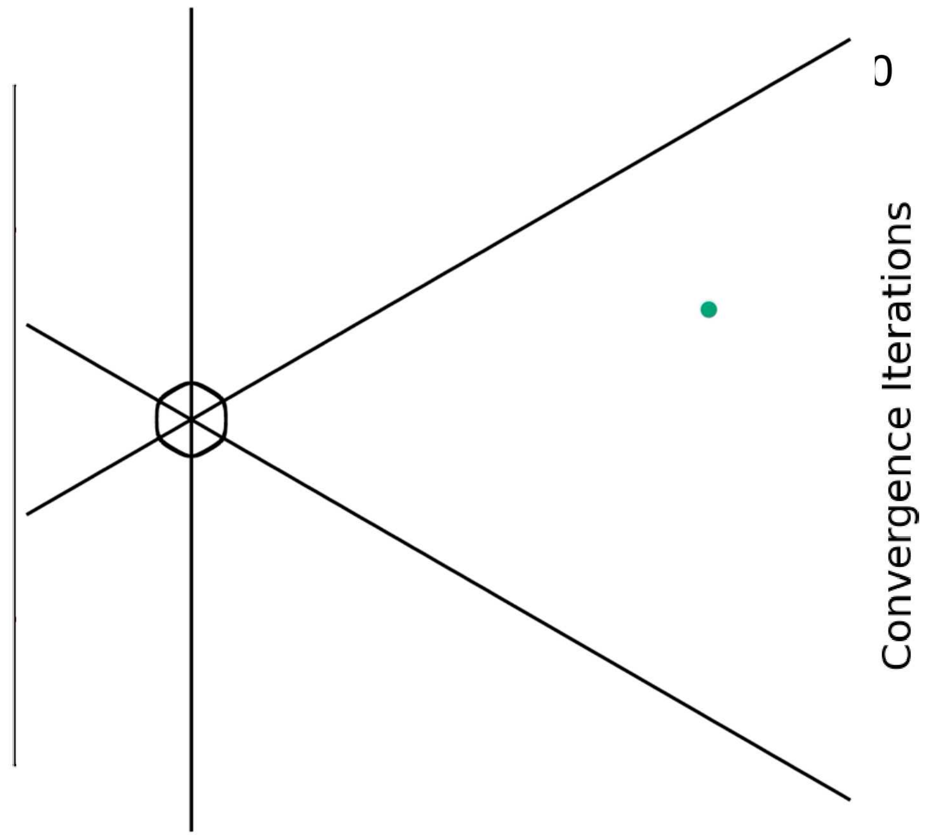




Johnson and Cook, 1985, *Eng. Frac. Mech.*, 21(1) 31-48

Numerical Implementation

- Robust numerical methods needed to solve various forms and complex load histories
  - "Textbook" implementations use the Newton-Raphson method
  - May fail to converge in variety of cases



Return Mapping Problem

- Elastic predictor/inelastic corrector; Fully implicit RMA-CPP
- Solution to non-linear problem $\{r\}^{(n+1)}\left(\{x\}\right) = \{0\}$

Residual Vector

$$\{r\} = \left[r_{ij}, r^f\right]^T \quad \left\{ \begin{aligned} r_{ij}^{\varepsilon(n+1)} &= -d\varepsilon_{ij}^{\mathrm{p}(n+1)} + d\kappa^{(n+1)} \frac{\partial \phi}{\partial \sigma_{ij}^{(n+1)}} \\ r^{f(n+1)} &= f\left(\sigma_{ij}^{(n+1)}, \kappa^{(n+1)}\right) \end{aligned} \right.$$

State Vector

$$\{x\} = \left[\sigma_{ij}, \kappa\right]^T$$

- Problem solved by iteratively updating the state vector

$$\{x\}^{(k+1)} = \{x\}^{(k)} + \alpha^{(k)} \{p\}^{(k)}$$

Step Size *Step Vector*

Existing Solution Approaches

- Newton-Raphson (NR)

$$\alpha^{(k)} = 1 \quad \forall k \qquad\qquad [J] = \frac{d\left\{r\right\}}{d\left\{x\right\}}$$

$$\left\{p\right\}^{\mathrm{NR}(k)} = -\left[J\right]^{-1}\left\{r\right\}^{(k)}$$

- Line-search augmented NR (LS-NR): As before but

$$\alpha^{(k)} = \min_{\alpha} \psi\left(\left\{r^{(k)}\left(\alpha\right)\right\}\right), \quad \alpha \in (0,1]$$

$$\psi\left(\left\{r\right\}\right) = \frac{1}{2}\left\{r\right\}^{T}\left[D\right]^{T}\left[D\right]\left\{r\right\}$$

(See Scherzinger, 2017, *CMAME*, 317, 526-553)

Trust-Region Based Solver

- Step 1: Construct a scaled model problem, $\tilde{m}^{(k)}\left(\{\tilde{p}\}\right)$
- Step 2: With $\alpha^{(k)} = 1$, find $\{\tilde{p}\}_{(k)}$ minimizing model problem in trusted domain,

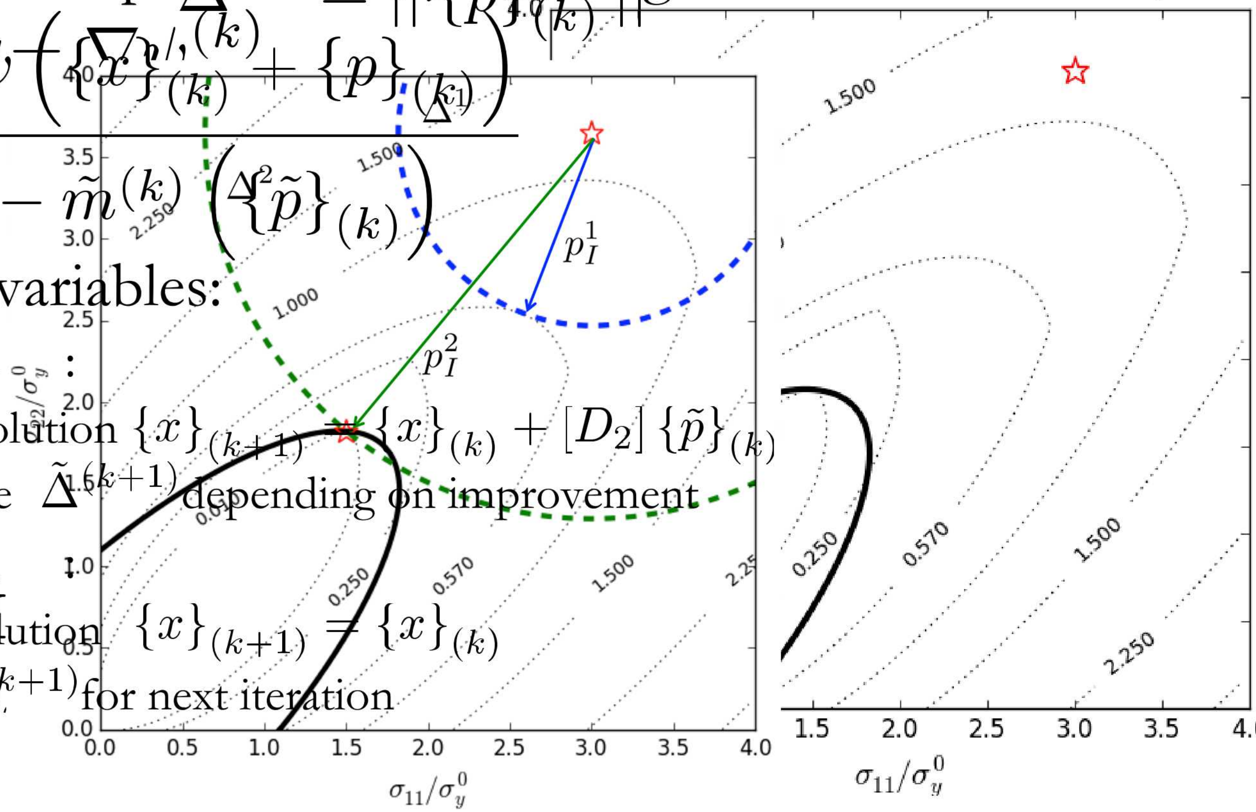
$$\tilde{m}^{(k)}\left(\{\tilde{p}\}\right) = \psi^{(k)} + \{\tilde{g}\}_{(k)}^T \{\tilde{p}\} + \frac{1}{2}\{\tilde{p}\}^T \left[\tilde{B}\right]^{(k)} \{\tilde{p}\}$$

$$\tilde{\Delta}^{(k)} = \left|\left|\{\tilde{p}\}_{(k)}\right|\right|^2$$

- Step 3: Calculate improvement, $\rho^{(k)}$, of a given trial increment, $\{\tilde{p}\}_{(k)}$

$$\rho^{(k)} = \frac{\psi\left(\{x\}_{(k)}\right) - \psi\left(\{x\}_{(k)} + \{p\}_{(k)}\right)}{\tilde{m}^{(k)}(0) - \tilde{m}^{(k)}\left(\{\tilde{p}\}_{(k)}\right)}$$

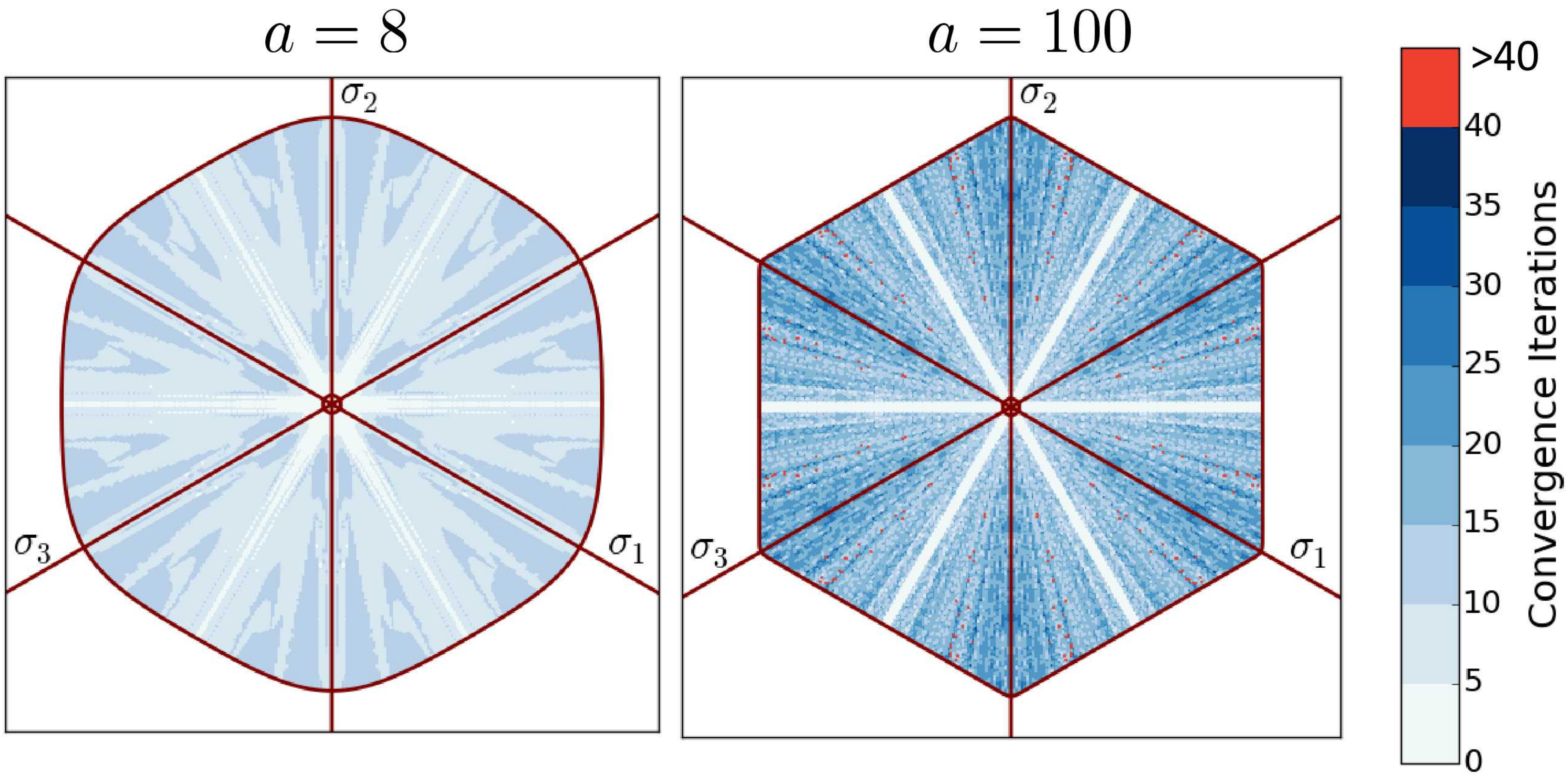
- Step 4: Update variables:
  - If $\rho^{(k)} \geq \text{tol}$:
    - Accept trial solution $\{x\}_{(k+1)} = \{x\}_{(k)} + [D_2]\{\tilde{p}\}_{(k)}$
    - Keep/increase $\tilde{\Delta}^{(k+1)}$ depending on improvement
  - If $\rho^{(k)} < \text{tol}$:
    - Reject trial solution $\{x\}_{(k+1)} = \{x\}_{(k)}$
    - Decrease $\tilde{\Delta}^{(k+1)}$ for next iteration



(Lester and Scherzinger, 2017, *IJNME*, 112, 257-282)

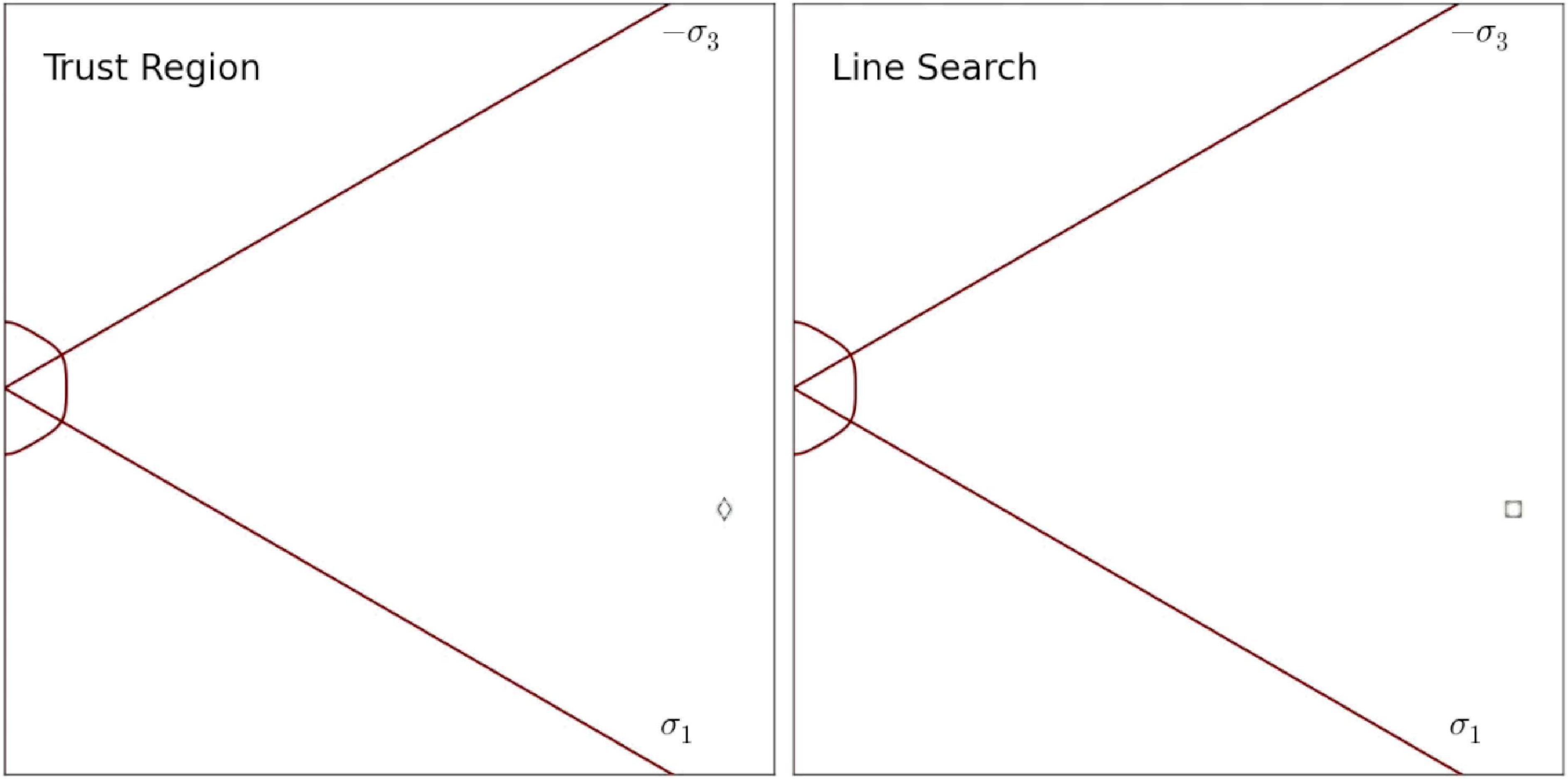
Convergence Maps

- Determine number of correction iterations needed for TR algorithm at $\phi\left(\sigma_{ij}\right) \leq 30\sigma_y^0$

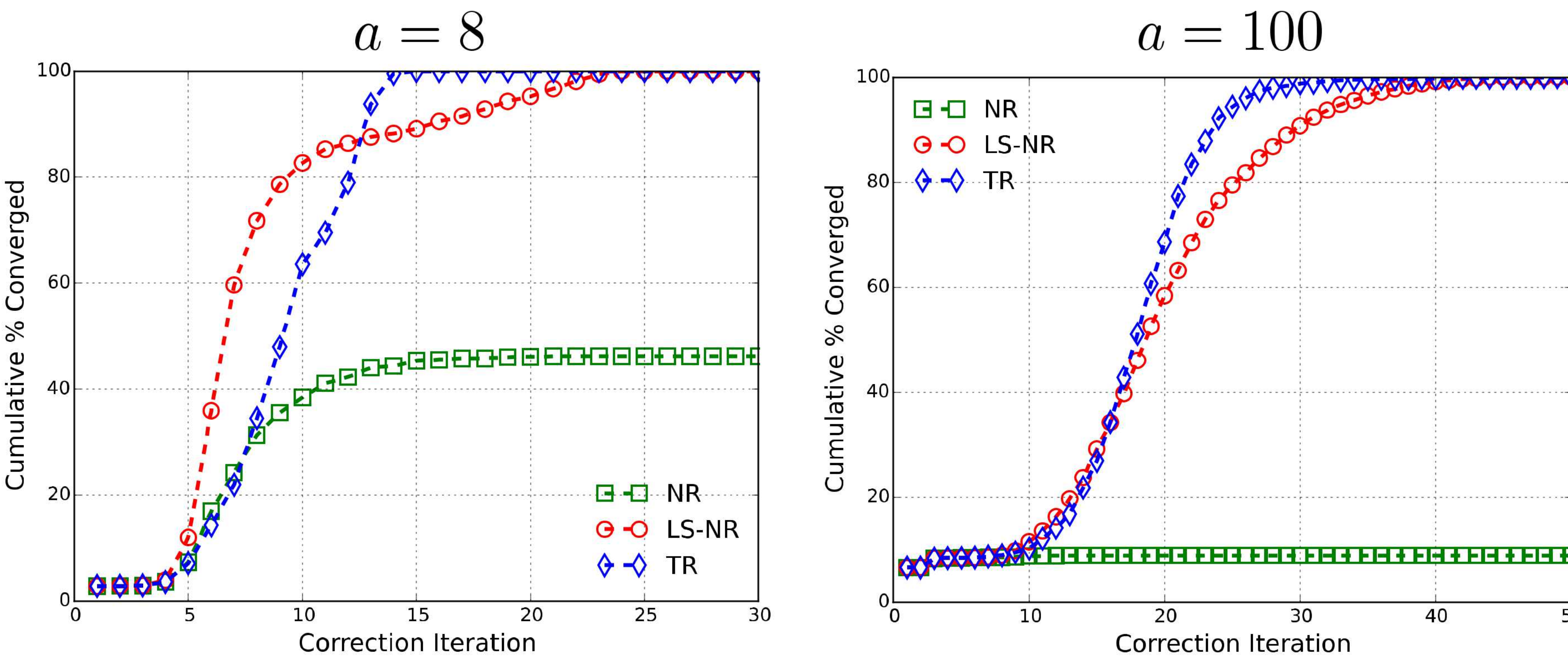


- Proposed algorithm converges in <40 iterations in almost every case

Return Trajectory Comparison (A)



Cumulative Convergence Distributions



- Convergence of TR method well in excess of traditional NR
  - Comparable with LS-NR
  - TR better at higher iterations

Verification

- Robust implementations enable a variety of descriptions
  - Different yield surfaces
  - Various rate and temperature dependencies

- Utilization/adoption require appropriate, flexible verification approaches
  - Combinatorics of different feature combinations
  - Variety of different loading conditions
  - Preferably leveraging analytical solutions

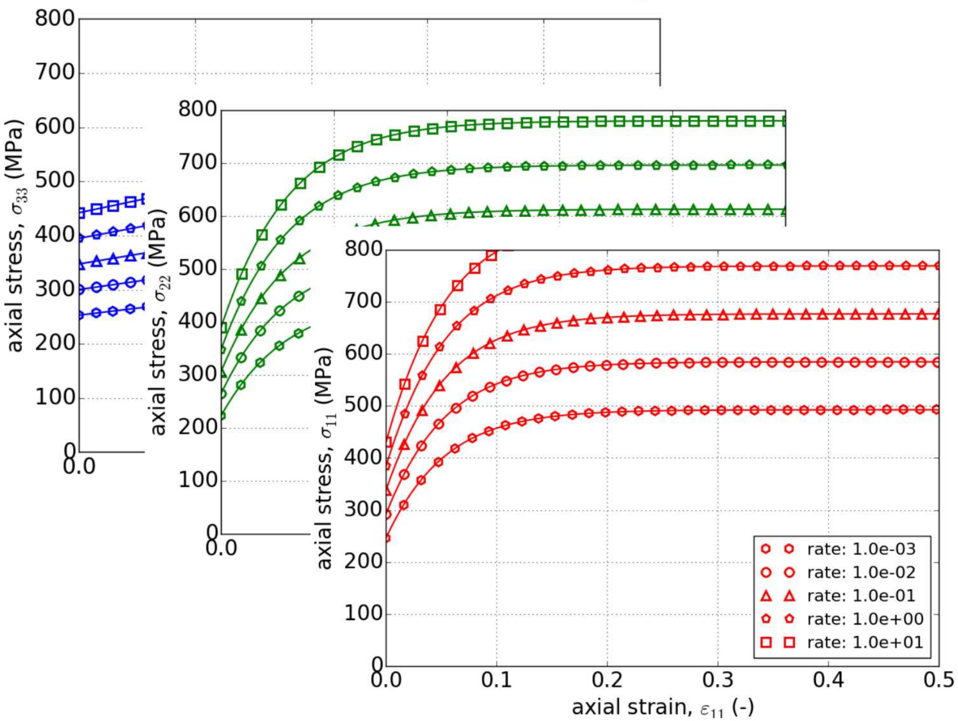
- Solution can be found assuming plastic deformation, *constant equivalent plastic* strain rate

$$\bar{\varepsilon}^{\mathrm{p}} = \dot{\bar{\varepsilon}}^{\mathrm{p}} t \rightarrow u\left(t\right) = \hat{u}\left(\dot{\bar{\varepsilon}}^{\mathrm{p}}, t\right)$$

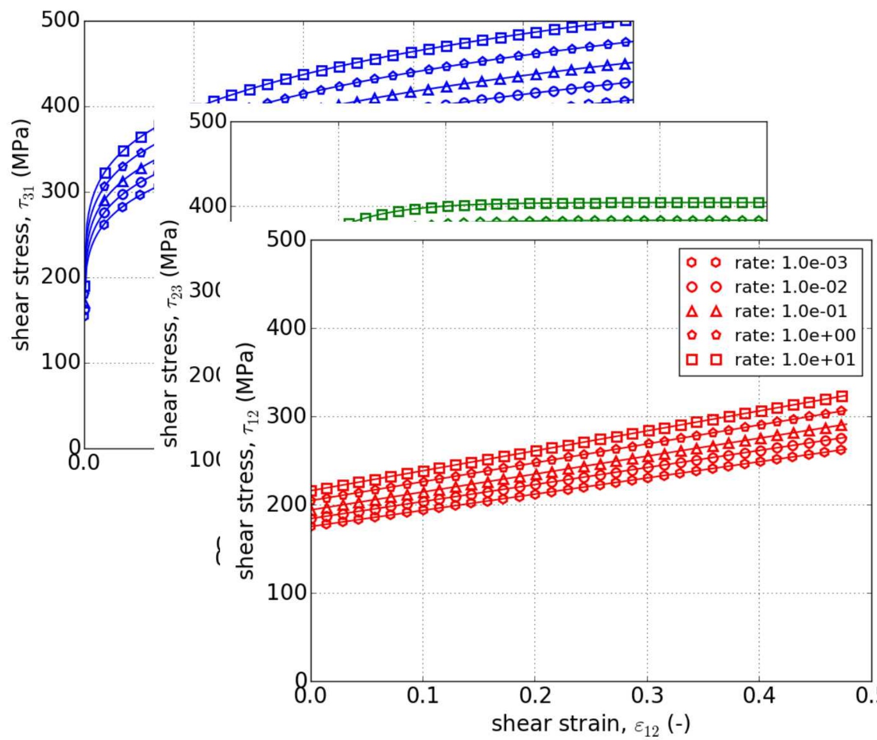
Verification

- 100's of analytical, automated tests
  - Done regularly to ensure consistent, correct responses
  - Solutions available for different loadings – e.g. uniaxial, pure shear, biaxial

Uniaxial – Barlat (Yld2004-18p)



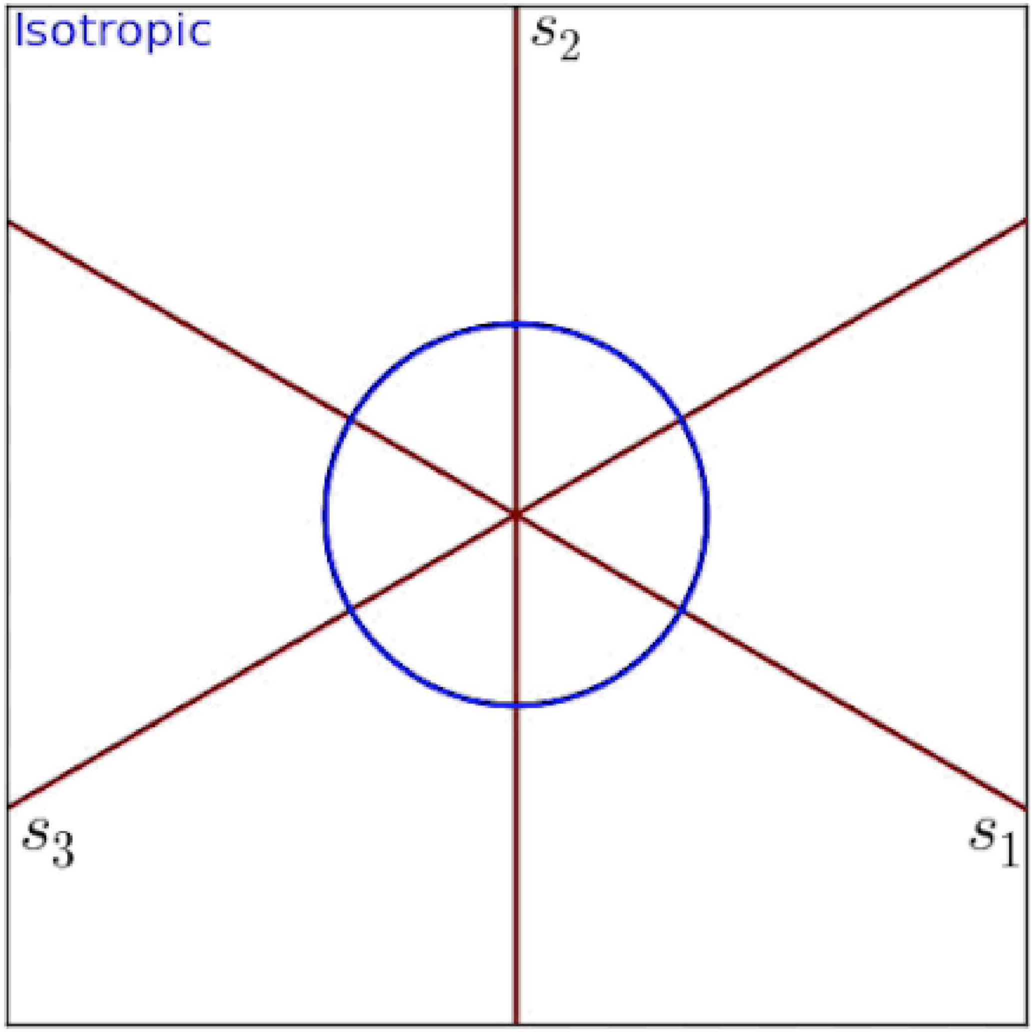
Pure Shear - Hill



Plasticity – Distortional Hardening

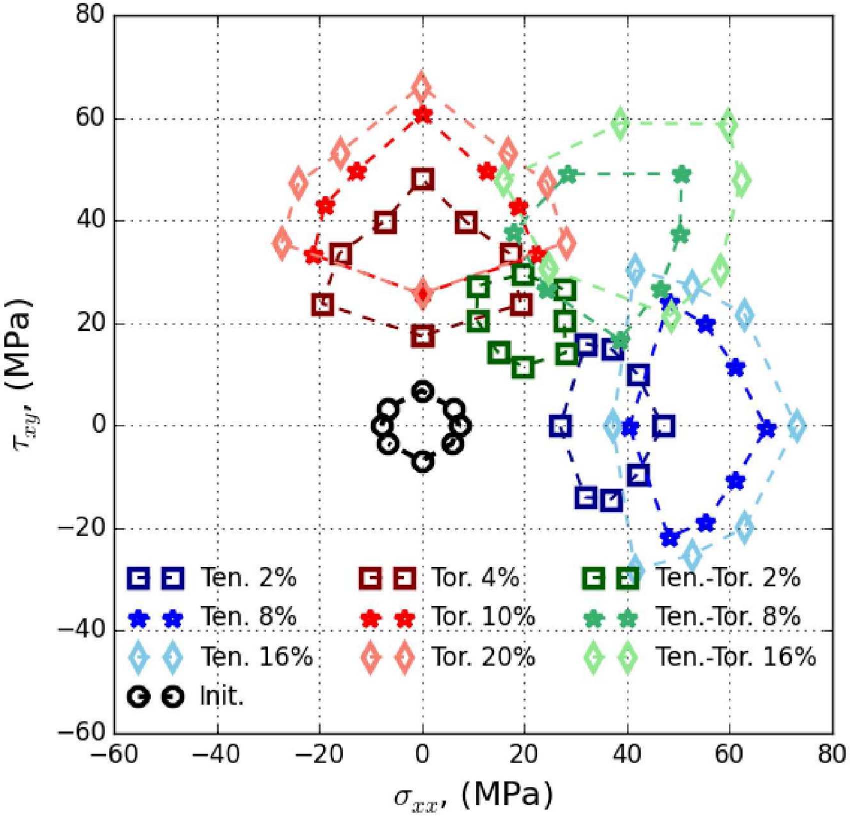
Plastic Hardening

- Capturing multiaxial, history dependent response requires description of anisotropic yield and *hardening*



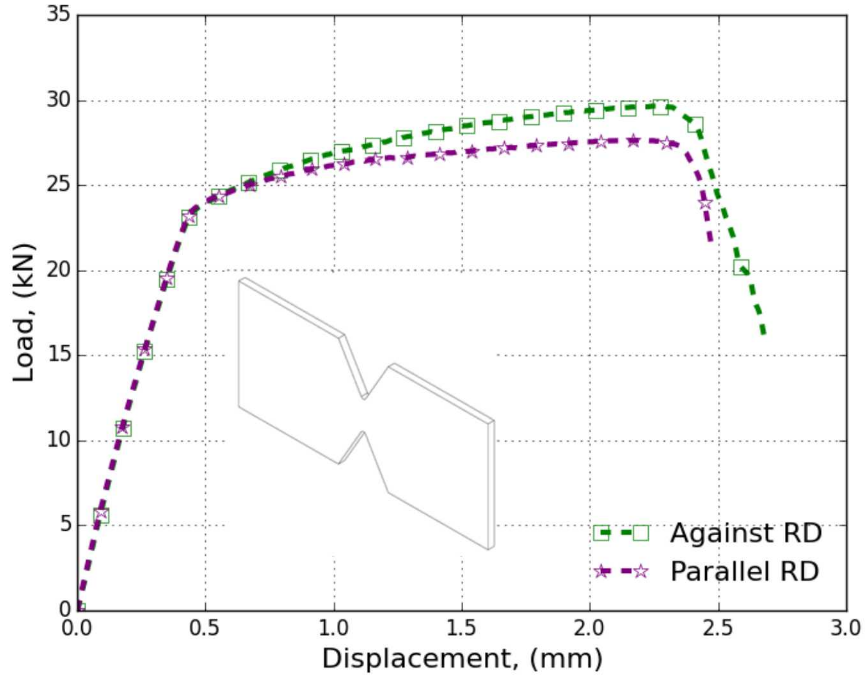
Distortional Hardening

- To expand capabilities, want to develop capabilities for distortional hardening to capture additional anisotropy



Data from Khan *et al.*, 2010, *Int. Jrnl. Plas.*, 26: 1421-1431

Notched Shear Calibration Data for SFC2



Boyce et al., 2016, *Int. Jrnl. Frac.*, 198: 5-100

(SFC2 Data Courtesy S. Kramer, B. Boyce, K. Karlson, J. T. Ostien et al., SNL)

Free Energy

State Variables

Traditional: $\varepsilon_{ij}^{\mathrm{el}}, \quad \kappa$ New Distortional ISV: η

Free Energy

$$\psi = \hat{\psi}\left(\varepsilon_{ij}^{\mathrm{el}}, \kappa, \eta\right) = \psi^{\mathrm{el}}\left(\varepsilon_{ij}^{\mathrm{el}}\right) + \psi^{\mathrm{iso}}\left(\kappa\right) + \psi^{\mathrm{dis}}\left(\eta\right)$$

$$\psi^{\mathrm{el}}\left(\varepsilon_{ij}^{\mathrm{el}}\right) = \frac{1}{2\rho}\varepsilon_{ij}^{\mathrm{el}}\mathbb{C}_{ijkl}\varepsilon_{kl}^{\mathrm{el}} \quad \psi^{\mathrm{iso}}\left(\kappa\right) = \frac{1}{\rho}g\left(\kappa\right) \quad \psi^{\mathrm{dis}}\left(\eta\right) = \frac{1}{\rho}h\left(\eta\right)$$

- Traditional State Variables:
  - Elastic Strain Tensor, $\varepsilon_{ij}^{\mathrm{el}}$
  - Isotropic Hardening Variable (IHV), κ
- Introduce single scalar ISV for distortional hardening, η
  - Encapsulates all microstructural effects of distortional hardening
  - Likely multiple mechanisms
- Assume isotropic and distortional energetic effects are independent and separable

Constitutive Behavior

$$\sigma_{ij} = \mathbb{C}_{ijkl}\varepsilon_{kl}^{\mathrm{el}} \qquad \varepsilon_{ij} = \varepsilon_{ij}^{\mathrm{el}} + \varepsilon_{ij}^{\mathrm{p}}$$

Dissipation Inequality

$$\mathcal{D} = \sigma_{ij}\dot{\varepsilon}_{ij}^{\mathrm{p}} - K\dot{\kappa} - N\dot{\eta} \geq 0$$

$$K := \rho\frac{\partial\psi}{\partial\kappa} = \frac{\partial g}{\partial\kappa} \qquad N := \rho\frac{\partial\psi}{\partial\eta} = \frac{\partial h}{\partial\eta}$$

(Lester and Scherzinger, 2018, *IJSS*, 143, 194-208)

Yield Function Definition

- Introduce a new "Evolving Effective Stress" (EES)
- Weighted sum of different definitions for desired features

$$f = f\left(\sigma_{ij}, K, N\right) = \phi\left(\sigma_{ij}, N\right) - \sigma_y\left(K\right)$$

- "Evolving" Effective Stress (EES)

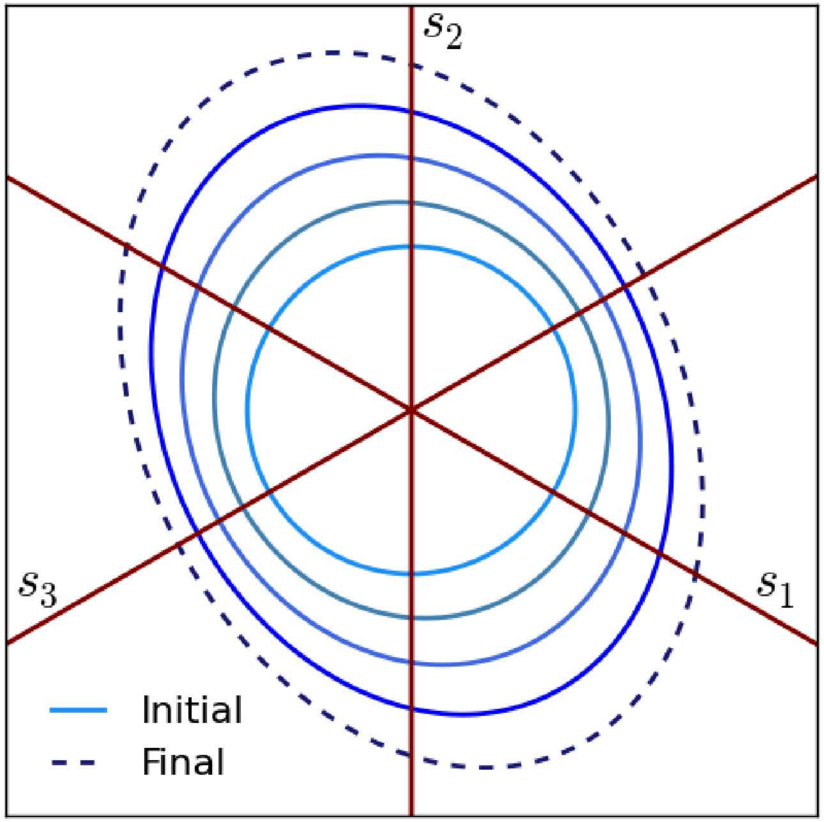
$$\phi\left(\sigma_{ij}, N\right) = \sum_{k=1}^{n_{\mathrm{es}}} \zeta^{(k)}\left(N\right)\phi^{(k)}\left(\sigma_{ij}\right)$$

- Weighting Function Constraints

$$\sum_{k=1}^{n_{\mathrm{es}}} \zeta^{(k)} = 1\ ;\ \zeta^{(k)} \geq 0$$

- Flow Stress

$$\sigma_y\left(K\right) = \sigma_y^0 + K$$



Evolution Equations

- Evolution equations found by trying to maximize dissipation
- Flow rules correspond to Karush-Kuhn-Tucker conditions

$$\dot{\kappa} = \lambda$$

$$\dot{\varepsilon}_{ij}^{\mathrm{p}} = \lambda \frac{\partial \phi}{\partial \sigma_{ij}} \qquad \lambda f\left(\sigma_{ij}, K, N\right) = 0$$

$$\dot{\eta} = -\lambda \frac{\partial \phi}{\partial N}$$

- Leads to rate of dissipation density of

$$\mathcal{D} = \left(\sigma_y^0 + N \frac{\partial \phi}{\partial N}\right) \dot{\kappa}$$

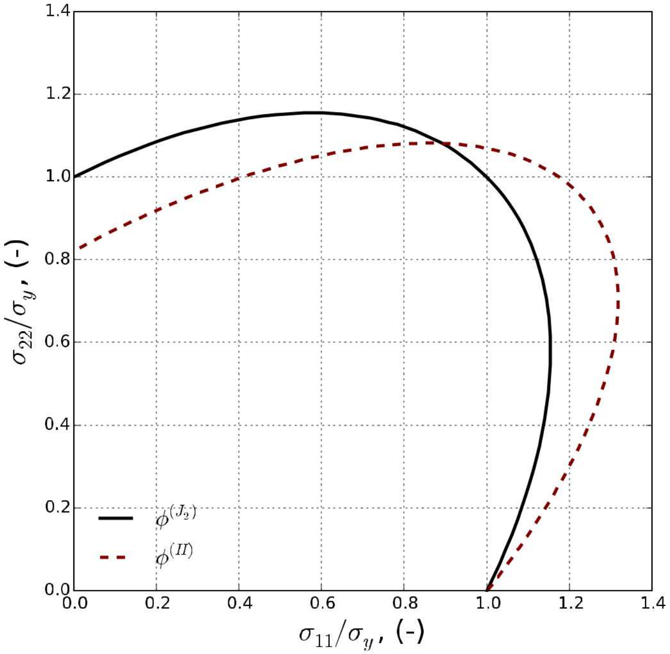
Can be positive or negative

Anisotropic Evolution

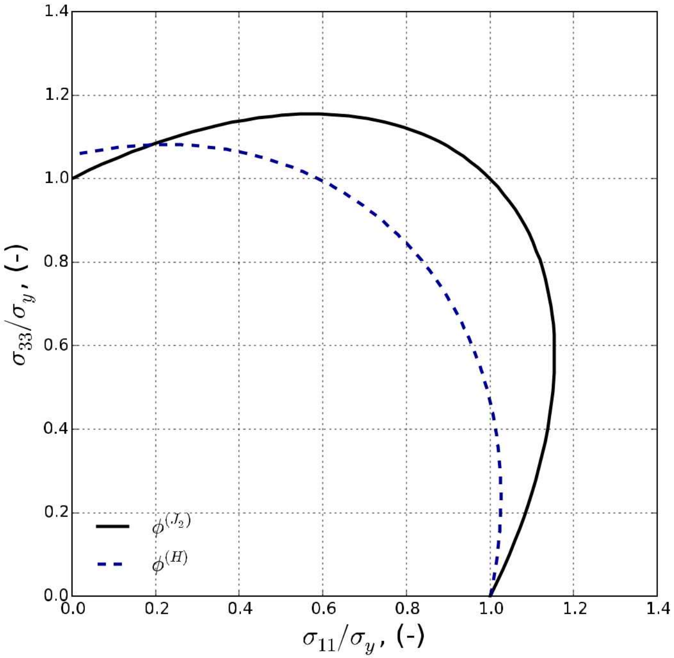
- Want to look at effect of evolving anisotropy
  - Consider case of von Mises evolving to anisotropic Hill ('48)

$$\left(\phi^{(\mathrm{H})}\left(\sigma_{ij}\right)\right)^2 = F\left(\hat{\sigma}_{22}-\hat{\sigma}_{33}\right)^2 + G\left(\hat{\sigma}_{33}-\hat{\sigma}_{11}\right)^2 + H\left(\hat{\sigma}_{11}-\hat{\sigma}_{22}\right)^2 + 2L\hat{\sigma}_{23}^2 + 2M\hat{\sigma}_{31}^2 + 2N\hat{\sigma}_{12}^2$$

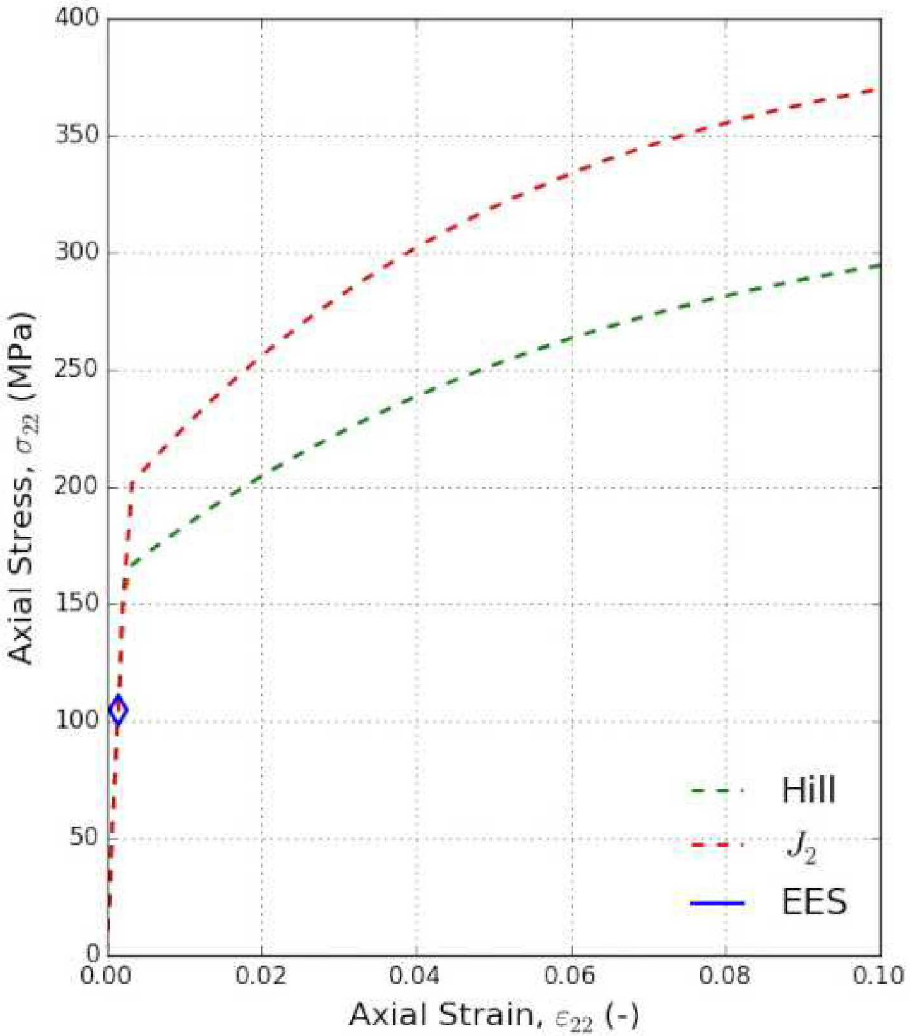
$\sigma_{11} - \sigma_{22}$ Yield Surfaces

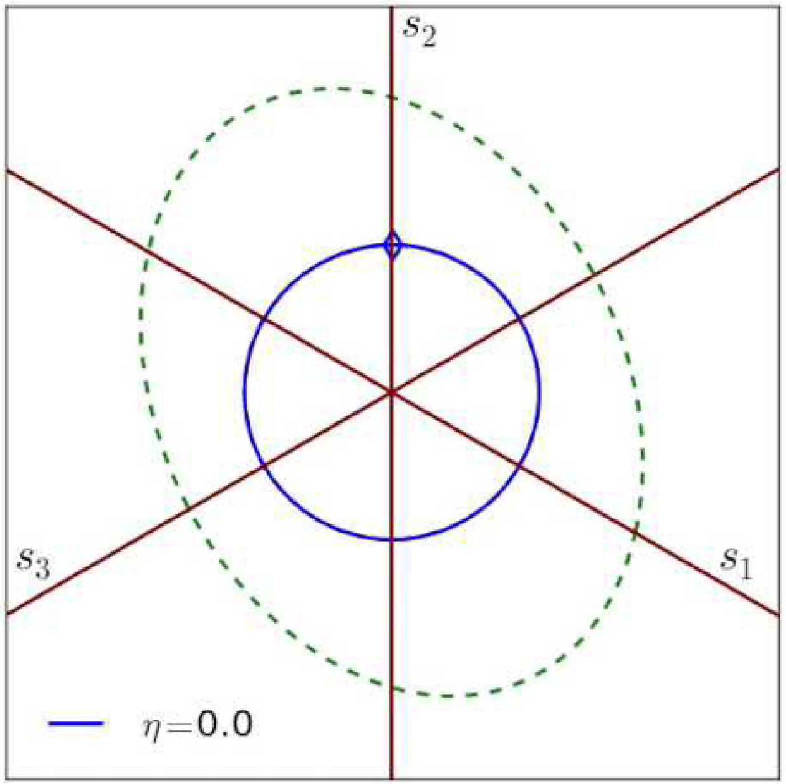


$\sigma_{11} - \sigma_{33}$ Yield Surfaces



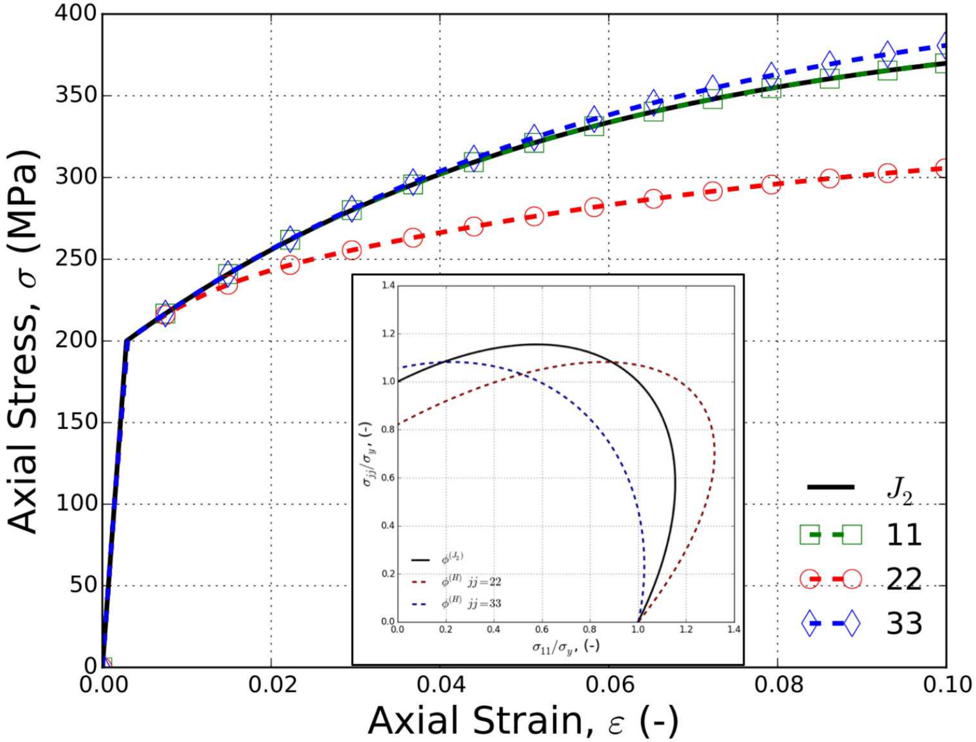
Evolving Effective Stress

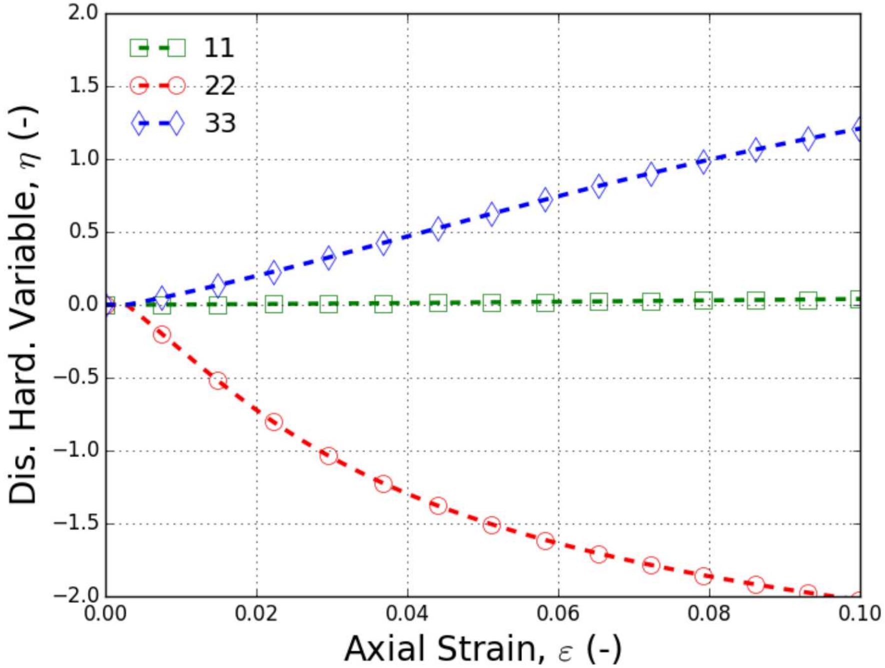




- Able to capture change of yield surface on hardening

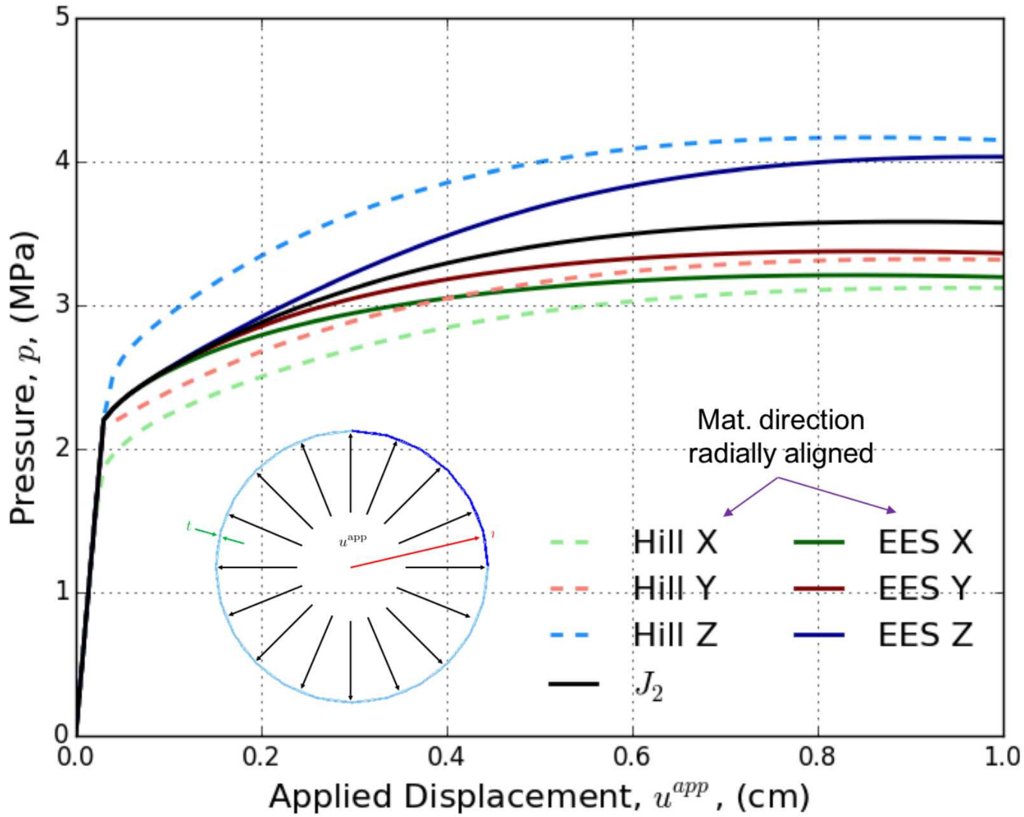
Constitutive Behavior - Hill

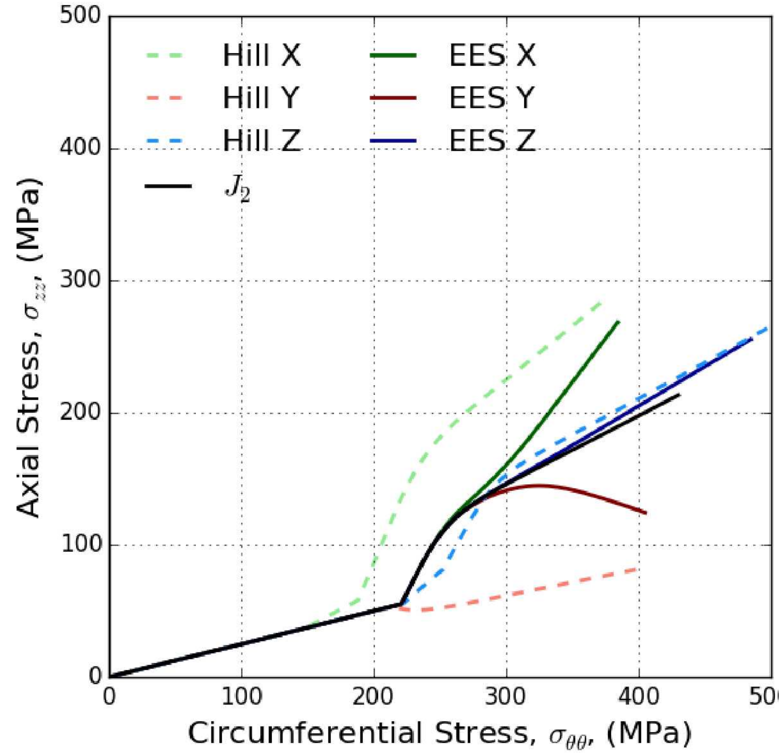




- Distortional hardening is anisotropic
  - Impact depends on difference on effective stresses
  - Different sign of distortional hardening variables

Pressurized Cylinder



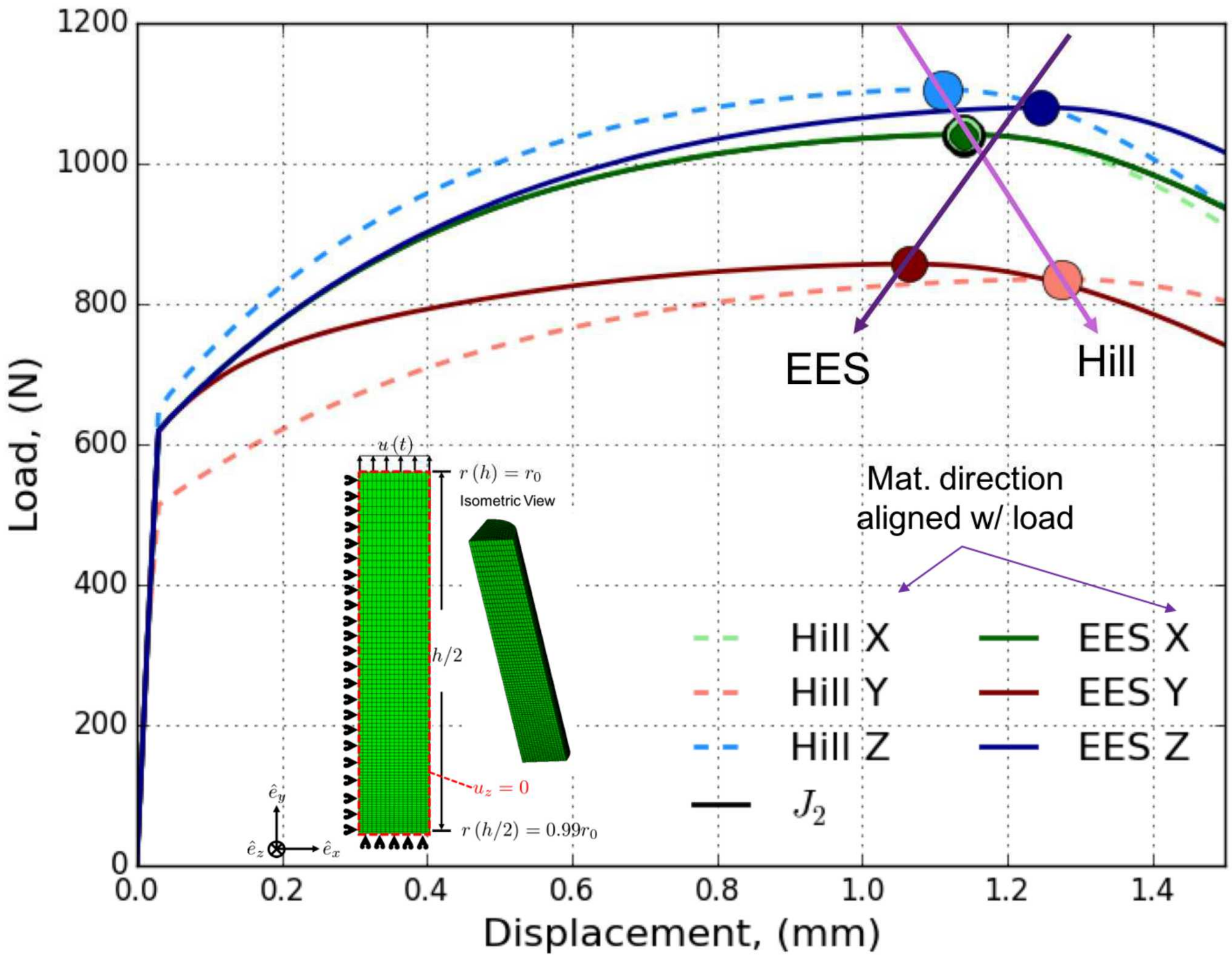


$$p = \frac{F}{(r + \bar{u}_r)\, h}$$

- Implementation is robust under complex, non-proportional, multiaxial loading paths

Tensile Cylinder

- Consider loading of a uniaxial tensile bar with the classic Hill'48 yield surface

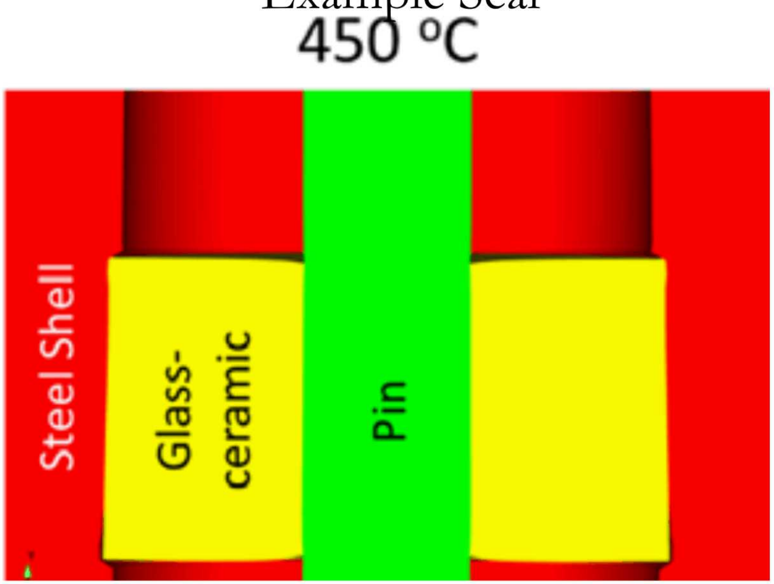


Glass-Ceramics

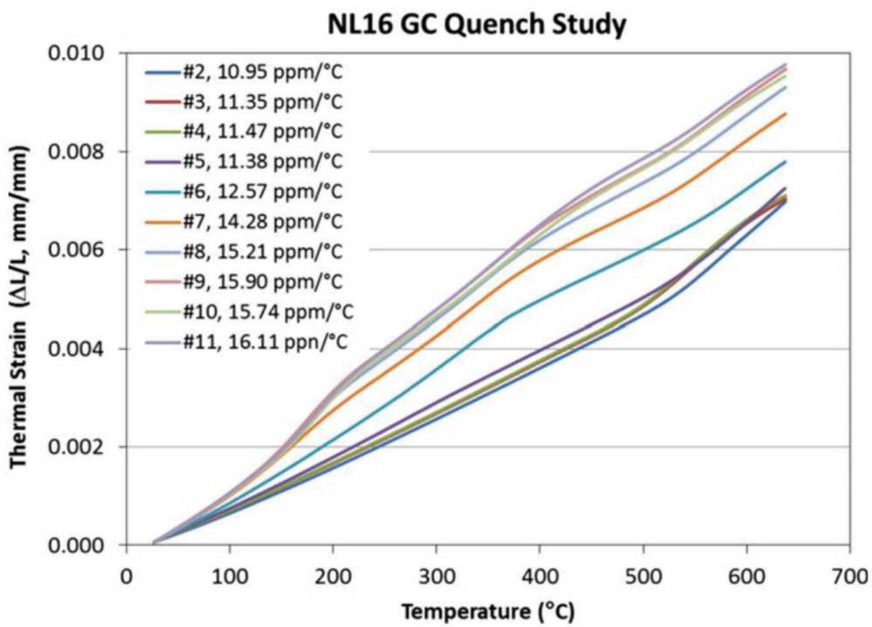
Glass-Ceramic Materials

- Glass-ceramics are produced by inducing a ceramic phase(s) in an inorganic base glass
  - Variety of industrial applications
  - Hermetic glass-ceramic to metal seals (GcTMS)
  - High CTEs

Example Seal



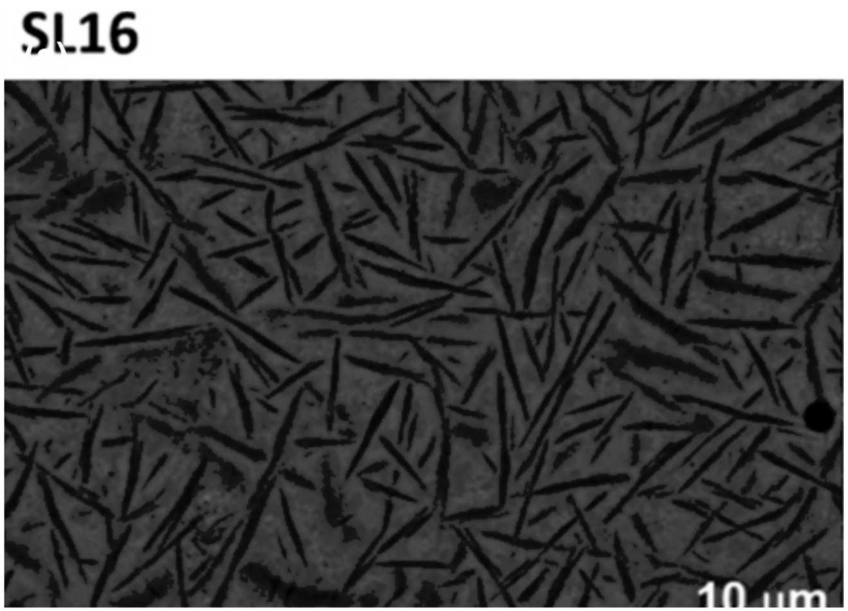
Dai *et al.*, 2017, *J Am Ceram Soc*, 100, pp.3652-3661



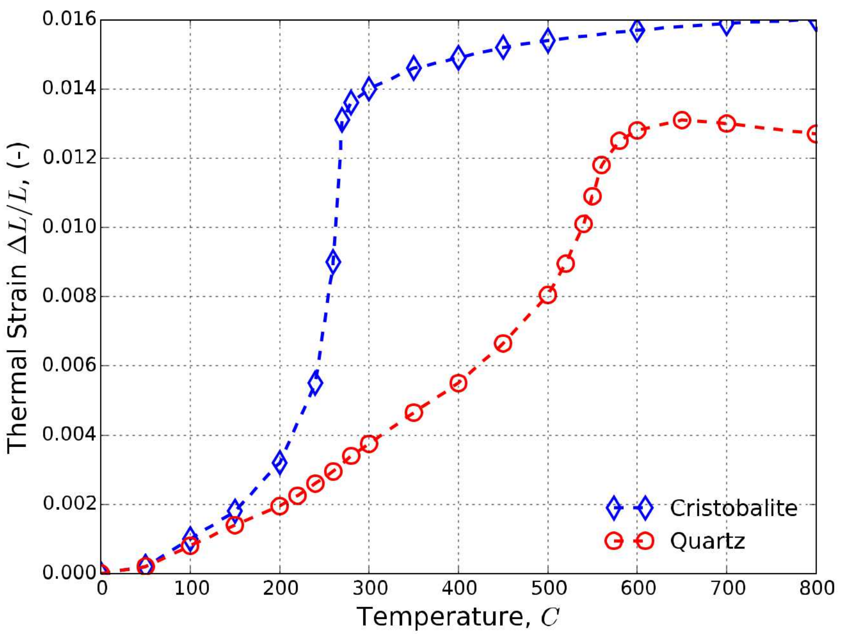
Dai *et al.*, 2016, *J Am Ceram Soc*, 99, pp.3719-3725

Glass-Ceramic Characteristics

- Glass-ceramics are microstructurally heterogeneous
- Multiple inelastic phases
  - Residual glass producing viscoelastic responses
  - Silica polymorphs (cristobalite and/or quartz) undergoing phase transformations



Rodriguez *et al.*, 2016, *J Am Ceram Soc*, 99(11), pp.3726-3733



Data from Bauleke, 1978, Kan. Geo. Survey, 211(4), p.23-27

Glass-Ceramic Model

- Need model capable of describing coupled phase transformation and viscoelasticity
  - Thermoviscoelastic theory for response of glassy phase
  - Utilize shape memory alloy (SMA) theory as basis (Lagoudas model) for phase transformations

$$G\left(\sigma_{ij}, T, t, \xi, \varepsilon_{ij}^{\mathrm{t}}; \delta^{i}\right) = G^{\mathrm{te}}\left(\sigma_{ij}, T, \xi; \delta^{i}\right) + G^{\mathrm{in}}\left(\sigma_{ij}, T, t, \xi, \varepsilon_{ij}^{\mathrm{t}}\right)$$

ξ	Low Cristobalite Volume Fraction
$\varepsilon_{ij}^{\mathrm{t}}$	Transformation Strain

$$G^{\mathrm{te}}\left(\sigma_{ij}, T, \xi\right) = \sum_{i=1}^{4} \delta^{i} G^{i}\left(\sigma_{ij}, T\right) + \delta^{\mathrm{C}}\left(\xi G^{\text{C-low}}\left(\sigma_{ij}, T\right) + (1-\xi)\, G^{\text{C-high}}\left(\sigma_{ij}, T\right)\right)$$

Constitutive Model

- Assume independent contributions of mechanisms
  - Use an integral based representation of viscoelasticity*
  - WLF shift factor

$$G^{\mathrm{in}} = -g_{\varepsilon}\left(\delta^{i}\right)\frac{1}{\rho}\sigma_{ij}\varepsilon^{\mathrm{t}}_{ij} + g_{h}\left(\delta^{i}\right)\frac{1}{\rho}h\left(\xi\right) + G^{\mathrm{neq}}\left(\sigma_{ij}, T, t; \delta^{i}\right)$$

- Coleman-Noll and 2nd Law arguments produce:

$$\varepsilon_{ij} = \frac{1}{2\bar{\mu}\left(\xi\right)}\sigma'_{ij} + \frac{1}{9\bar{K}\left(\xi\right)}\sigma_{kk}\delta_{ij} + g_{\varepsilon}\varepsilon^{\mathrm{t}}_{ij} + \bar{\alpha}\left(\xi\right)\left(T - T_0\right)\delta_{ij}$$

$$g_v\frac{\Delta\mu}{2\mu^{\mathrm{eq}}\mu^{\mathrm{g}}}H^2_{ij} - g_v\frac{\Delta K}{9K^{\mathrm{eq}}K^{\mathrm{g}}}H^1\delta_{ij} + g_v\Delta\alpha H^3\delta_{ij}$$

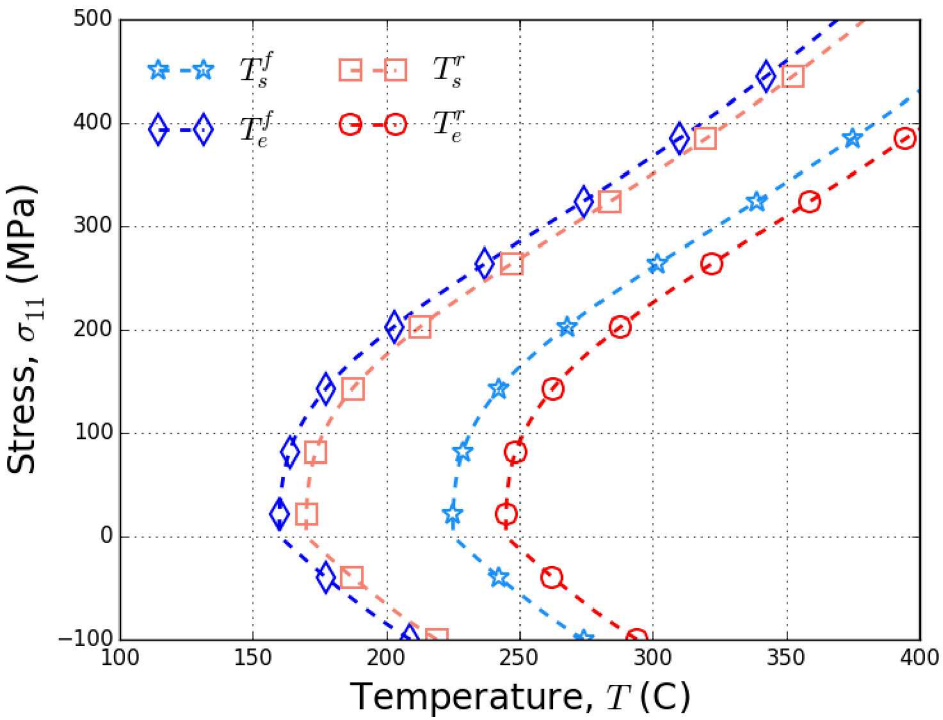
$H^1,\ H^2_{ij},\ H^3$ Viscoelastic Hereditary Integrals

*Caruthers *et al.*, 2004, *Polymer*, 45, pp. 4577-4597

Transformation Function

- For transformation behavior use $J_2 - I_1$ description
  - Associative form of evolution equations
  - Combines parts of Qidwai & Lagoudas (2000) and Lagoudas *et al.* (2012)

$$f(X_{ij}, p) = [\phi(X_{ij}) - p]^2 - p_0^2$$



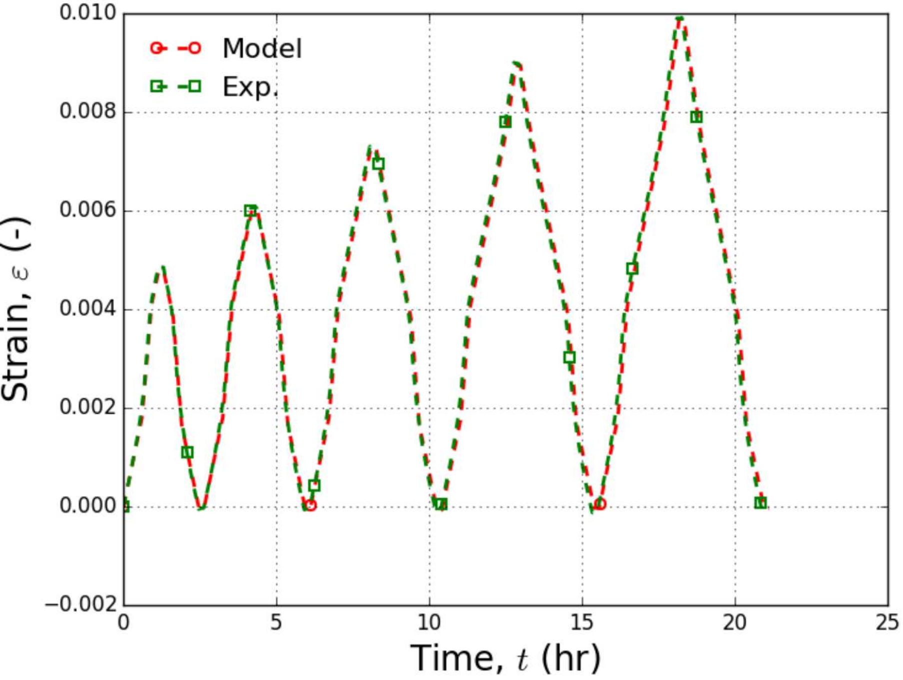
$$X_{ij} := g_\varepsilon \sigma_{ij}$$

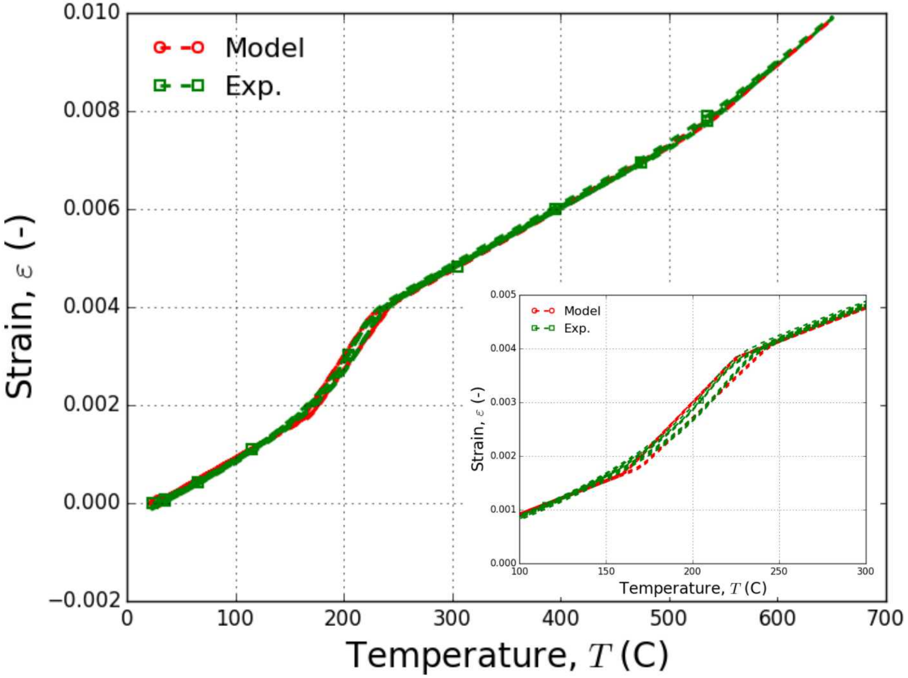
$$p := \rho \frac{\partial G^{\mathrm{te}}}{\partial \xi} + g_h \frac{\partial h}{\partial \xi}$$

$$\phi(X_{ij}) = \gamma_1(J_2)\sqrt{3J_2} - \gamma_2 I_1$$

Validation

- Validated model against no-load thermal sweeps





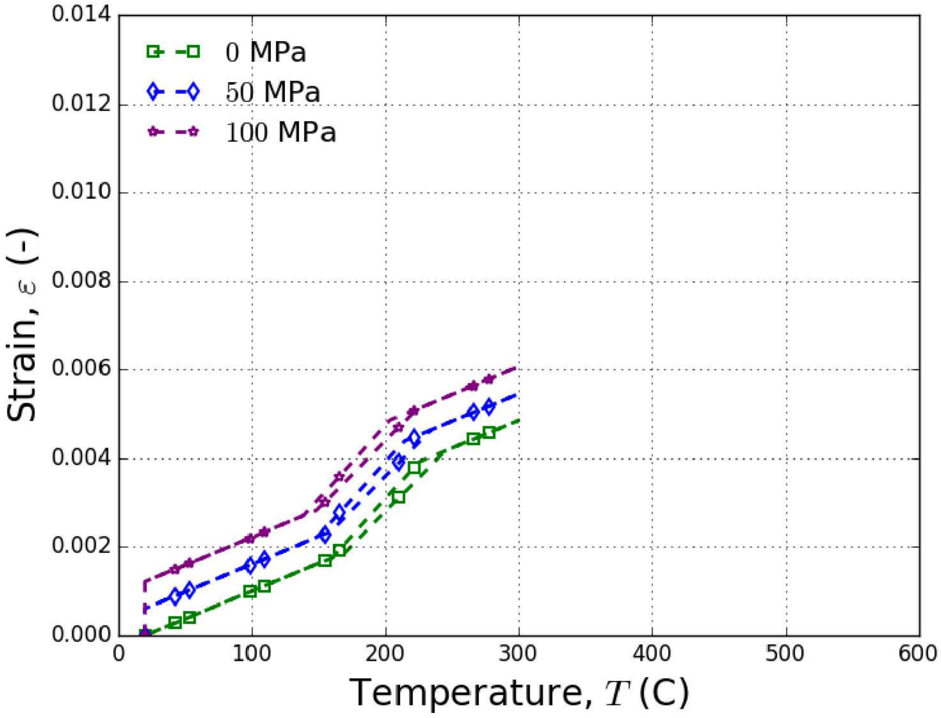
- Working on extending validation against other experiments

Experiments courtesy S. Dai (SNL)

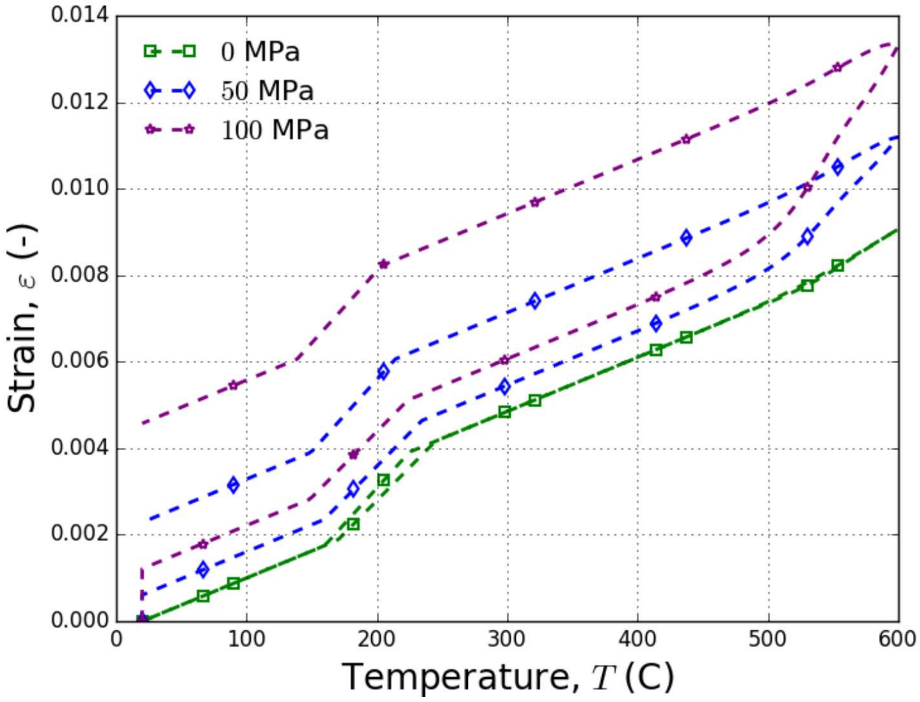
Glass-Ceramics

- Initial model can also be used for consideration of interaction of mechanism

Transformation Only



Transformation and Viscoelasticity



- 3D formulation being implemented

Conclusion and Summary

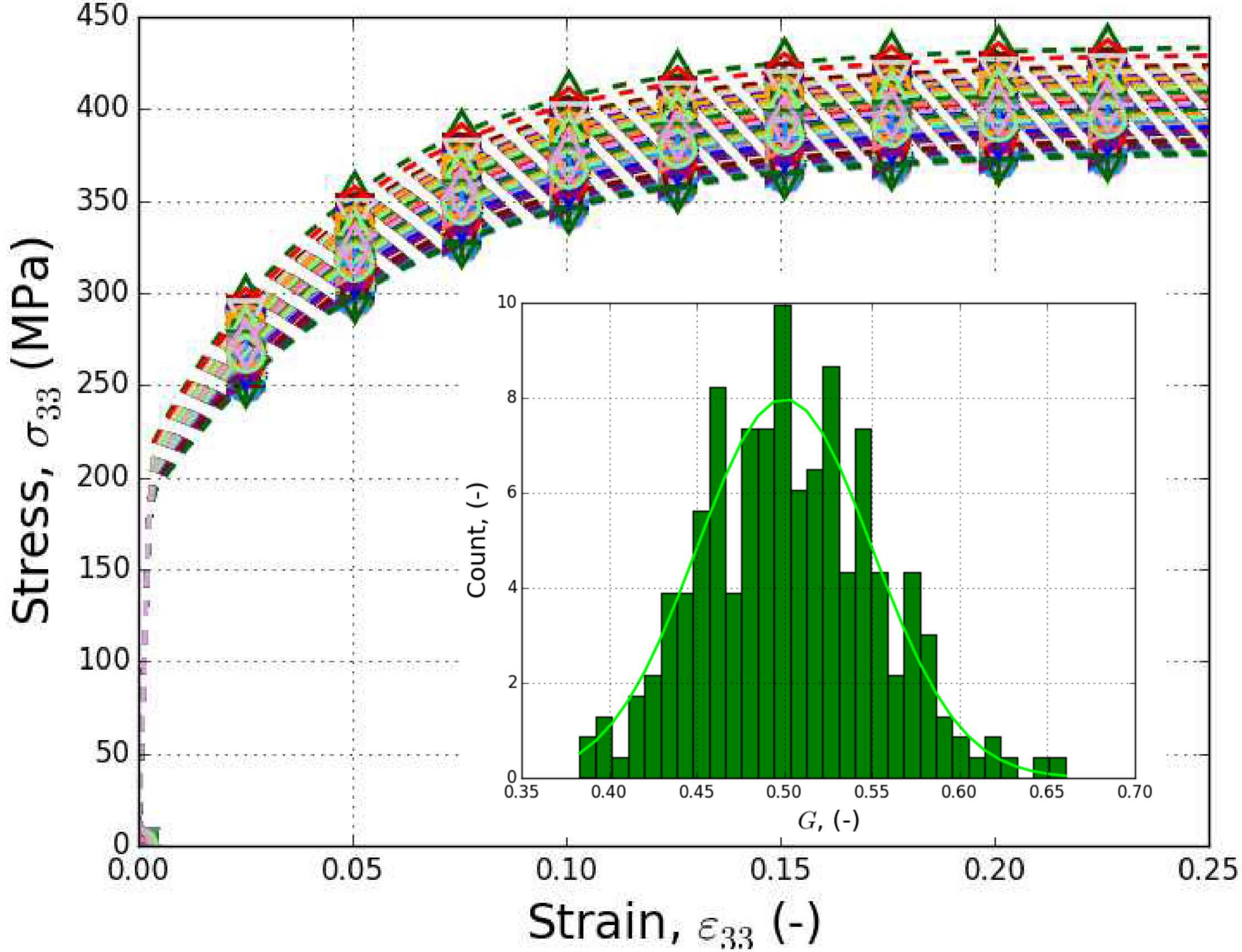
- Discussed development and implementation of two model classes:
  - Anisotropic distortional hardening plasticity
  - Glass-ceramic materials

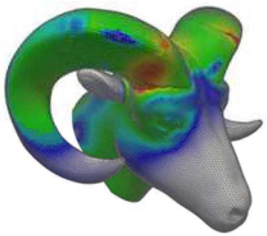
- Tried to emphasize continuing needs for model application beyond development
  - Implementation
  - Verification

- Future work
  - Continually expanding descriptions of material responses
    - Continuum descriptions of multiscale/multiphysics
  - Novel and efficient calibration procedures (full-field)
  - Model form error/uncertainty

Model Form

- What is the impact of model error selection?





Research and Application of Mechanics of Structures (RAMS) Institute

National Security Mission

Sandia National Laboratories delivers essential science and technology to resolve the nation's most challenging security issues. A strong science, technology, and engineering foundation enables Sandia's mission through a capable research staff working at the forefront of innovation, collaborative research with universities and companies, and mission directed research projects. We recruit the best and the brightest, equip them with world-class research tools and facilities, and provide opportunities to collaborate with technical experts from many different scientific disciplines.

Institute Description

Sponsored by Sandia's Engineering Sciences Center, the Research and Applications of Mechanics of Structures (RAMS) Institute provides students an opportunity to work with outstanding technical staff in providing engineering solutions to national security mission deliverables. Institute participants will research, develop, and apply computational capabilities to define mechanical environments and simulate response of complex structural systems subjected to extreme loading conditions.

Students work in a collaborative environment and participate in frequent technical and team building activities throughout their internship, including career discussions, tours, and speaker presentations.

Interns Needed

Highly qualified graduate and undergraduate engineering students with an interest in structural mechanics research and applications, including environments definitions, structural mechanics simulation, material mechanics, and shock physics are needed to support on-going programs during the summer of 2020. Undergraduate students transitioning from the Junior to Senior year and graduate students having completed at least one year of studies toward an MS or Ph.D. degree are preferred. Successful candidates will be assigned a staff mentor and work as part of a team of interns from across the United States. Students will be challenged to conduct independent and group work, and to actively engage in mission activities.

Applying

Minimum GPAs of 3.0 on a 4.0 scale are required at Sandia for student internships. Preference will be given to students that meet a more rigorous standard of 3.3 undergraduate and 3.7 graduate GPAs. Applicants must be eligible to pursue a Department of Energy security clearance. More information and applications are available at the Sandia recruiting web site: http://www.sandia.gov/careers. Search for specific internship postings: **#668783 (Graduate), #668808 (Undergraduate).** Please direct any questions to Lisa Zimmer Raver at lzimmer@sandia.gov.

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Questions?

Model Extension

- EES introduces tractable description of anisotropic hardening
- Still missing some experimentally observed characteristics (e.g. kinematic hardening, directional dependence)
- Can model be extended appropriately?

Free Energy

$$\psi\left(\varepsilon_{ij}^{\mathrm{el}}, \kappa, \eta, \beta_{ij}\right) = \psi^{\mathrm{el}}\left(\varepsilon_{ij}^{\mathrm{el}}\right) + \psi^{\mathrm{iso}}(\kappa) + \psi^{\mathrm{dis}}(\eta) + \psi^{\mathrm{kin}}(\beta_{ij})$$

$$\psi^{\mathrm{dis}}(\eta) = \frac{1}{\rho} h(\eta) \qquad \psi^{\mathrm{kin}}(\beta_{ij}) = \frac{1}{2\rho} H \beta_{ij}\beta_{ij}$$

Dissipation Inequality

$$\mathcal{D} = \sigma_{ij}\dot{\varepsilon}_{ij}^{\mathrm{p}} - K\dot{\kappa} - N\dot{\eta} - B_{ij}\dot{\beta}_{ij} \geq 0$$

$$K := \rho\frac{\partial \psi}{\partial \kappa} = \frac{\partial g}{\partial \kappa} \qquad N := \rho\frac{\partial \psi}{\partial \eta} = \frac{\partial h}{\partial \eta} \qquad B_{ij} := \rho\frac{\partial \psi}{\partial \beta_{ij}} = H\beta_{ij}$$

Extended Evolving Effective Stress (E3S)

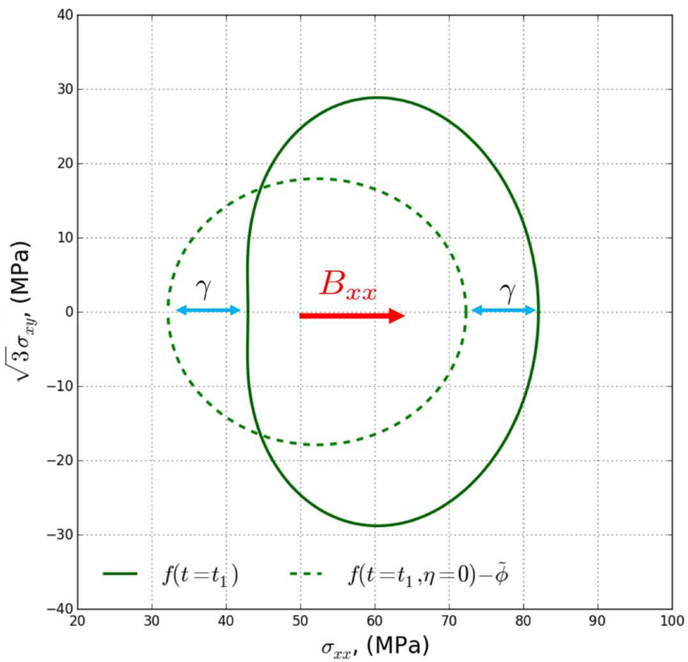
- Next need to capture kinematic hardening and directional dependence
- Consider extended evolving effective stress (E3S)

EES

$$f\left(\sigma_{ij}, K, N\right) = \phi\left(\sigma_{ij}, N\right) - \sigma_y^0 - K$$

E3S

$$f\left(\sigma_{ij}, K, N, B_{ij}\right) = \phi\left(X_{ij}, N\right) - \sigma_y^0 - K - \tilde{\phi}\left(\sigma_{ij}, N, B_{ij}\right)$$



- Use effective stress tensor for kinematic hardening

$$X_{ij} = \sigma_{ij} - B_{ij}$$

$$\phi\left(X_{ij}, N\right) = \sum_{k=1}^{n_{\mathrm{es}}} \zeta^{(k)}\left(N\right) \phi^{(k)}\left(X_{ij}\right)$$

- Introduce perturbation term for direction dependence

$$\tilde{\phi}\left(\sigma_{ij}, N, B_{ij}\right) = \gamma\omega\left(N\right) \frac{X'_{ij} B_{ij}}{||X'_{mn}|| \, ||B_{mn}||}$$

Evolution Equations

- Use Frederick-Armstrong non-linear kinematic hardening law
- Requires use of non-associated, plastic potential, F

$$F\left(\sigma_{ij}, K, N, B_{ij}\right) = f\left(\sigma_{ij}, K, N, B_{ij}\right) + \frac{1}{2}\frac{b_1}{H}B_{ij}B_{ij}$$

- Evolution equations:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \lambda\frac{\partial F}{\partial \sigma_{ij}} = \dot{\kappa}\left(\frac{\partial \phi}{\partial X_{ij}} - \frac{\partial \tilde{\phi}}{\partial \sigma_{ij}}\right)$$

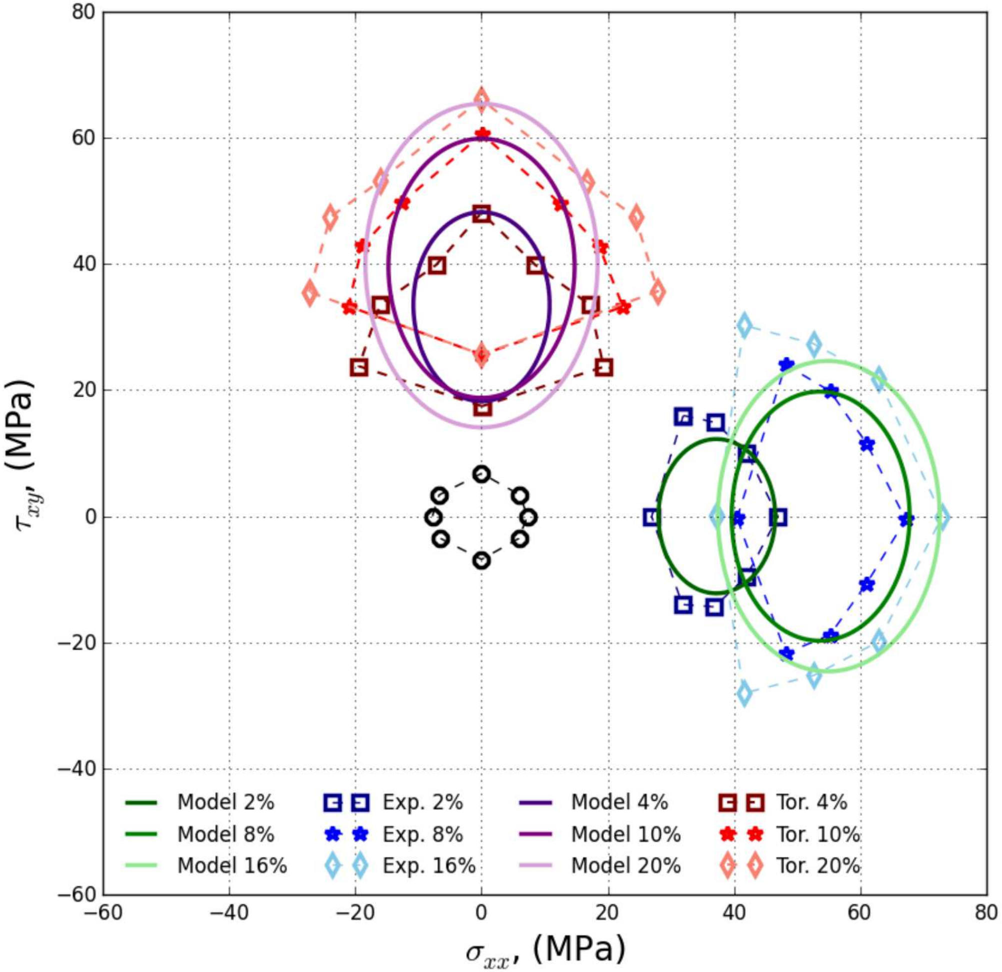
$$\dot{\kappa} = -\lambda\frac{\partial F}{\partial K} = \lambda$$

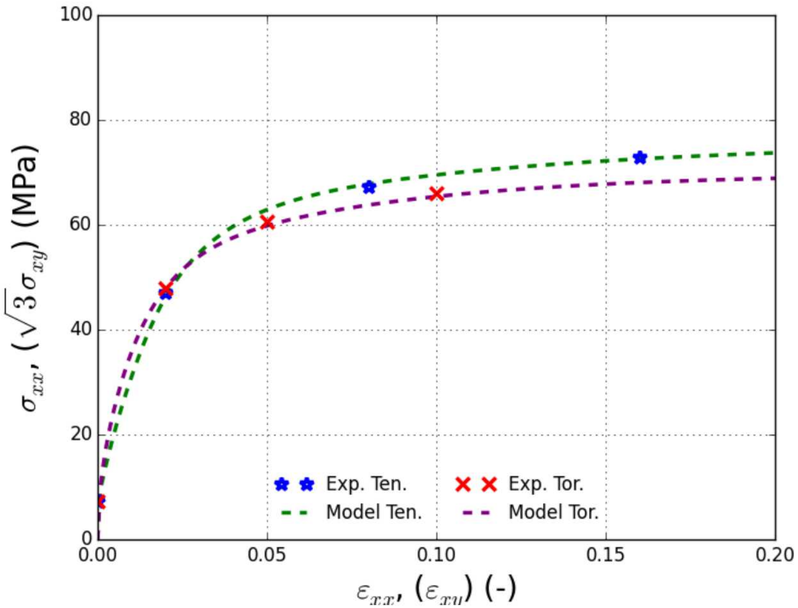
$$\dot{\eta} = -\lambda\frac{\partial F}{\partial N} = -\dot{\kappa}\left(\frac{\partial \phi}{\partial N} - \gamma\frac{\partial \omega}{\partial N}\frac{X'_{ij}B_{ij}}{||X'_{mn}||||B_{mn}||}\right)$$

$$\dot{\beta}_{ij} = -\lambda\frac{\partial F}{\partial B_{ij}} = \dot{\kappa}\left(\frac{\partial \phi}{\partial X_{ij}} - b_1\beta_{ij} - \frac{\partial \tilde{\phi}}{\partial B_{ij}}\right)$$

Model Validation (Ongoing)

- Fit model using just tensile loading; predict pure torsion
- Reasonable fit although some refinement ongoing



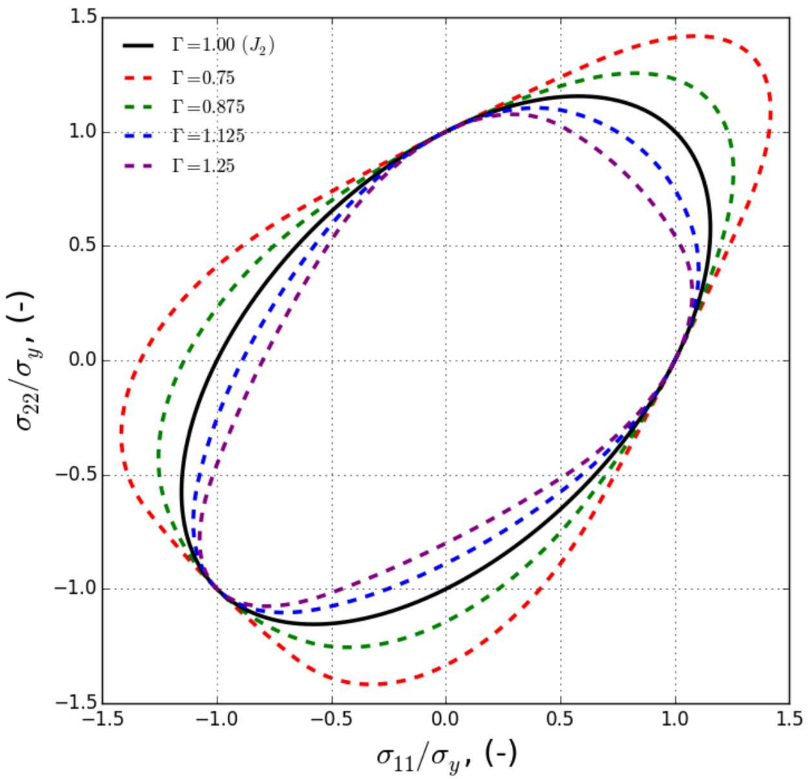


(Exp. Data from Khan *et al.*, 2010, *Int. Jrnl. Plas.*, 26: 1421-1431)

Strength-Differential Evolution

- Want to look at effect of developing a strength-differential effect
  - Consider isotropic form of Cazacu *et al.* effective stress

$$\phi^{(C)} = \{[|s_1| - k_c s_1]^a + [|s_2| - k_c s_2]^a + [|s_3| - k_c s_3]^a\}^{1/a}$$



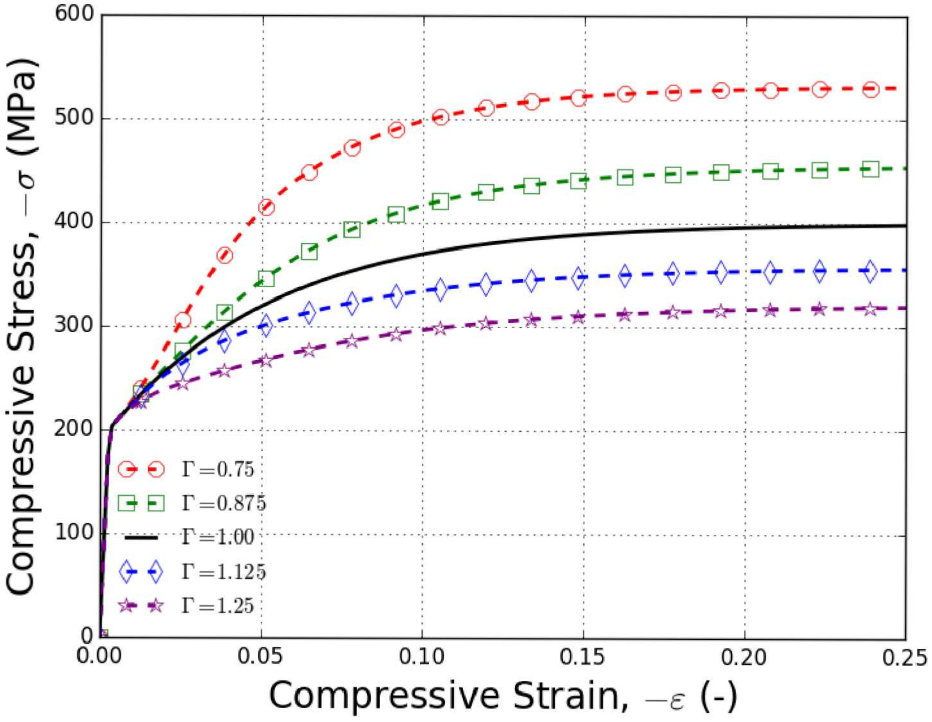
$$\Gamma = \frac{\sigma_y^{0(t)}}{\sigma_y^{0(c)}}$$

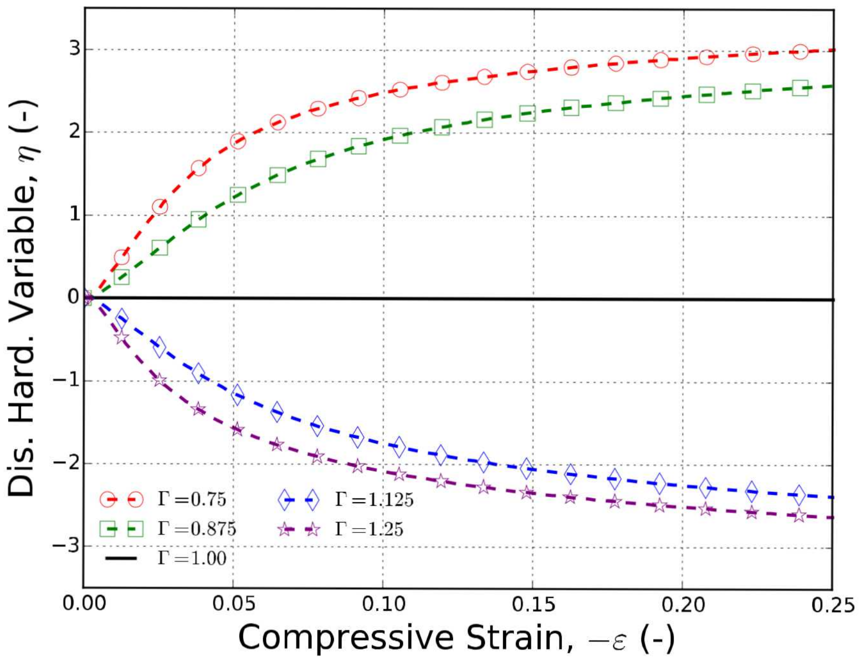
$$k_c = \frac{1 - h(\Gamma)}{1 + h(\Gamma)}$$

$$h(\Gamma) = \left[\frac{2^a - 2\Gamma^a}{(2\Gamma)^a - 2}\right]^{\frac{1}{a}}$$

(Cazacu *et al.*, 2006, IJP, 22, pp.1171-1194)

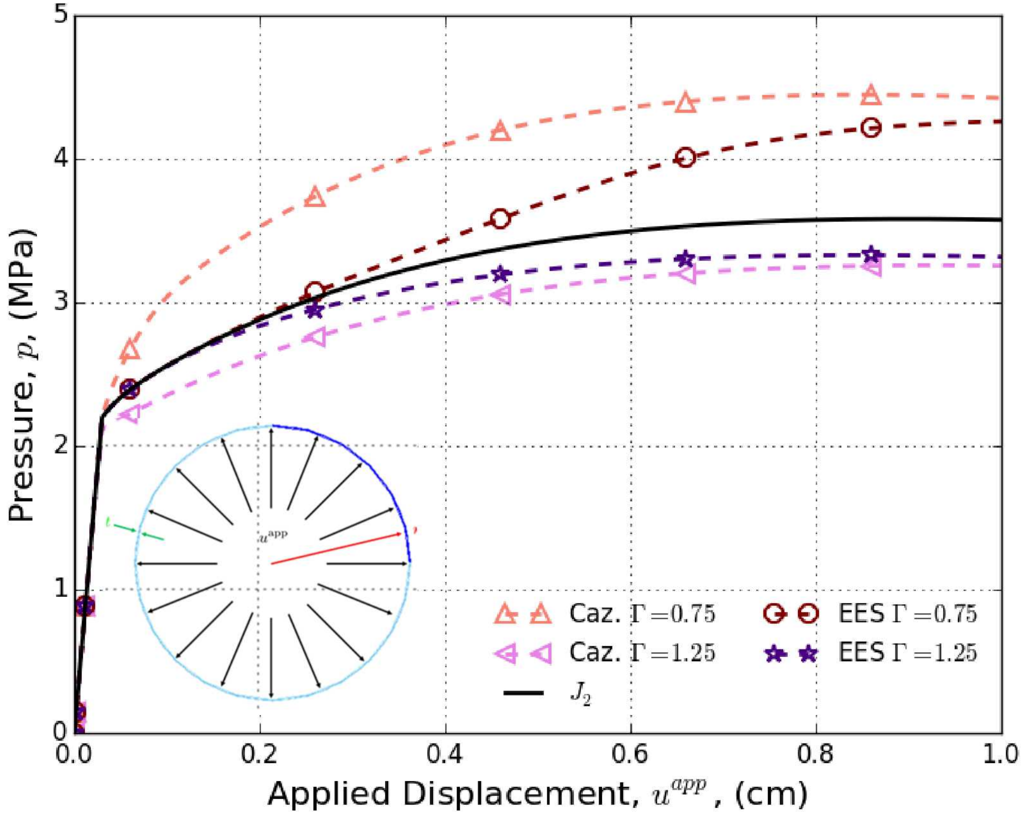
Constitutive Behavior

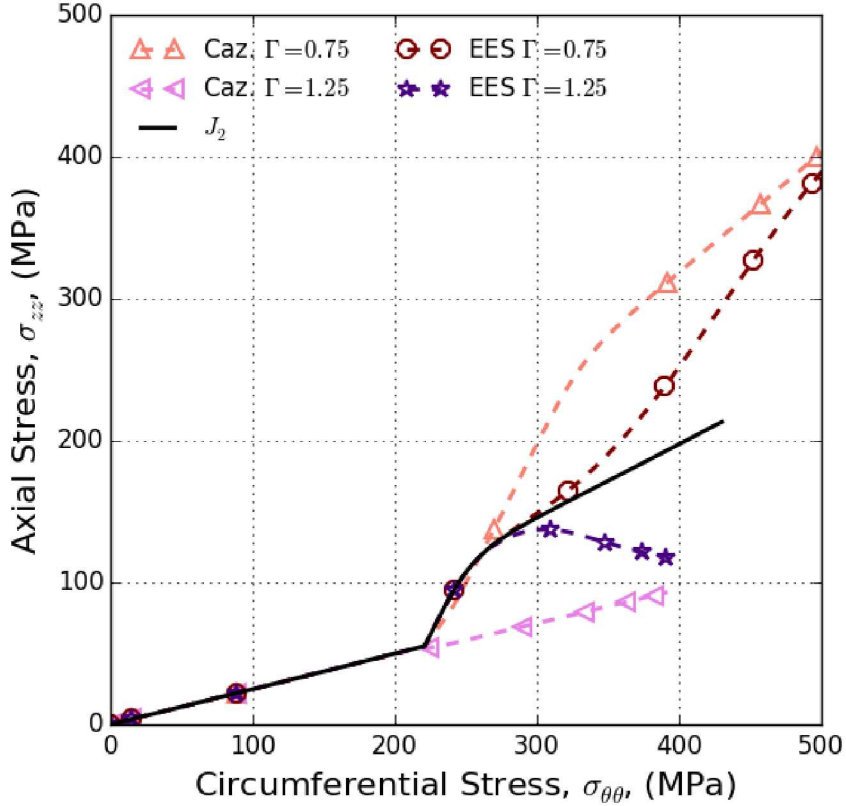




- EES approach enables the description of developing tension-compression asymmetry

Pressurized Cylinder





$$p = \frac{F}{(r + \bar{u}_r)\, h}$$

- Implementation is robust under complex, non-proportional, multiaxial loading paths

Merit Function

- For optimization methods need to introduce a merit function
  - Assess convergence
  - Gauge improvement over an increment

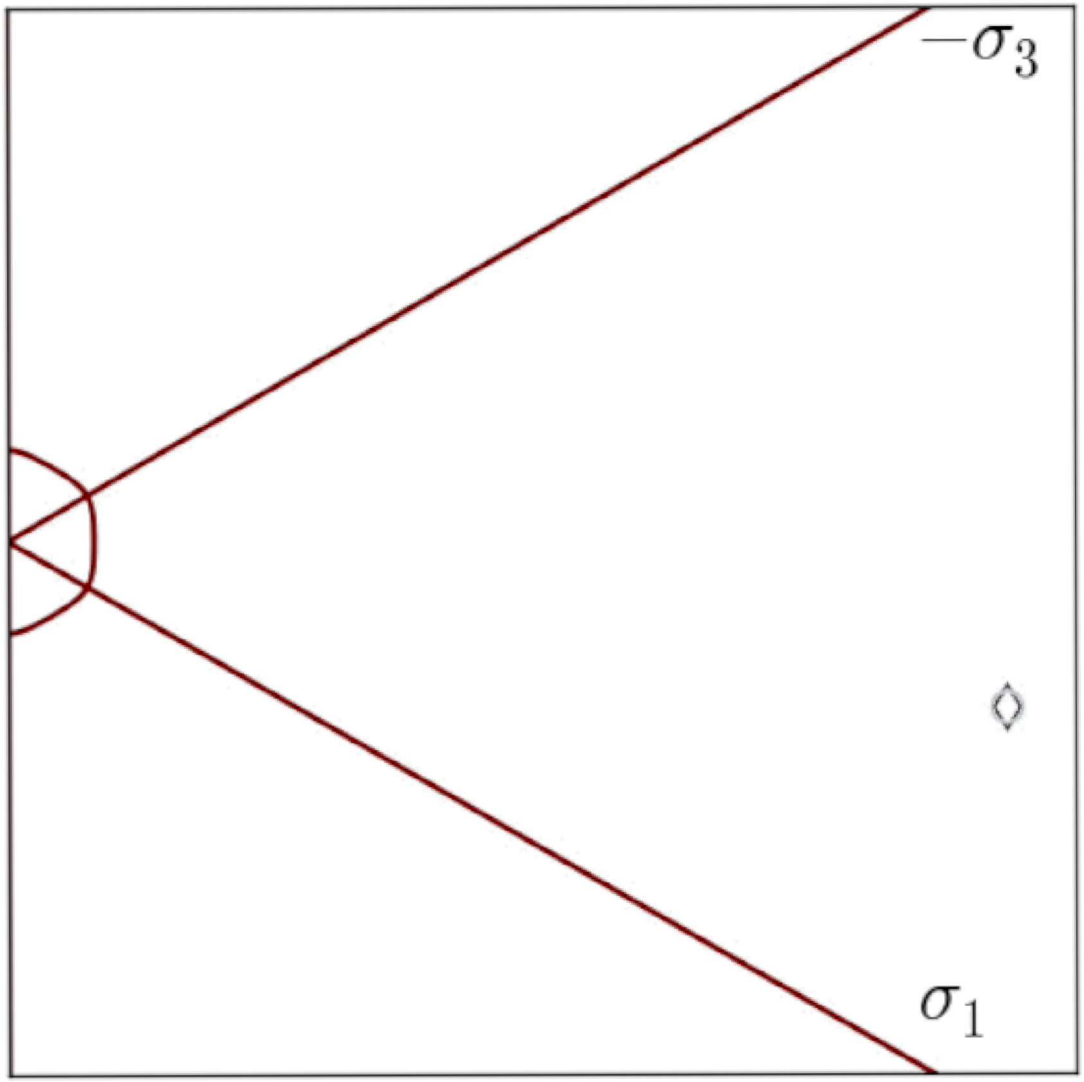
$$\psi\left(r_I\right) = \frac{1}{2} D^1_{JK} r_K D^1_{JL} r_L$$

$$D^1_{IJ} = \begin{bmatrix} c^{N\varepsilon} c^{W\varepsilon} \mathbb{I}_{ijkl} & 0_{ij} \\ 0_{ij} & c^{Nf} c^{Wf} \end{bmatrix} \begin{array}{l} c^{N\varepsilon},\ c^{Nf} \rightarrow \text{Normalization} \\ c^{W\varepsilon},\ c^{Wf} \rightarrow \text{Weight} \end{array}$$

- With an equal weighted, stress-normalization

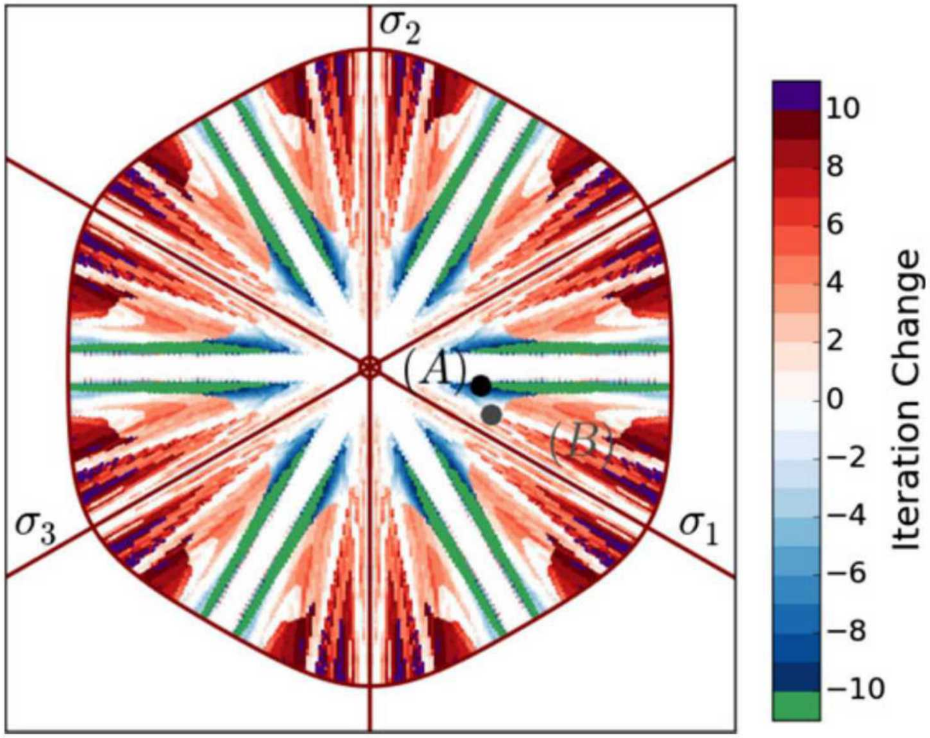
$$\psi\left(r_I\right) = \frac{1}{2} \left(\left(\frac{E}{\sigma_y^0} \right)^2 r^{\varepsilon}_{ij} r^{\varepsilon}_{ij} + \left(\frac{r^f}{\sigma_y^0} \right)^2 \right)$$

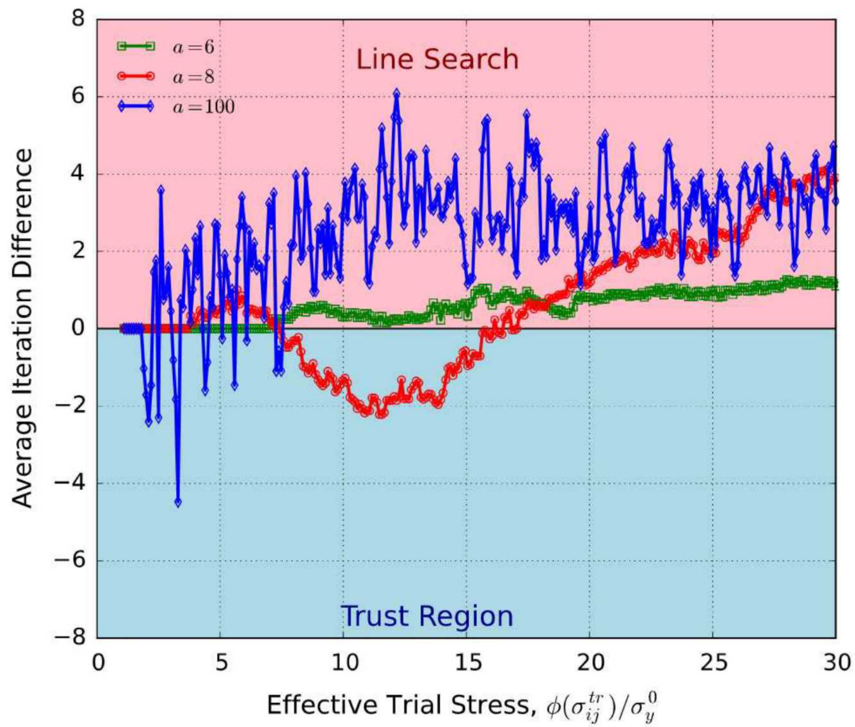
Trust-Region Return Trajectory



Method Comparison

Iter(TR) – iter(LS-NR)





- LS-NR generally outperforms TR based approach
- Preferential algorithms depend on loading state

Weighting Function Definition

- For current cases consider a two effective stress definition

$$\phi\left(\sigma_{ij}, N\right) = \zeta\left(N\right)\phi^{(1)}\left(\sigma_{ij}\right) + \left(1 - \zeta\left(N\right)\right)\phi^{(2)}\left(\sigma_{ij}\right)$$

$$\frac{\partial \phi}{\partial N} = \frac{\partial \zeta}{\partial N}\left(\phi^{(1)} - \phi^{(2)}\right)$$

- For weighting functions want:
  - Non-zero initial derivatives
  - Satisfy positivity constraints
  - Eventually saturate
  - Continuous

$$\zeta = \exp\left(-kN\right) \qquad N\left(\eta\right) = \frac{1}{2}P^{\mathrm{mod}}\eta^2$$

$k,\ P^{\mathrm{mod}}$ Fitting constants