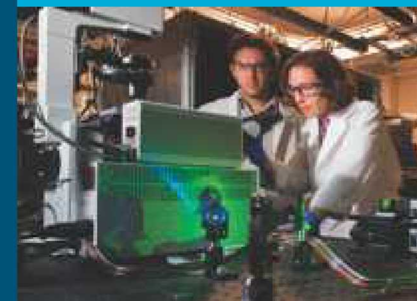
SAND2018-6615PE

Constitutive Modeling: An Introduction



William M. Scherzinger

Brian T Lester

Solid Mechanics
Sandia National Laboratories

NOMAD Institute
Albuquerque, NM
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What is a Constitutive Model?

- "Constitutive model" is an oft used but infrequently defined term

- Meaning and interpretation often vary by individual
  - Constitutive equations are, "… equations characterizing the individual material and its reaction to applied loads… they describe the macroscopic behavior resulting from the internal constitution of the materials." (L. E. Malvern, 1969, *Introduction to the Mechanics of a Continuous Media*)

  - Constitutive equations "… relate the stress tensor and the heat-flux vector to the motion." (C. Truesdell and Noll, 2004, *The Non-Linear Field Theories of Mechanics*)

  - Constitutive relations "…relate stress to displacement (more particularly, to the strain that is derived from the displacement)… Such relations are characteristic of the materials or materials of which the body is made…" (J. Lubliner, 2008, *Plasticity Theory*)

What is a Constitutive Model?

- "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)

- Commonly provides closure relation(s) connecting field variables

- Different models are needed for different physics/materials

- Variety of approaches to developing/deriving constitutive models

Closure relations

- Constitutive models often referred to as "closure relations" – Why?

- Typical BVP requires solving for stress, strain, and displacement
  - 6 strain components, ε_{ij}
  - 6 stress components, σ_{ij}
  - 3 displacement components, u_i

Kinematics

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \quad \text{6 Eqn.}$$

Equilibrium

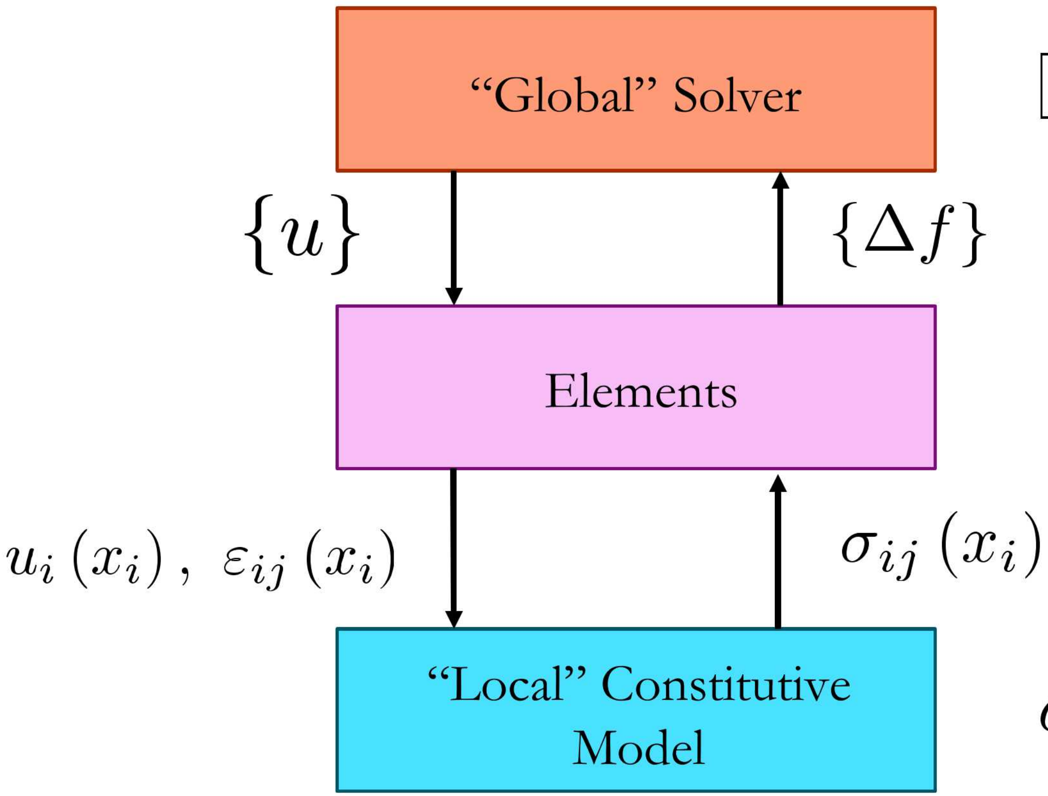
$$\sigma_{ij,j} + \rho b_i = \rho \ddot{u}_i \quad \text{3 Eqn.}$$

- Physically derivable relations (kinematics, equilibrium) yield **only 9 equations for 15 unknowns**

- Constitutive equations provide the final 6 equations to close the system that is specific to the response of the body
  - Isotropic vs. anisotropic? (Same response in all directions or not?)
  - Homogeneous vs. heterogeneous? (Comprised of one material or many?)

Constitutive Models in FEA

- Most modern analysis performed via finite element analysis (FEA)
- What role do constitutive models play in FEA?
  - Displacements found via "global" solver enforcing equilibrium
  - Constitutive models solve "local" problem connecting stress to displacement



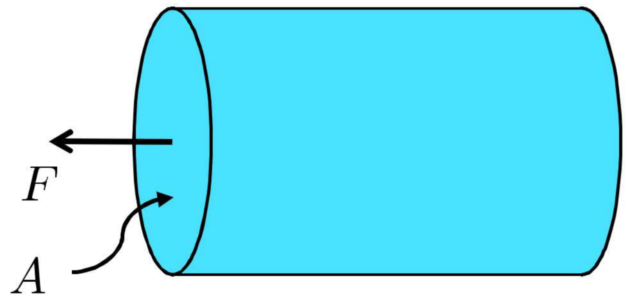
$$[K]\{u\} = \{\Delta f\}$$

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

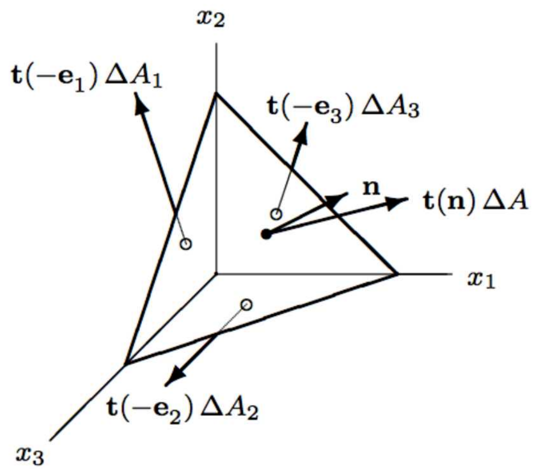
Stress

- Classically, force per unit area

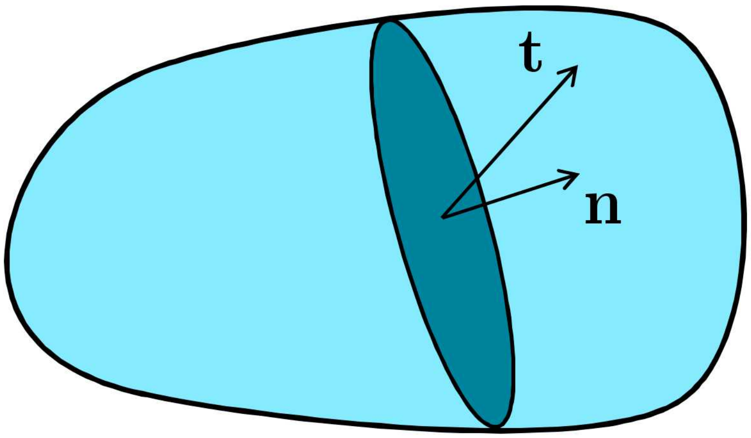
$$\sigma = \frac{F}{A}$$



- More completely, stress is a rank two tensor mapping a vector to a vector
  - The stress relates the traction (force per unit area) to the normal to the area (geometry)



(J. Lubliner, 1990, *Plasticity Theory*)



$$t_i = \sigma_{ji} n_j$$

Outline

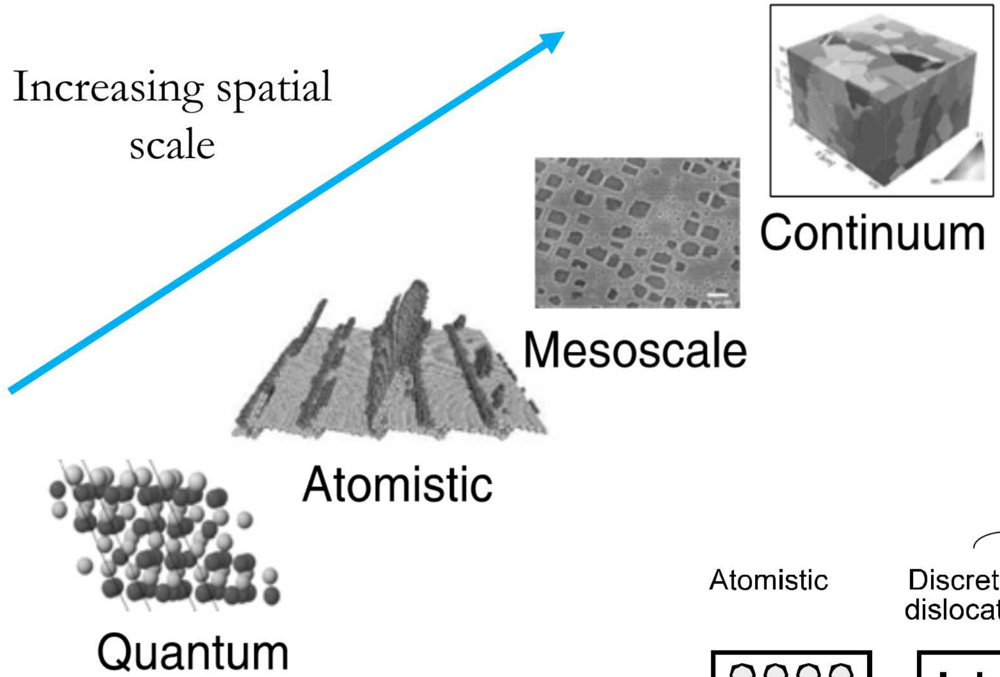
- Methods for development of constitutive models

- Constitutive model examples/utilization
  - Survey of common models/types
  - Example case: metal plasticity

- Open research topics
  - Numerical integration of constitutive models
  - Development of distortional hardening plasticity model

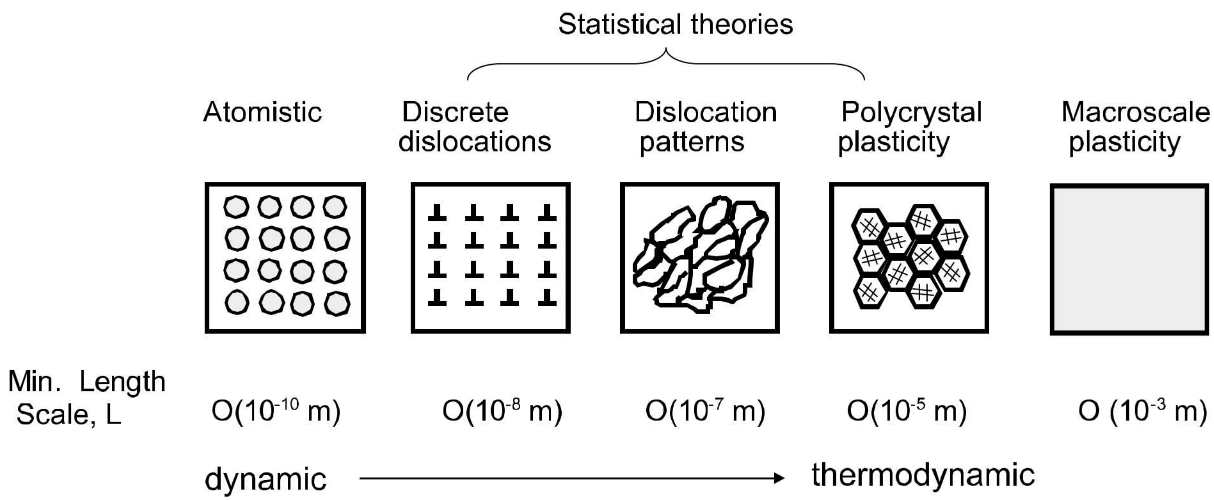
Constitutive Model Development

Multiscale Modeling



- Multiscaling modeling "upscales" (homogenizes) information
- Allows for detailed physics representations

- Lower scale models can be expensive



(Figures from D. McDowell, 2010, *IJP*, **26**, pp. 1280-1309)

Material Modeling – Atomistic Scale

- Methodologies explicitly resolve forces between different atoms/molecules (e.g. molecular dynamics)

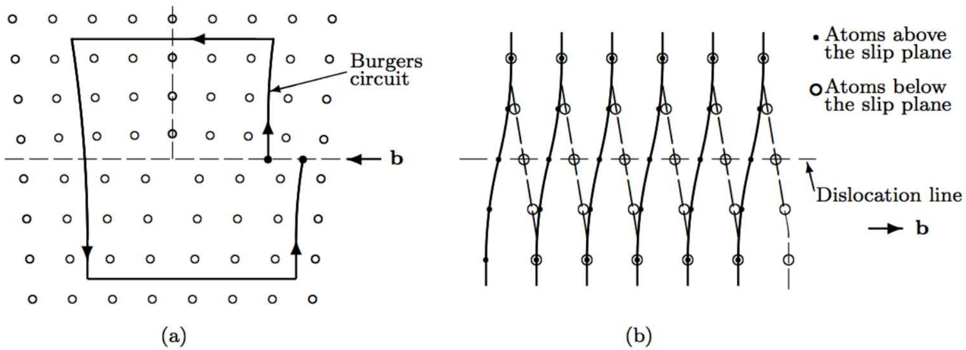


Figure 2.2.6. Dislocation in a crystal: (a) edge dislocation; (b) screw dislocation.

(J. Lubliner, 1990, *Plasticity Theory*)

- *Limitation*: Cost in resolving both spatial and temporal scales
  - Modeling 1cm^3 of material requires order of 10^{22} atoms
  - Small size scale/cost also typically restricts analysis to short time scales

Material Modeling – Dislocation Scale

- Methodologies (e.g. dislocation dynamics) study impact/interactions of dislocation(s) on response
- Resolution on the scale of crystal lattice(s)
- One cm^3 of material can have order of km of dislocation motion

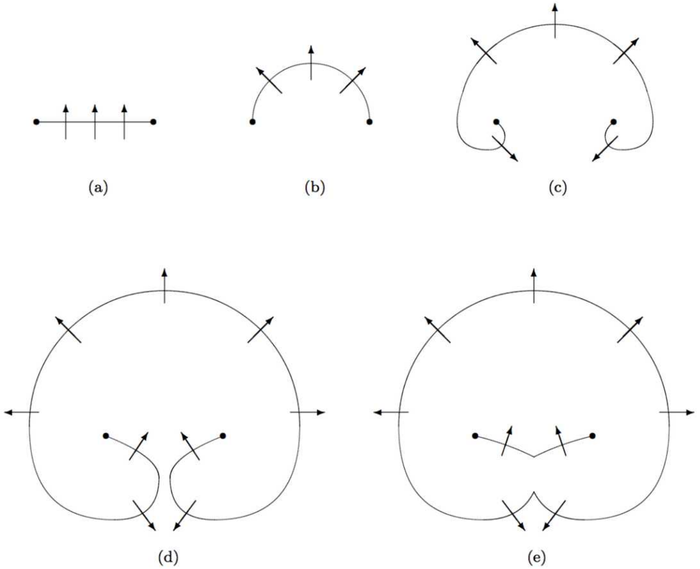
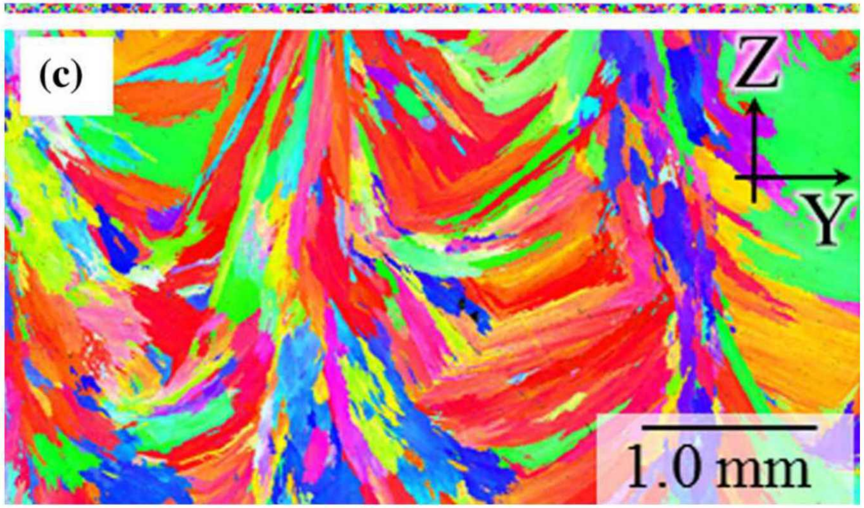


Figure 2.2.8. Frank–Read source (after Read [1953]).

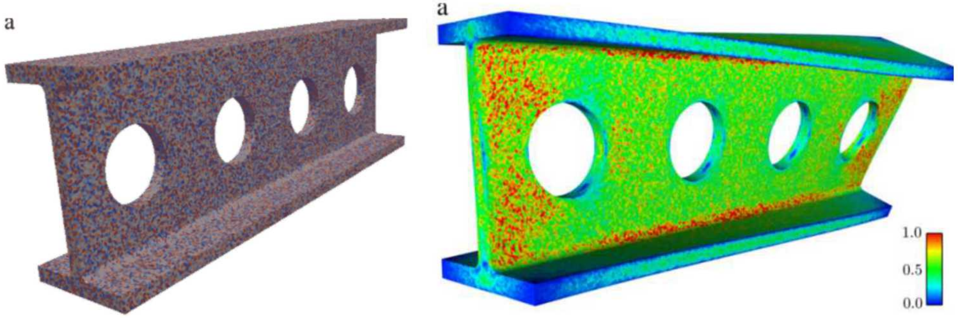
(J. Lubliner, 1990, *Plasticity Theory*)

Material Modeling – Mescoscale

- Mesoscale models focus on resolving microstructure
  - Polycrystalline texture
  - Inhomogenieties
- Polycrystalline materials
  - Grain sizes ~ order one to hundreds of micrometers
  - 10^6 to 10^{12} grains per cm^3
- Methodologies include
  - Analytical (Eshelby's method)
  - Direct numerical simulation



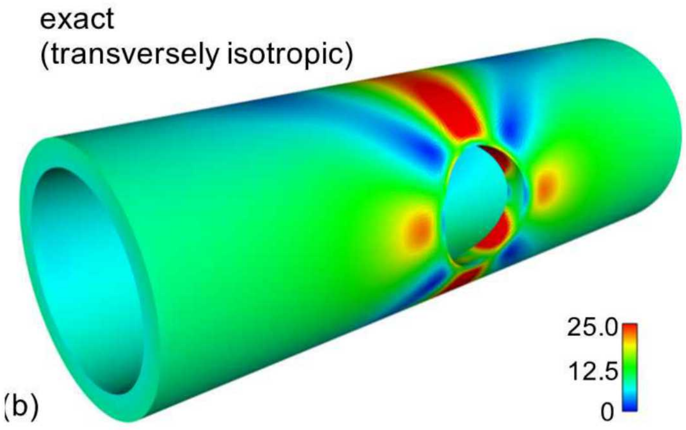
(Brown *et al.*, 2017, *MMTA,* **48A**, p. 6055-6069)



(Bishop *et al.*, 2015, *CMAME,* **287**, p. 262-289)

Material Modeling – Continuum Scale

- Continuum scale models seek to analyze structures
- Each analysis point encapsulates all of the lower scale features previously identified
- Typical scale of interest to constitutive models



(Bishop and Brown, 2018, *CMAME*, Accepted)

- Development of constitutive models can rely upon:
  - Upscaling/bridging the scales to homogenize lower scale results
  - Deriving mathematical relationships of phenomena of interest (phenomenological modeling)

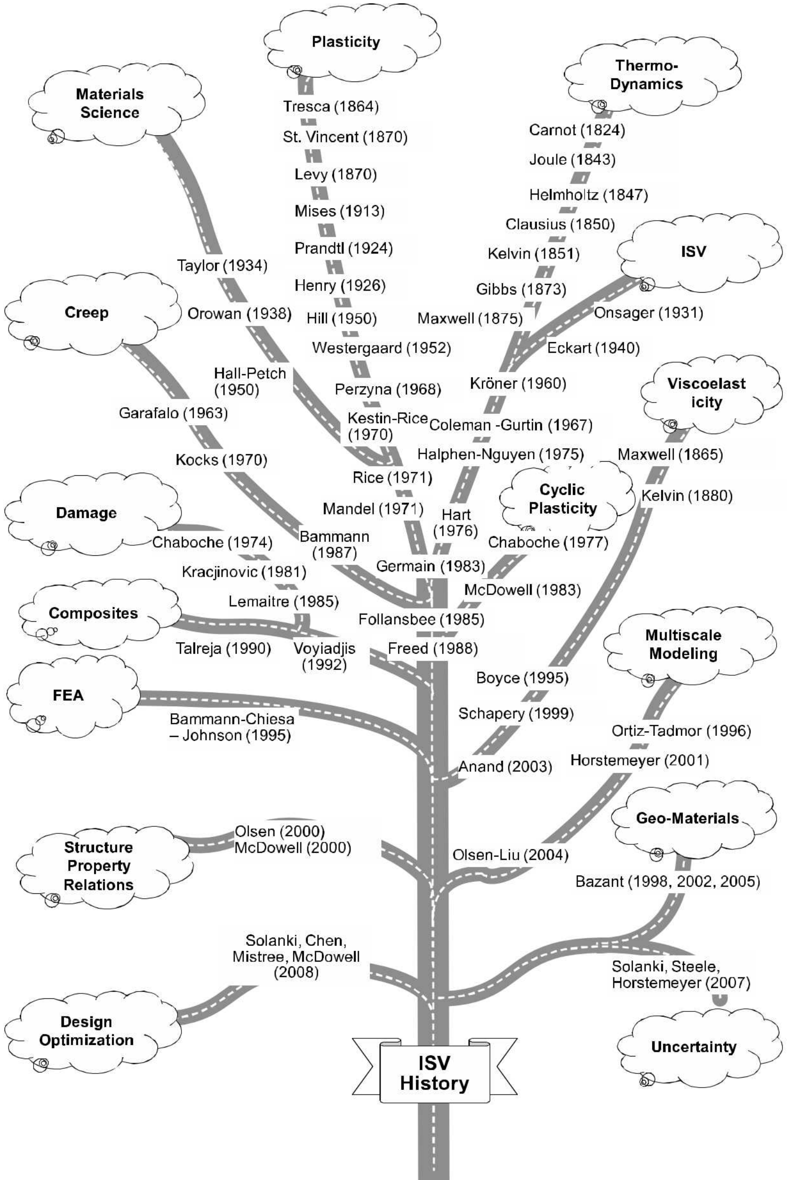
Phenomenological Modeling

- Experiments may also be used characterize a materials response to different stimuli
  - However, for history-dependent materials, "…an infinite number of experiments would be needed to quantify its response." (J. Fish, 2014, *Practical Multiscaling*, Wiley)
  - Instead characterize and understand *phenomena*

- *Phenomenological modeling* focuses on constructing mathematical models capable of describing specific physical phenomena
  - Seek to accurately and efficiently describe *relevant* phenomena
  - Variety of ways to develop constitutive model
    - Explicit curve fitting
    - Continuum thermodynamics/internal state variable (ISV)
      - Coleman and Noll, 1963, *ARMA*, **13**, pp. 167-178
      - Rice, 1971, *JMPS*, **19**, pp. 433-455
      - Horstmeyer and Bammann, 2010, *IJP*, **26**, pp.1310-1334

ISV Phenomenological Modeling

- ISV phenomenological models exist for wide range of materials/physics
- Development/utilization of model requires:
  - Theoretical formulation
  - Solution/computational Implementation
  - Calibration procedure
- All three elements needed for appropriate model usage



(Figure from Horstmeyer and Bammann, 2010, *IJP*, **26**, pp.1310-1334)

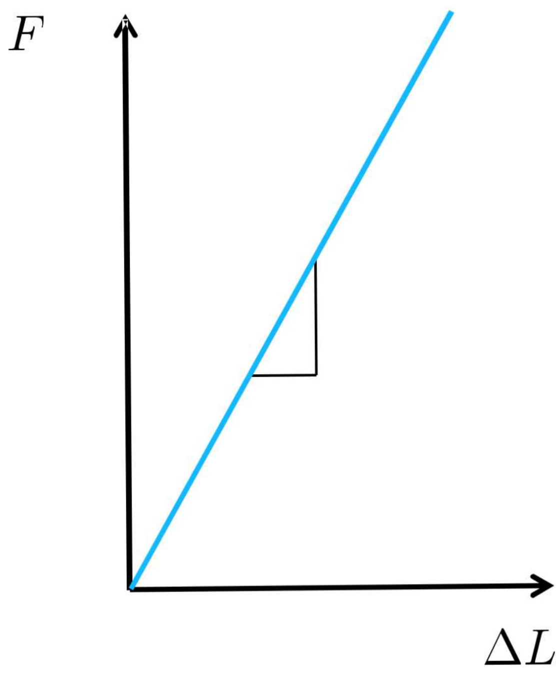
Constitutive Model Examples

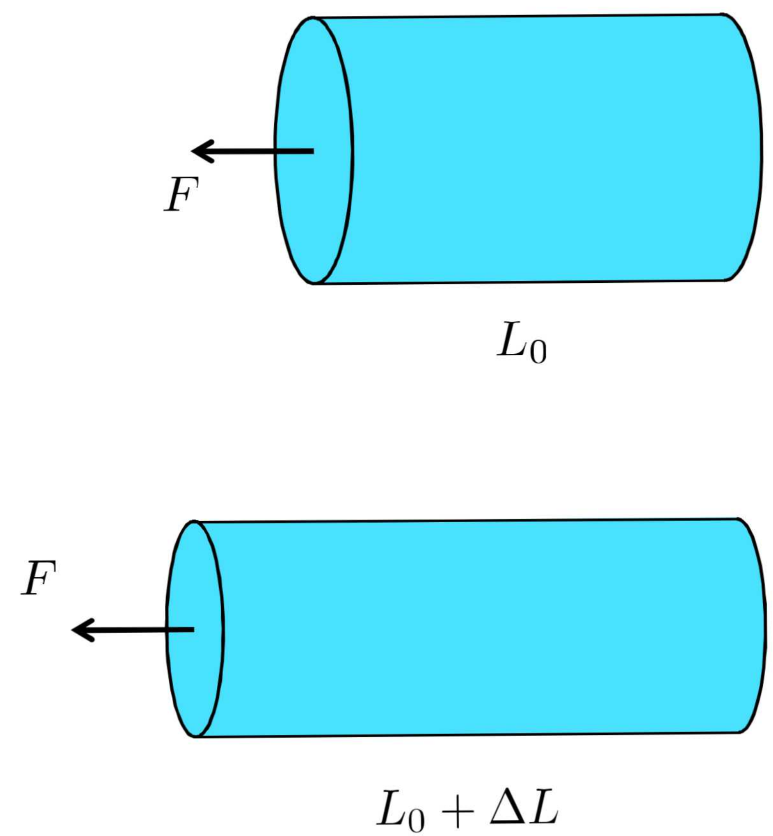
Common Constitutive Models

- Literature is replete with examples of constitutive models
  - Posed for different phenomena/combinations of phenomena
  - Often multiple models exist for same phenomena
- (Some) common classes of constitutive models
  - Elastic
  - Viscoelastic
  - Plastic
  - Viscoplastic
  - Geomechanics
  - Micromechanics/composites
- Each class may have multiple variants/types
  - Finite vs. infinitesimal deformations
  - Isotropic vs anisotropic
  - Etc…

Elastic

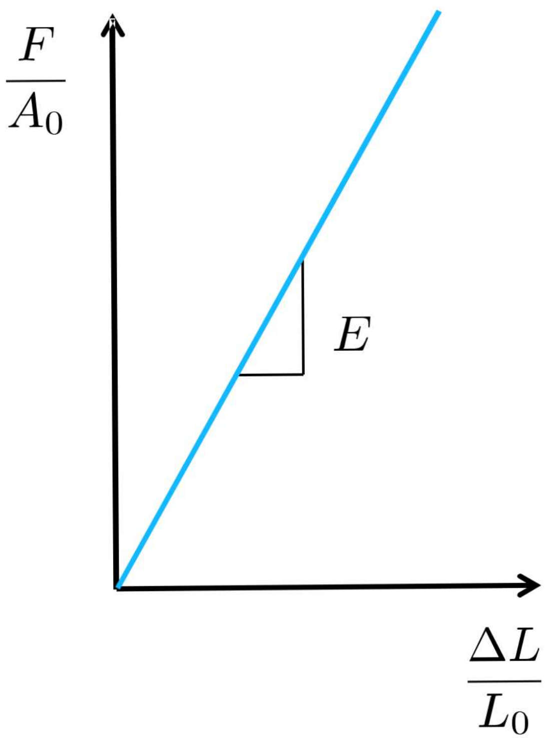
- Axial force is proportional to axial elongation

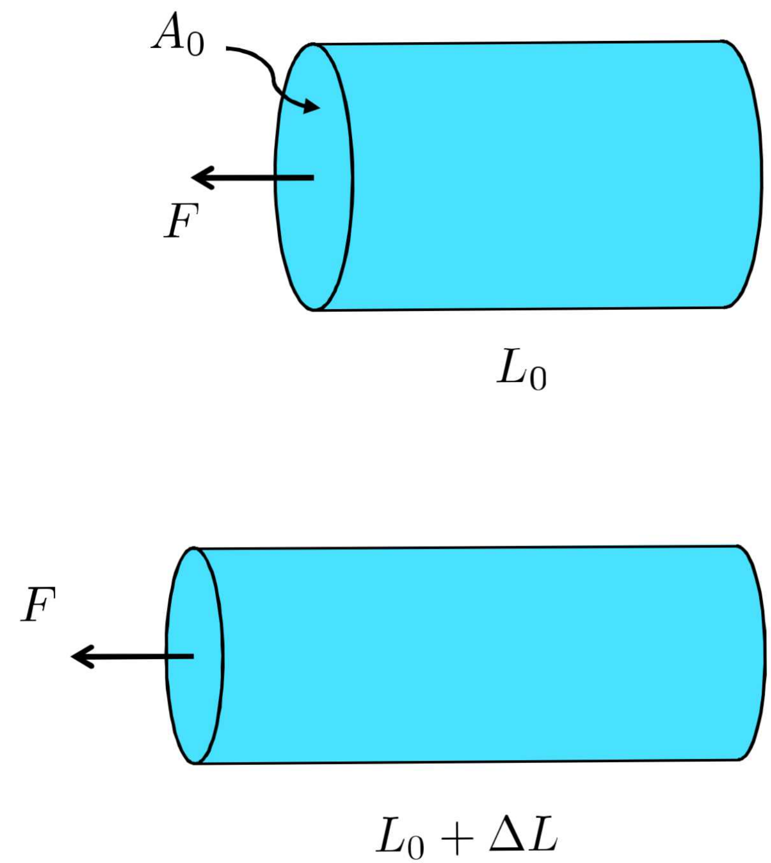




Elastic

- Axial *stress* is proportional to axial *strain*





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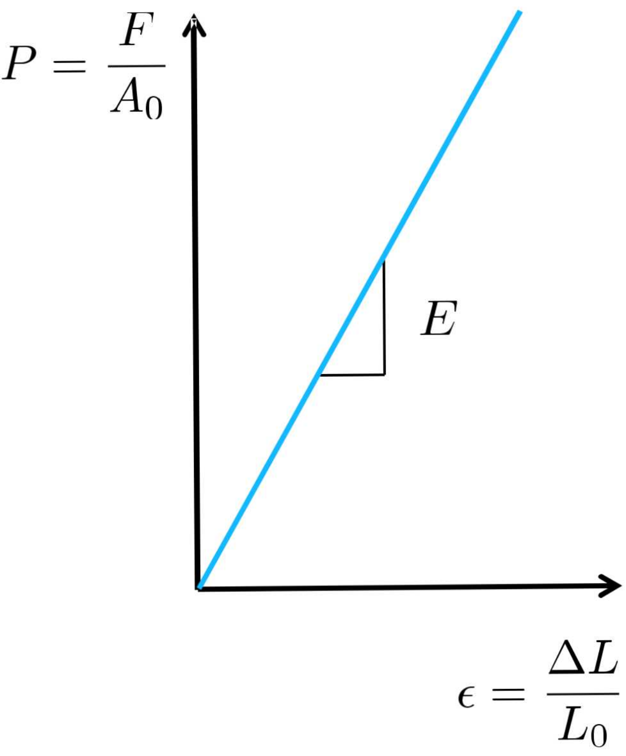
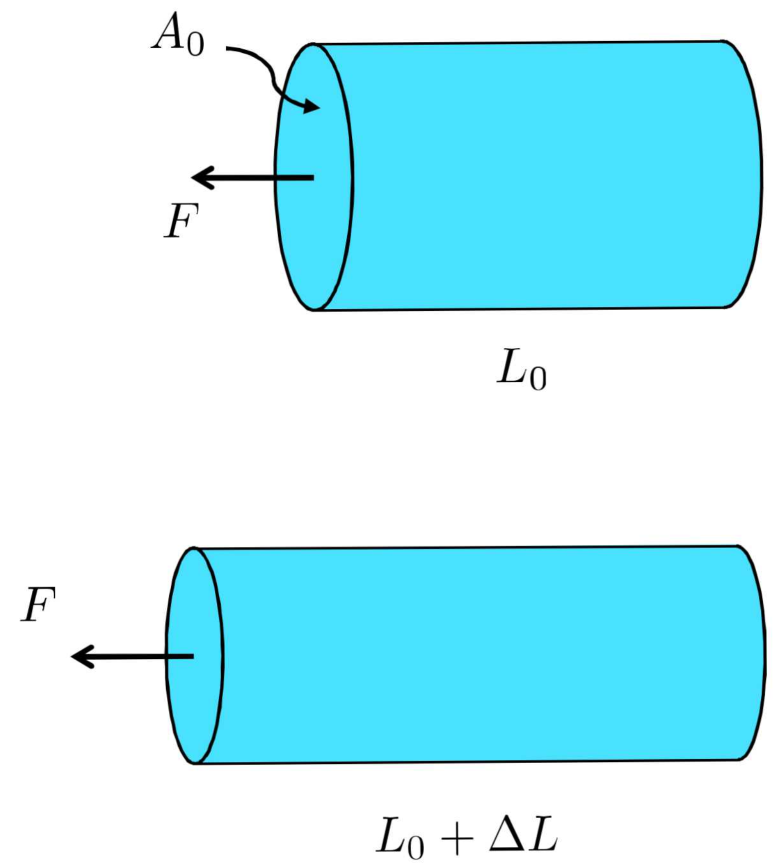
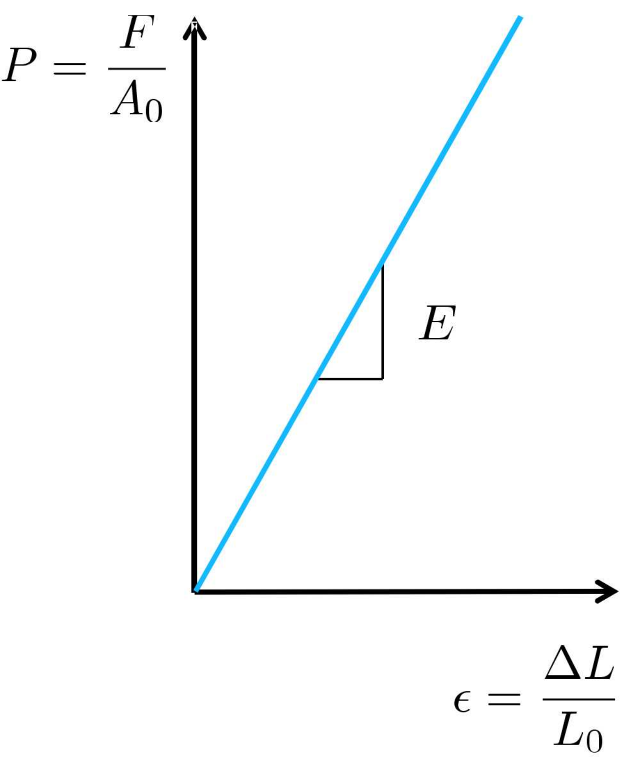


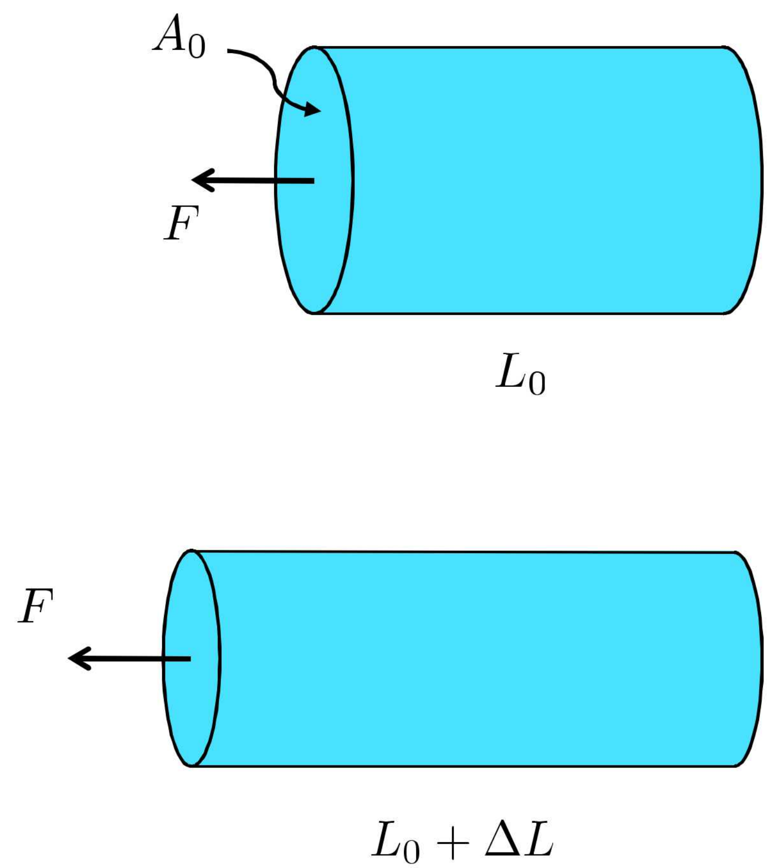


Elastic

- Axial *stress* is proportional to axial *strain*
- Linear relationship → no history dependence
- Propose corresponding model



$$P = E\epsilon$$



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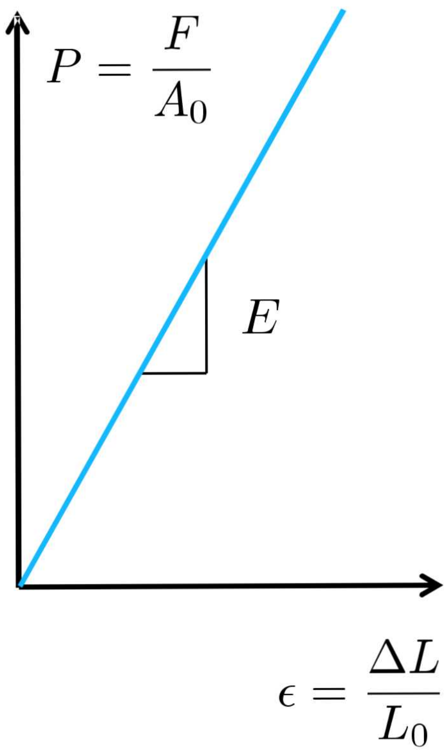


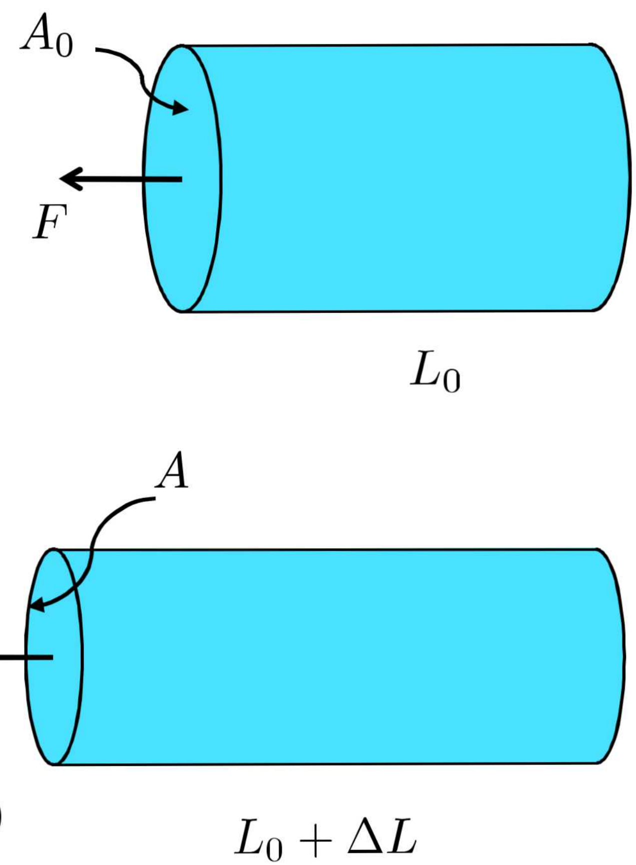
True Stress:

$$\sigma = \frac{F}{A}$$

True Strain:

$$d\varepsilon = \frac{dL}{L}$$

$$\varepsilon = \int_{L_0}^{L_0+\Delta L} \frac{dL}{L} = \ln(1+\varepsilon)$$



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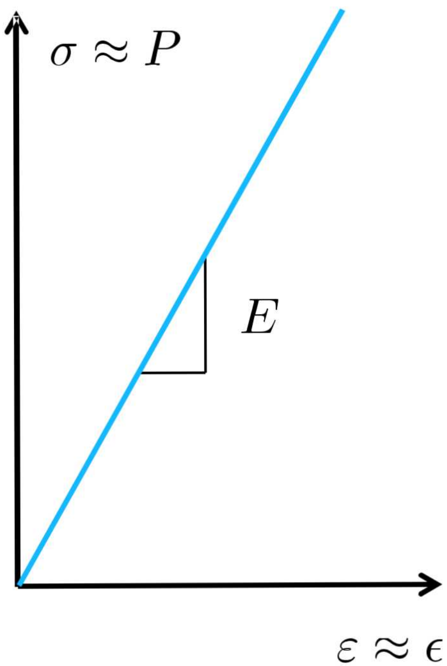

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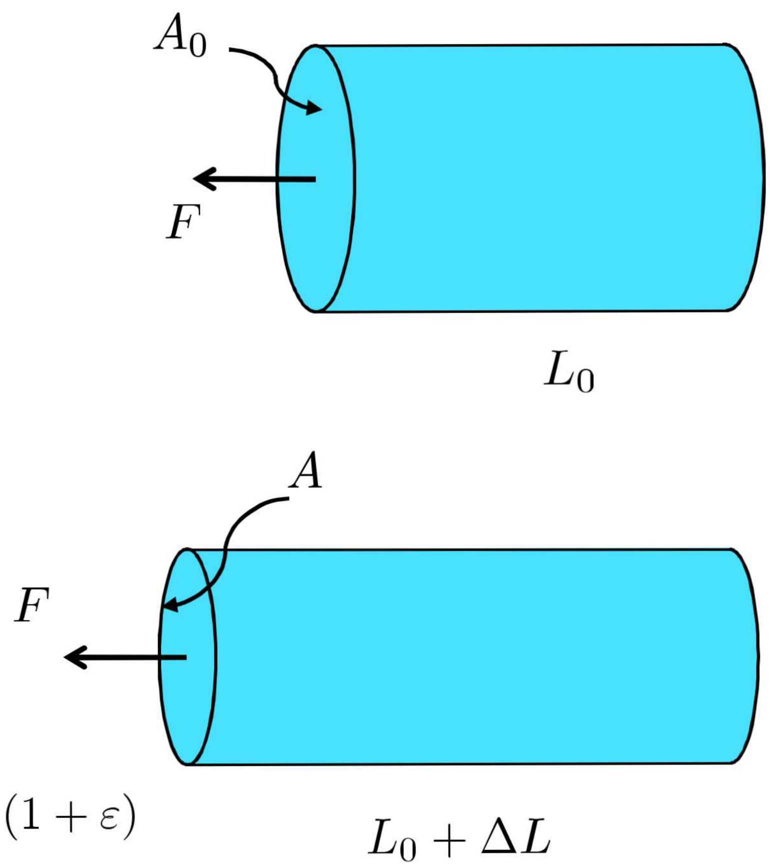
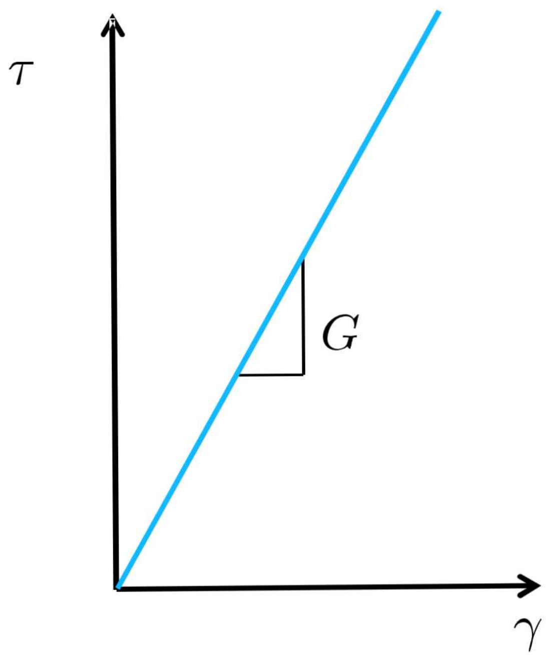
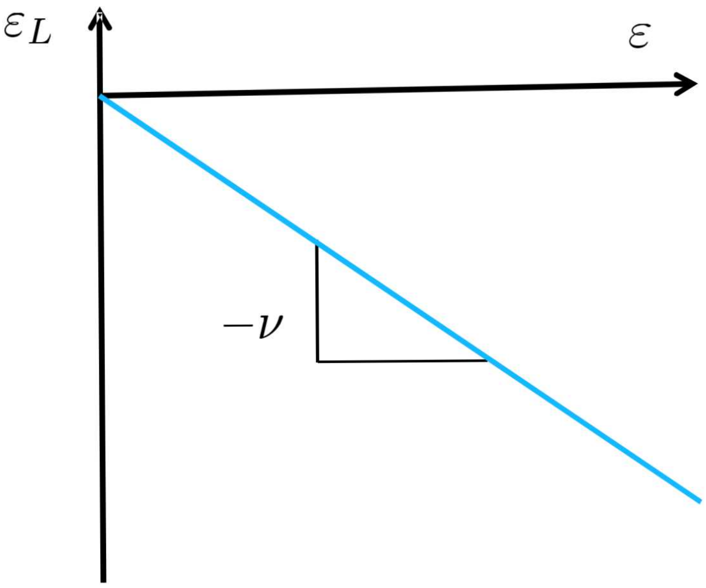


Elastic

Shear Response



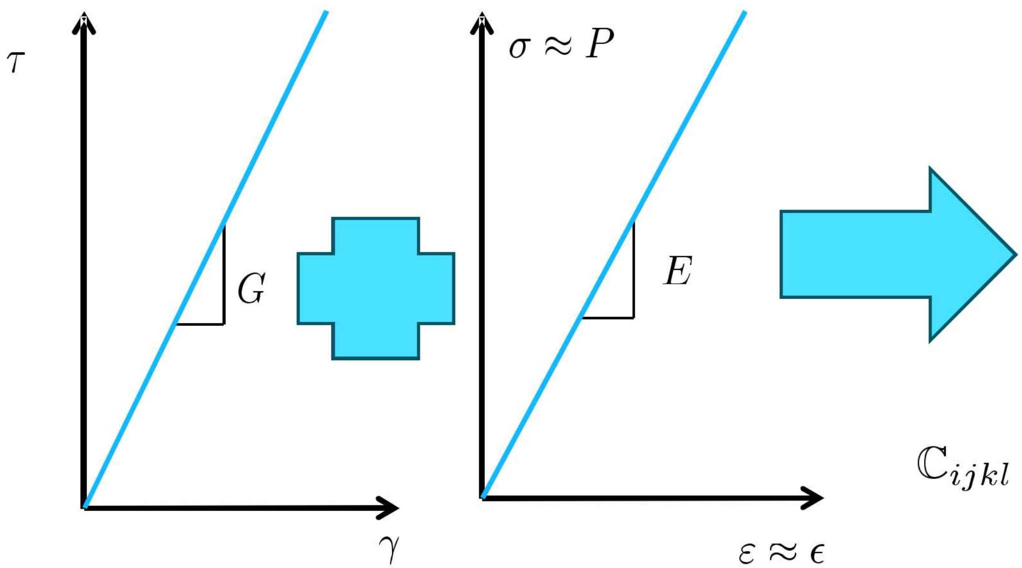
Lateral Strains



$$\nu = \frac{E}{2G} - 1$$

Elastic

- Combining previous observations can be used to determine 3D constitutive form



$$\sigma_{ij} = \mathbb{C}_{ijkl}\varepsilon_{kl}$$

$$\mathbb{C}_{ijkl} = \frac{E}{1+\nu}\left[\frac{\nu}{1-2\nu}\delta_{ij}\delta_{kl} + \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\right]$$

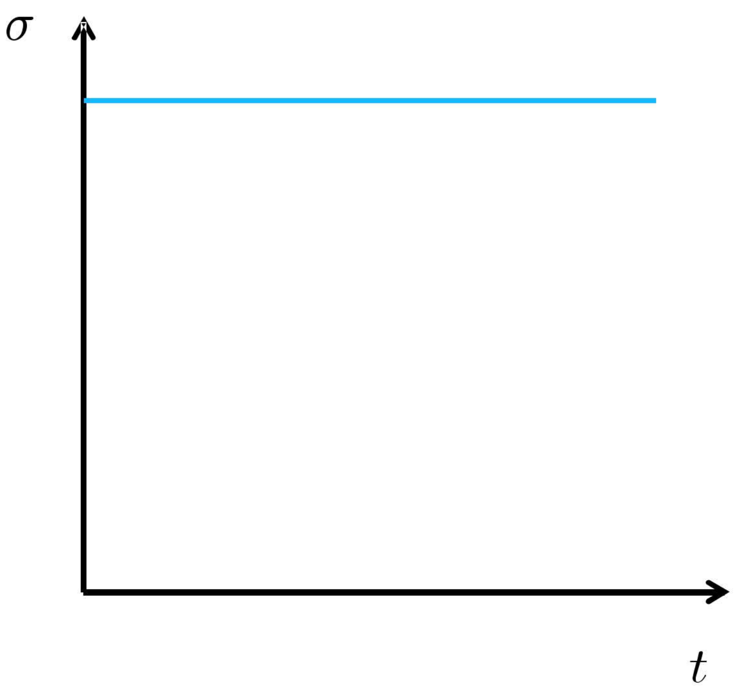
$$\mathbb{C}_{ijkl} = K\delta_{ik}\delta_{jl} + G\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right)$$

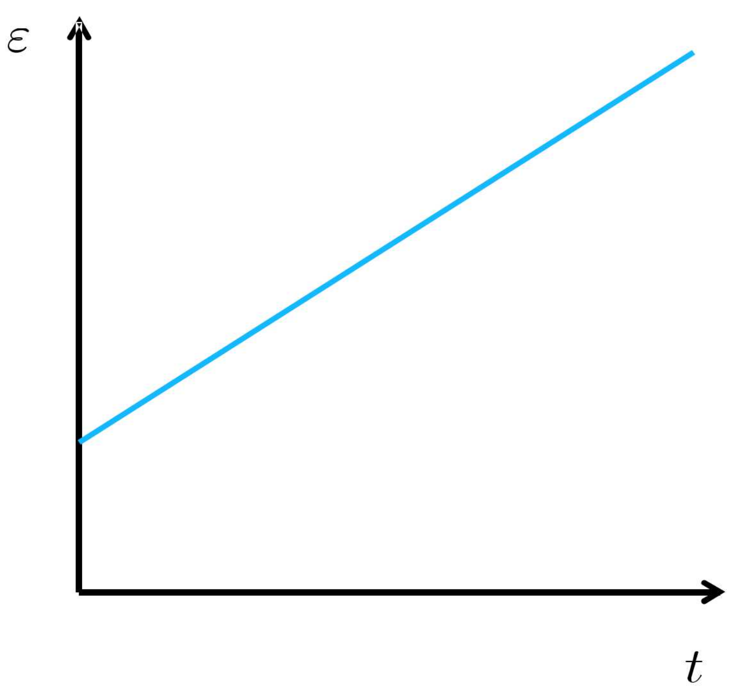
Bulk Shear

Viscoelasticity

- Viscoelastic materials exhibit history dependence
  - Stress/strain functions of *time*
  - Linear viscoelasticity: stress proportional to strain rate, $\sigma \propto \dot{\varepsilon}$
- Common for amorphous materials (e.g. polymers, glasses)
- Two common characteristic responses

Creep





(See Christensen, 1982, *Theory of Viscoelasticity*, for details)

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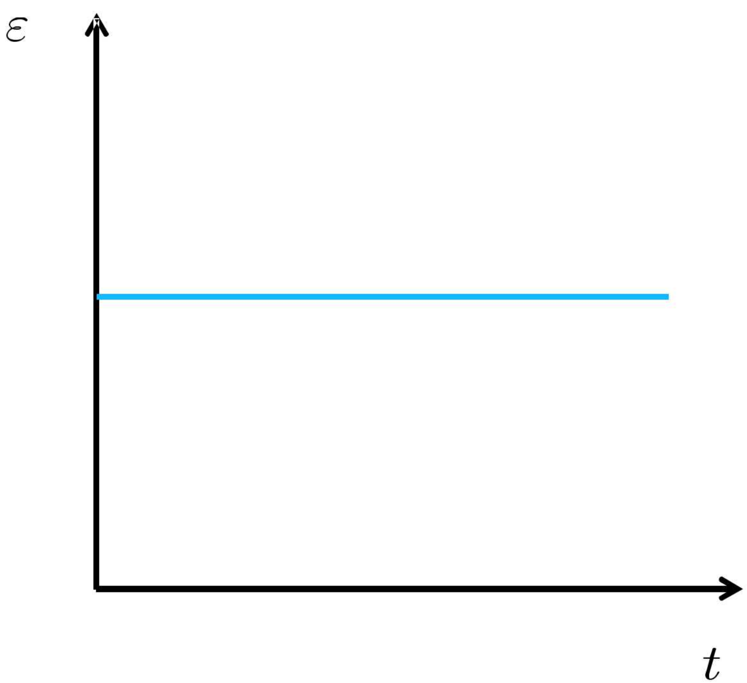
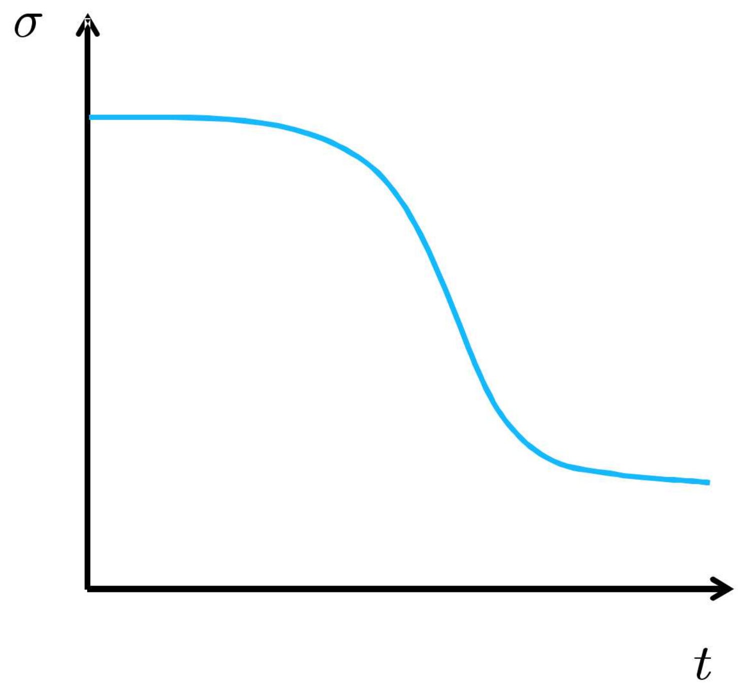
Stress Relaxation

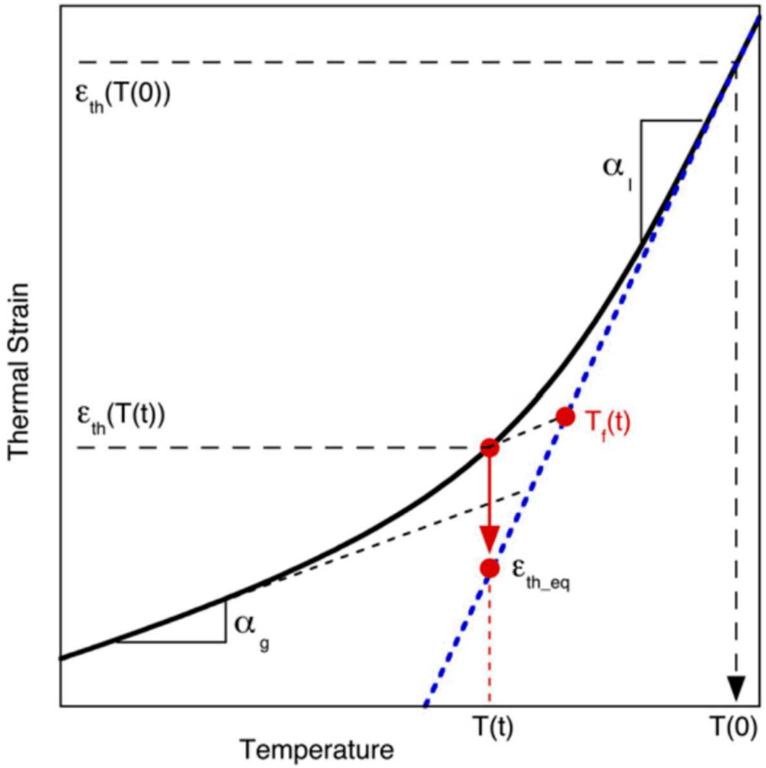


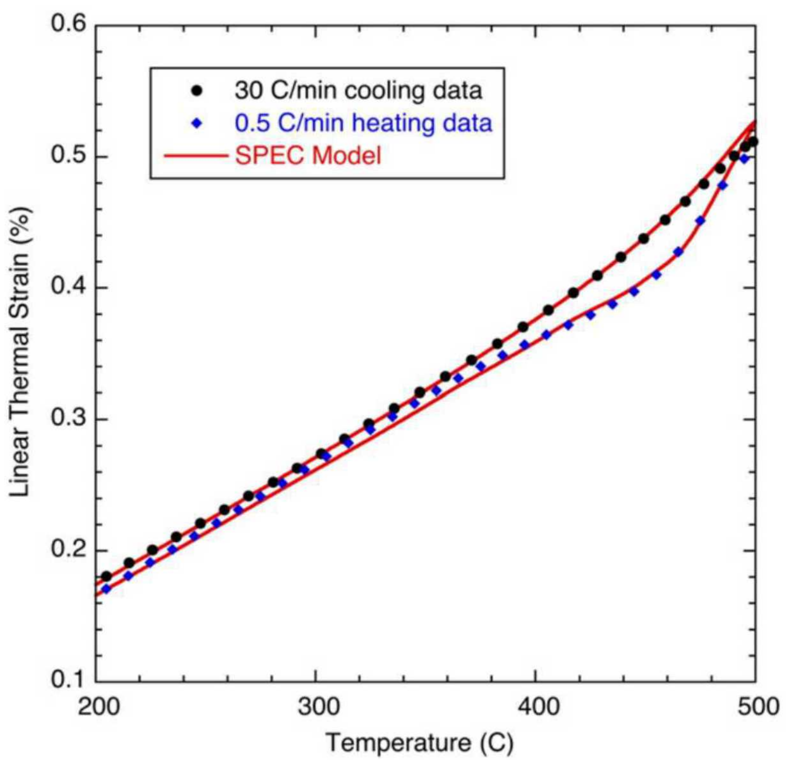


(See Christensen, 1982, *Theory of Viscoelasticity*, for details)

Nonlinear Viscoelasticity

- Nonlinear theories of viscoelasticity exist in literature
  - Capture complex, large-deformation behavior
  - Treatment of glass transition
  - E.g., "Potential Energy Clock" Model of Caruthers, Adolf, Chambers, and Shrikhande, 2004, *Polymer*, **45**, pp. 4577-4597

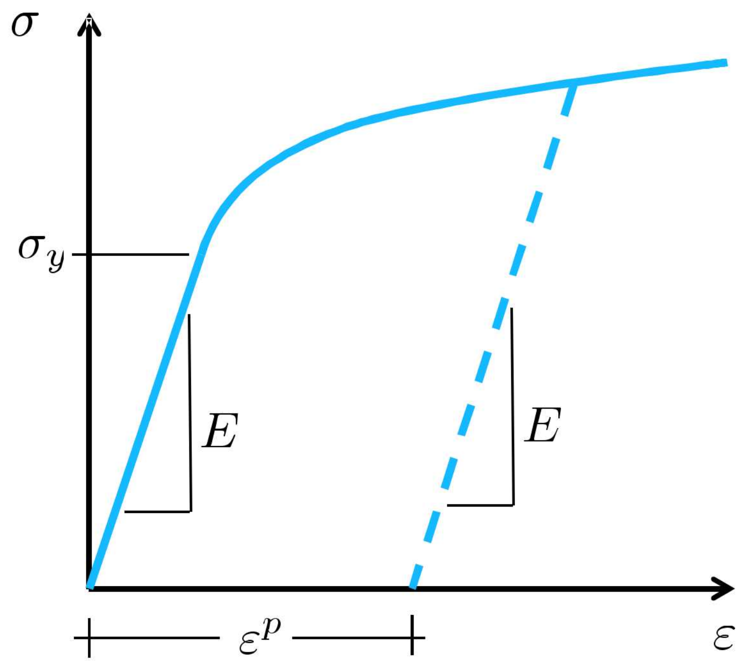




(Figures from Chambers *et al.*, 2016, *Jrnl. Non-Crystl. Solids*, **432**, pp. 545-555)

Elastic-Plastic

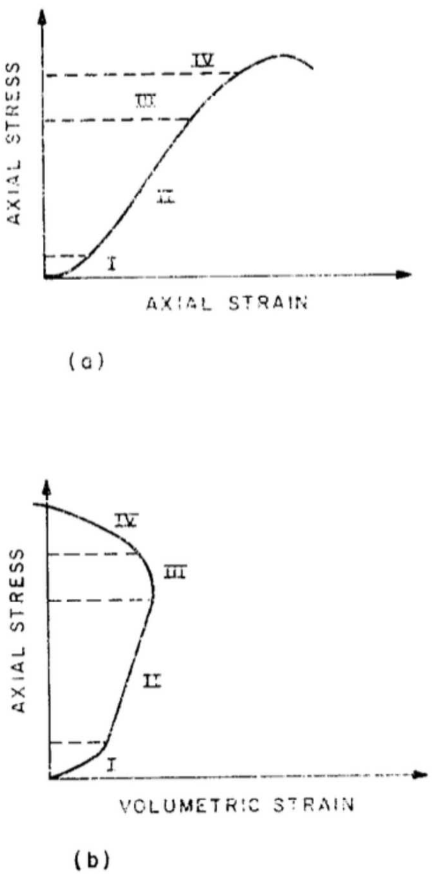
- Permanent deformations arising from dislocation motion (slip)
- Common for metals
- One of most popular/common class of material models



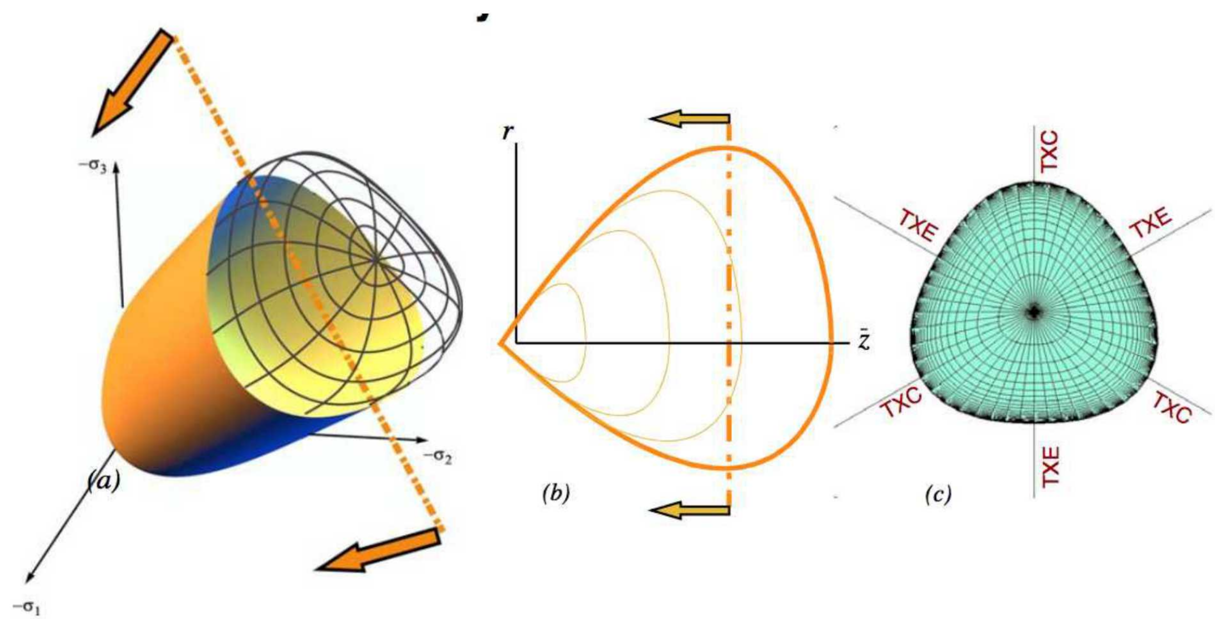
- Material yields at yield stress, σ_y
- Material unloads elastically before AND after yield
- Yielding produces permanent deformation after unload

Geomechanics

- Generally, formulations are complex extensions of plasticity-type models (e.g. pressure sensitivity)



(Rudnicki and Rice, 1975, *JMPS*, **23**, pp. 371-394)



(Brannon, Fossum, and Strack, 2009, SAND2009-2282)

Micromechanics

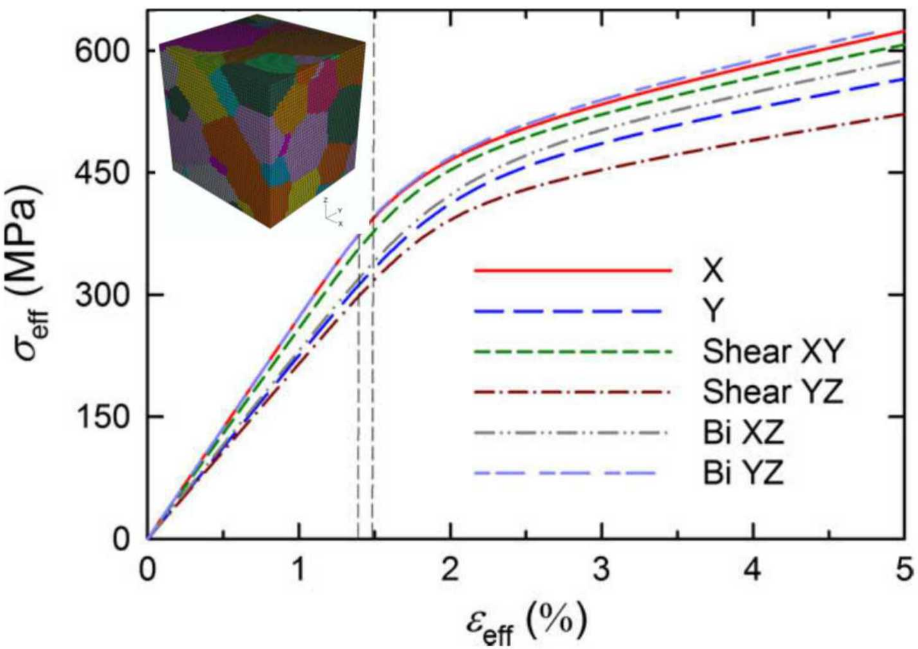
- "Micromechanical" models broad class of models used to describe heterogeneous media (e.g. composites, textured metals etc.)
- Many, many schemes/efforts dedicated to such efforts (see review of Pindera *et al.*, 2009, *Comp: Part B*, 40, pp. 349—378)

Analytical

$$k_{23}^{*} = K_m + \frac{\mu_m}{3} + \frac{c_f}{1/[K_f - K_m + (\mu_f - \mu_m)/3] + c_m/(K_m + 4/3\mu_m)}$$

(Pindera *et al.*, 2009, *Comp: Part B*, **40**, pp. 349--378)

Numerical

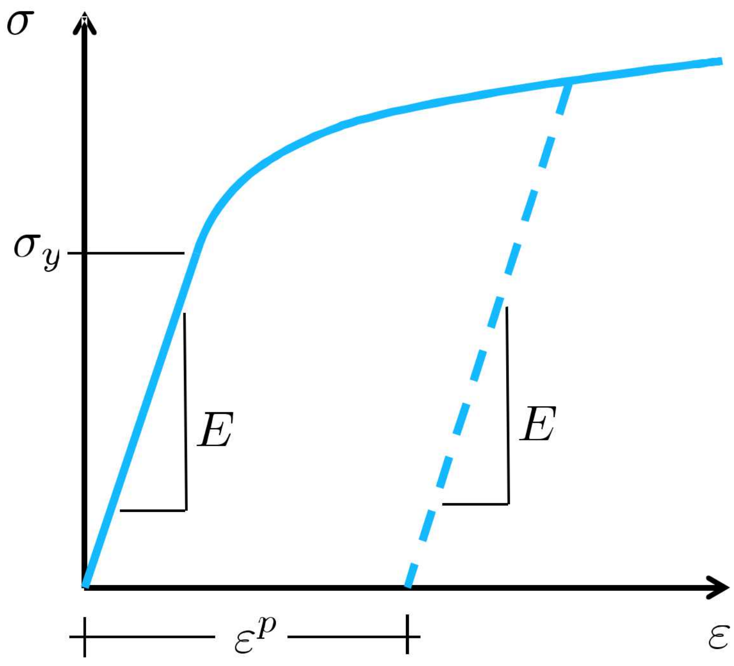


(Qidwai, Lewis, and Geltmacher, 2009, *Acta Mat*, **57**, pp. 4233--4247)

Elastic-Plastic

- Return to elastic-plastic models and look at some details

$$\sigma_{ij} = \mathbb{C}_{ijkl}\varepsilon^{\mathrm{el}}_{kl} \rightarrow \sigma_{ij} = \mathbb{C}_{ijkl}\left(\varepsilon_{kl} - \varepsilon^{\mathrm{p}}_{kl}\right)$$



- Need to capture:
  - Permanent deformations
  - Description of yield
  - Post-yield stress behavior (hardening)
  - Development of plastic-strain
- All can be derived via continuum thermodynamics
- Then look at structural impact/examples

Yield Function

- Yield surface defines elastic domain in multidimensional state

$$f\left(\sigma_{ij}, \bar{\varepsilon}^p\right) = \phi\left(\sigma_{ij}\right) - \bar{\sigma}\left(\bar{\varepsilon}^p\right) \qquad ; \qquad \bar{\sigma}\left(\bar{\varepsilon}^p\right) = \sigma_y^0 + K\left(\bar{\varepsilon}^p\right)$$

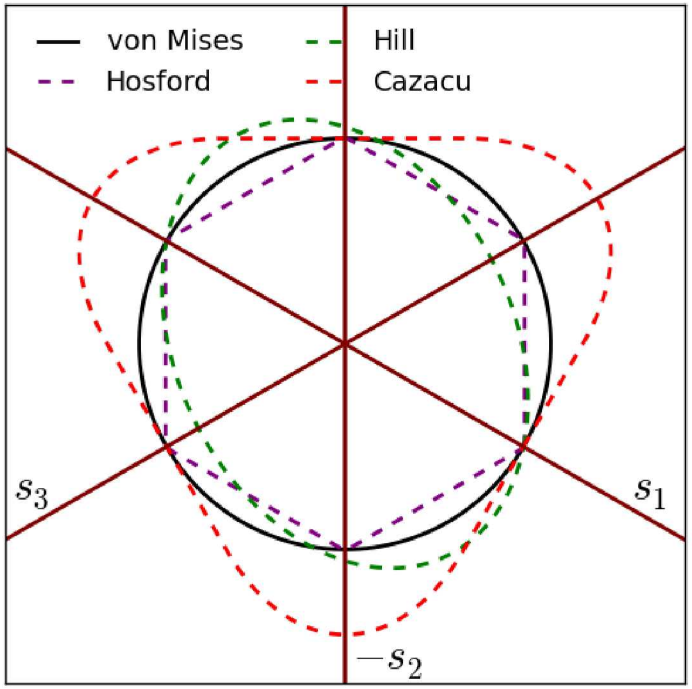
Effective Stress

Initial Yield Stress

Hardening Law

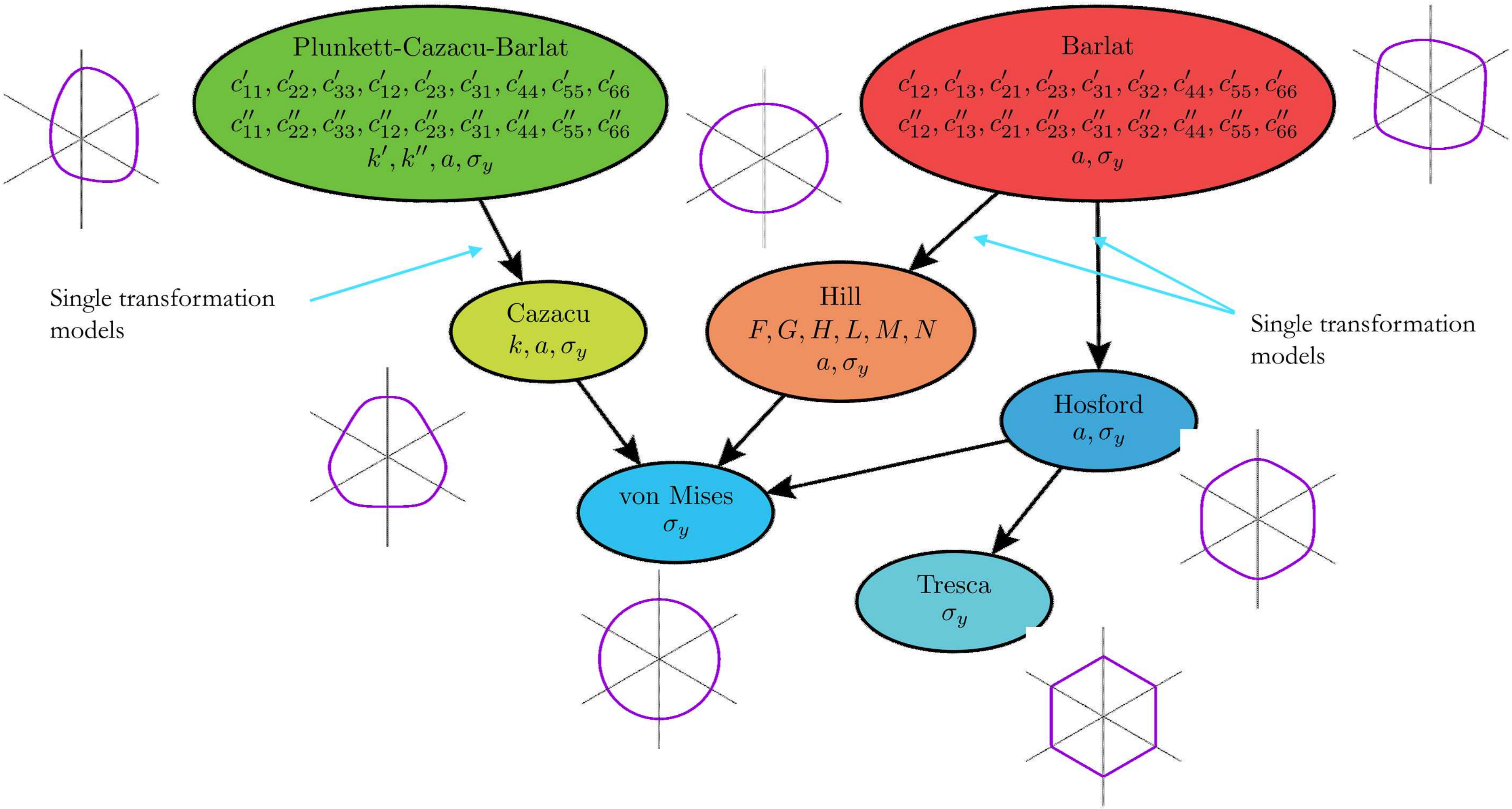
$f < 0 \longrightarrow$ Elastic

$f = 0 \longrightarrow$ Inelastic/plastic



- Enforcing $f = 0$ is referred to as consistency condition
- Enables problem solution

Family of Yield Surfaces



Flow Rule

- Need expression for evolution of plastic strain
- Referred to as flow rule

$$\dot{\varepsilon}^p_{ij} = \dot{\bar{\varepsilon}}^p \frac{\partial \Omega}{\partial \sigma_{ij}}$$

- Plastic potential, Ω

$$\Omega = f \longrightarrow \text{Associative}$$

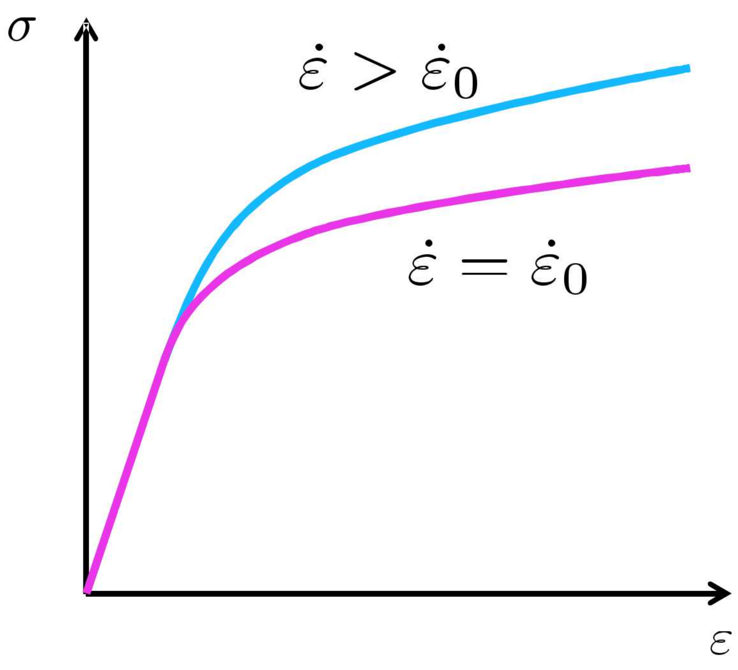
$$\Omega \neq f \longrightarrow \text{Non-associative}$$

- For associative (and most non-associative) yield surface gives *directionality* of plastic flow and strength

Viscoplasticity

- Viscoplasticity is rate-dependent plasticity
- Common example: Johnson-Cook model
  - Johnson and Cook, 1985, *Eng. Fract. Mech.*, 21(1), pp. 31-48

$$\bar{\sigma} = \left(A + B\varepsilon_p^n\right)\left(1 + C\ln\left(\dot{\varepsilon}/\dot{\varepsilon}_0\right)\right)\left(1 - T^{*\,m}\right)$$



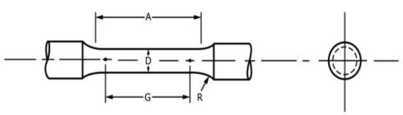
- Strain rate increases yield
- Temperature decreases yield

Uniaxial Tension

- Look at the response of a uniaxial tension test-specimen
- Model parameterization
  - Anisotropic parameters correspond to an Al 2090-T3 given by Barlat *et al.* (IJP 2005, **21**, pp. 1009-1039)
  - Consider both a rate independent and rate dependent formulation

Standard Test Methods for Tension Testing of Metallic Materials

E8/E8M − 16a



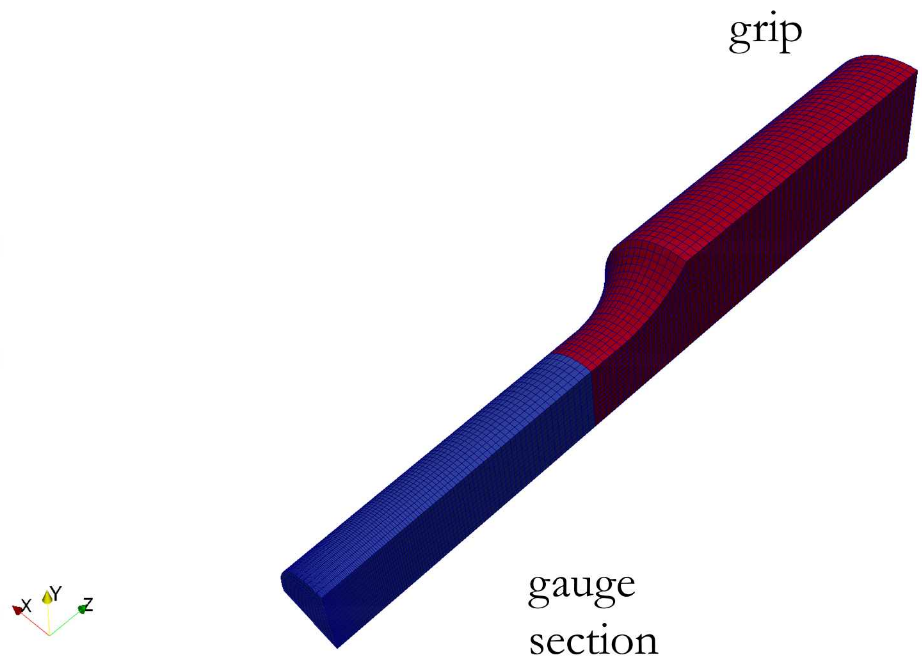
Dimensions, mm [in.]
For Test Specimens with Gauge Length Four times the Diameter [E8]

	Standard Specimen	Small-Size Specimens Proportional to Standard			
	Specimen 1	Specimen 2	Specimen 3	Specimen 4	Specimen 5
G—Gauge length	50.0 ± 0.1 [2.000 ± 0.005]	36.0 ± 0.1 [1.400 ± 0.005]	24.0 ± 0.1 [1.000 ± 0.005]	16.0 ± 0.1 [0.640 ± 0.005]	10.0 ±0.1 [0.450 ± 0.005]
D—Diameter (Note 1)	12.5 ± 0.2 [0.500 ± 0.010]	9.0 ±0.1 [0.350 ± 0.007]	6.0 ± 0.1 [0.250 ± 0.005]	4.0 ± 0.1 [0.160 ± 0.003]	2.5 ± 0.1 [0.113 ± 0.002]
R—Radius of fillet, min	10 [0.375]	8 [0.25]	6 [0.188]	4 [0.156]	2 [0.094]
A—Length of reduced parallel section, min (Note 2)	56 [2.25]	45 [1.75]	30 [1.25]	20 [0.75]	16 [0.625]

Dimensions, mm [in.]
For Test Specimens with Gauge Length Five times the Diameter [E8M]

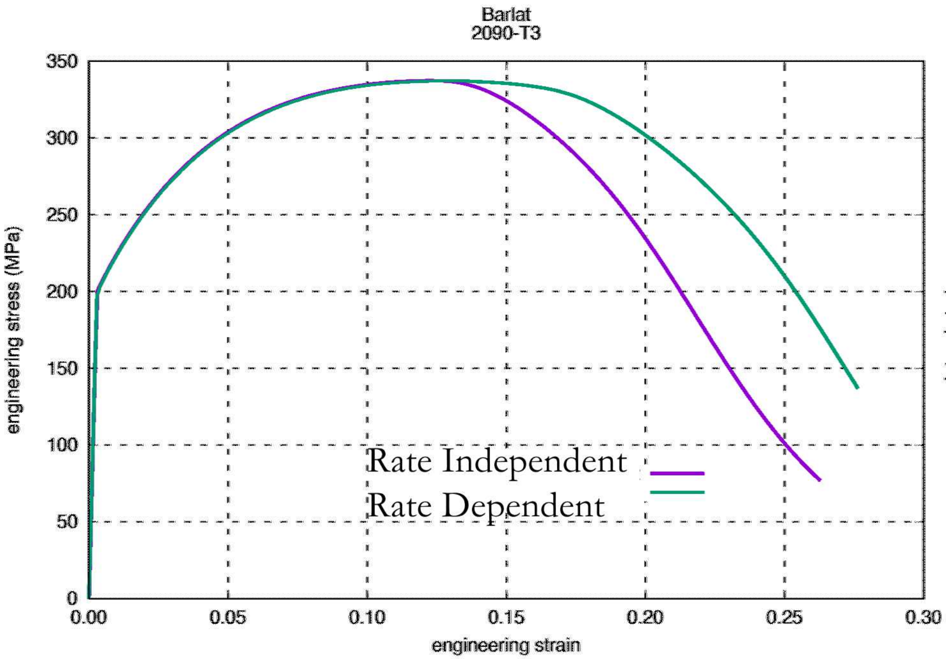
	Standard Specimen	Small-Size Specimens Proportional to Standard			
	Specimen 1	Specimen 2	Specimen 3	Specimen 4	Specimen 5
G—Gauge length	62.5 ± 0.1 [2.500 ± 0.005]	45.0 ± 0.1 [1.750 ± 0.005]	30.0 ± 0.1 [1.250 ± 0.005]	20.0 ± 0.1 [0.800 ± 0.005]	12.5 ± 0.1 [0.565 ± 0.005]
D—Diameter (Note 1)	12.5 ± 0.2 [0.500 ± 0.010]	9.0 ± 0.1 [0.350 ± 0.007]	6.0 ± 0.1 [0.250 ± 0.005]	4.0 ± 0.1 [0.160 ± 0.003]	2.5 ± 0.1 [0.113 ± 0.002]
R—Radius of fillet, min	10 [0.375]	8 [0.25]	6 [0.188]	4 [0.156]	2 [0.094]
A—Length of reduced parallel section, min (Note 2)	75 [3.0]	54 [2.0]	36 [1.4]	24 [1.0]	20 [0.75]

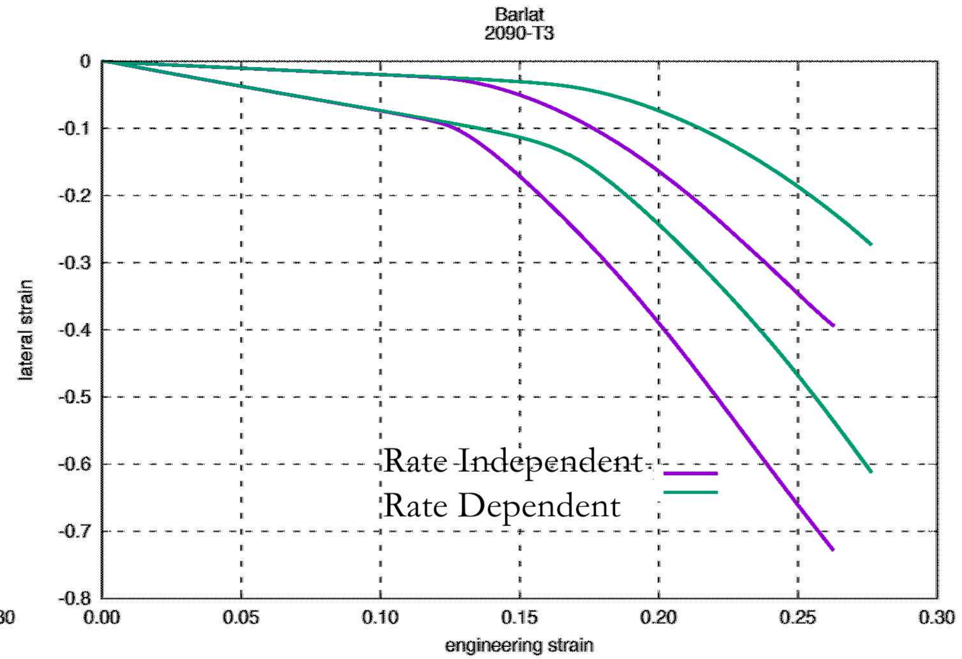
Geometry corresponds to ASTM E8 specification



mesh for a 1/8th symmetry model

Uniaxial Tension Results



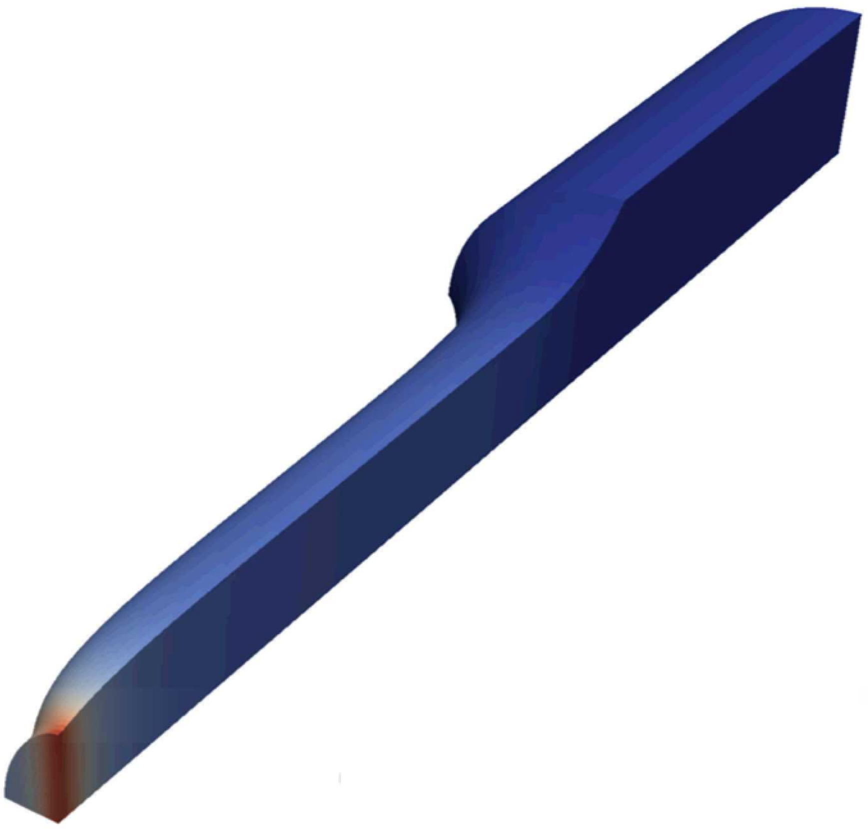


- Prior to maximum load models are the same
- Rate dependence affects post-max load behavior
  - Delays onset of necking
  - Reduces lateral strains at the neck

Uniaxial Tension Results

Rate Independent Model

anisotropic
lateral strains



- Anisotropic yield/flow leads to non-circular cross section at neck

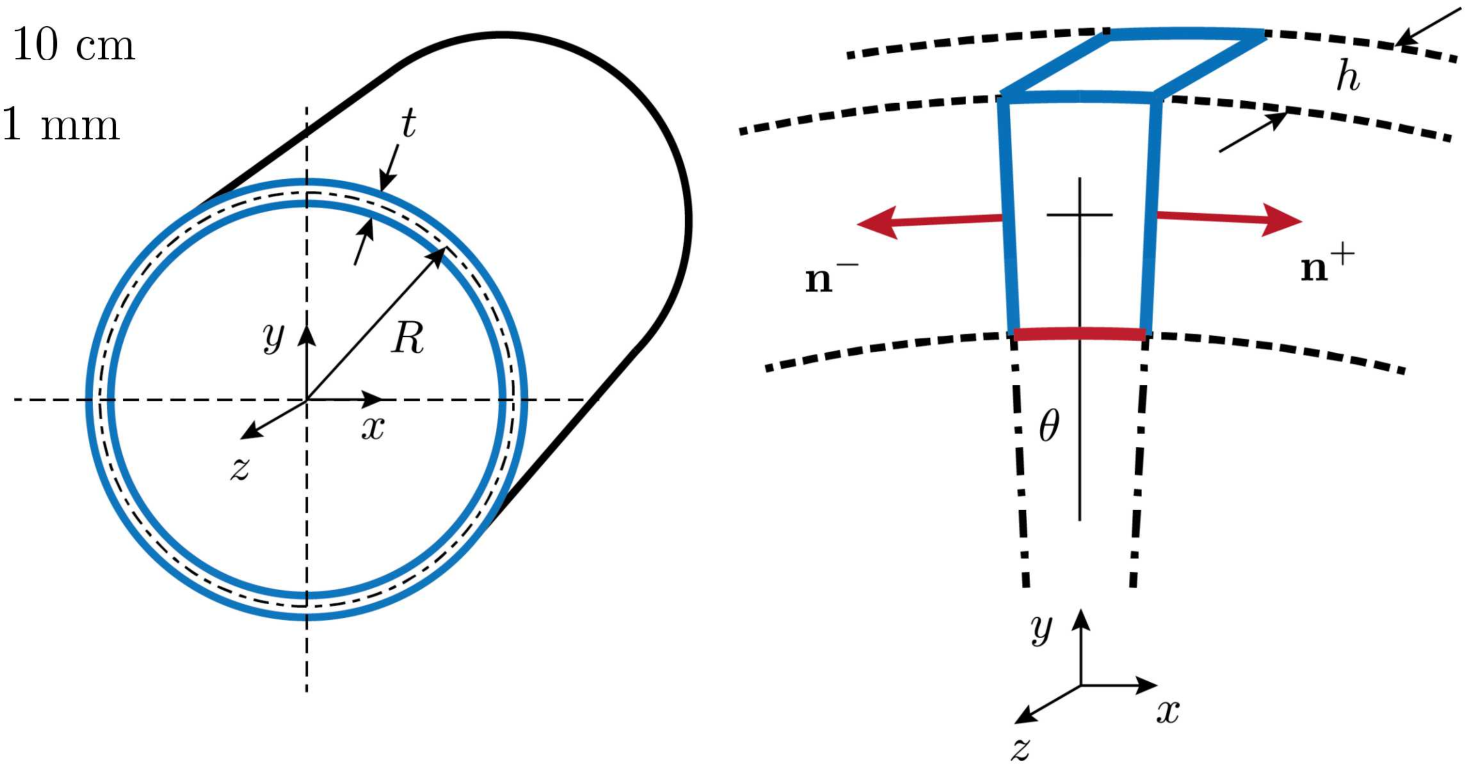
Internal Pressurization of a Cylinder

- Example from Scherzinger, 2017, "A return mapping algorithm for isotropic and anisotropic plasticity models using a line search method", *CMAME,* 317, p. 526-553

Model parameterization based on 2090-T3 Al fit of Barlat, et. al. (IJP 2005 **21** pp. 1009-10039)

$R = 10$ cm

$h = 1$ mm

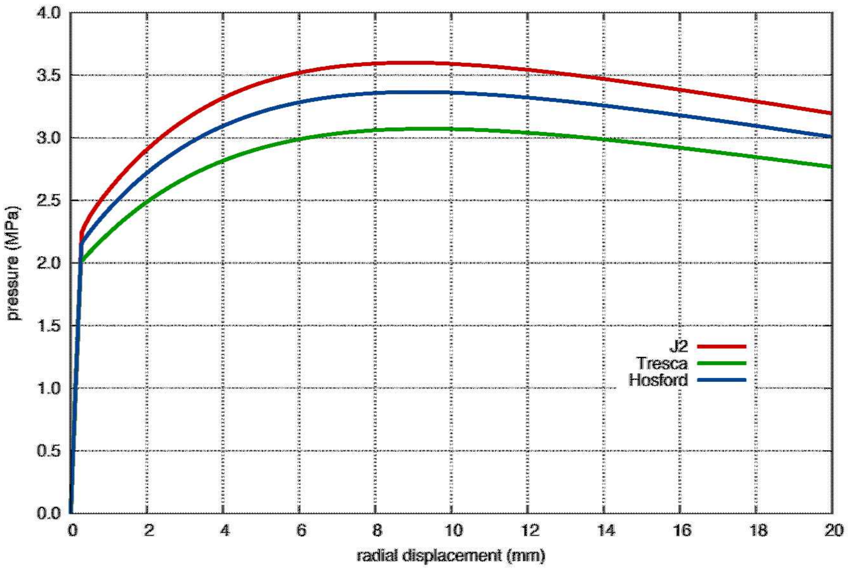


$$\bar{\sigma} = 200\,(1 - \exp(-20\,\bar{\varepsilon}^p))\ \text{MPa} \quad \rightarrow \quad \sigma_y = 200\ \text{MPa}$$

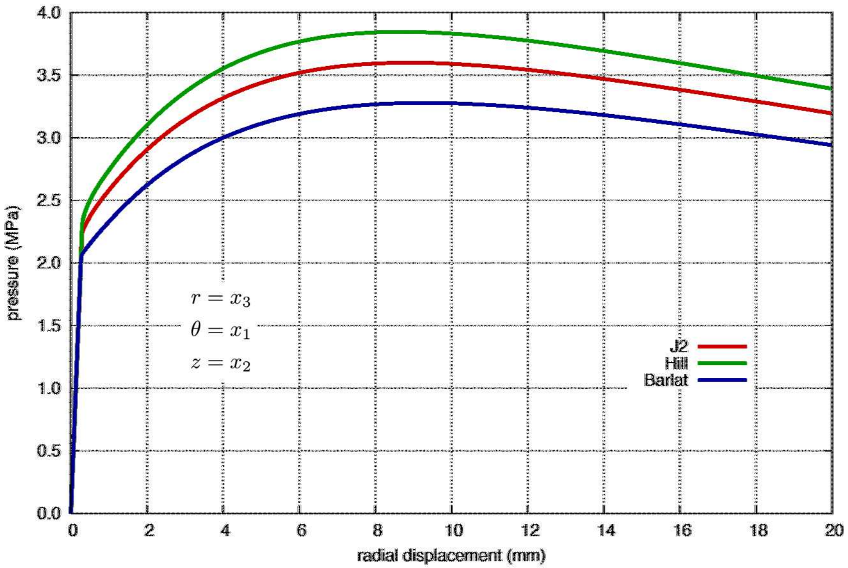
Internal Pressurization of a Cylinder

- Clear impact of yield surface on structural response

Isotropic Yield Surfaces



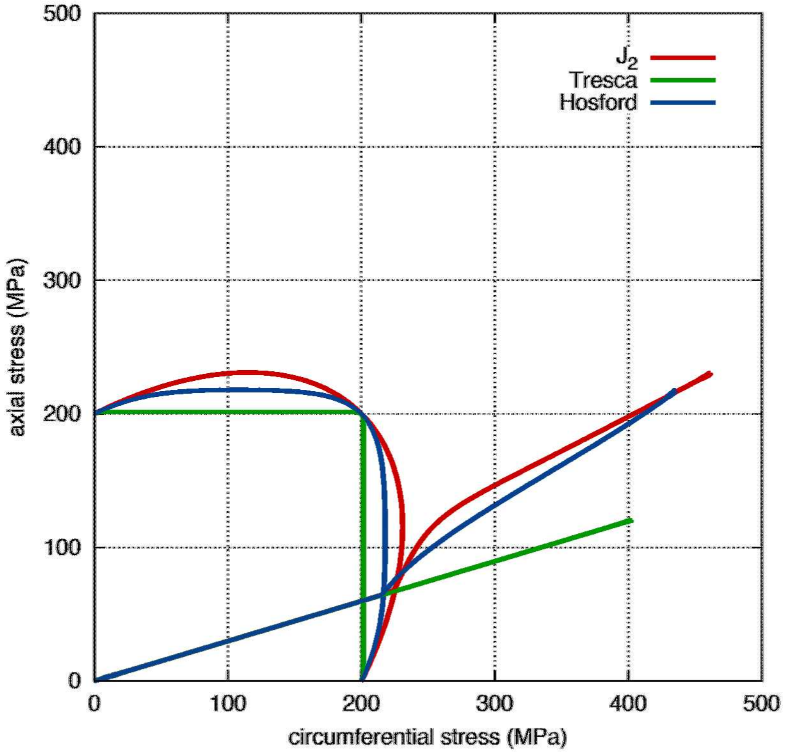
Anisotropic Yield Surfaces



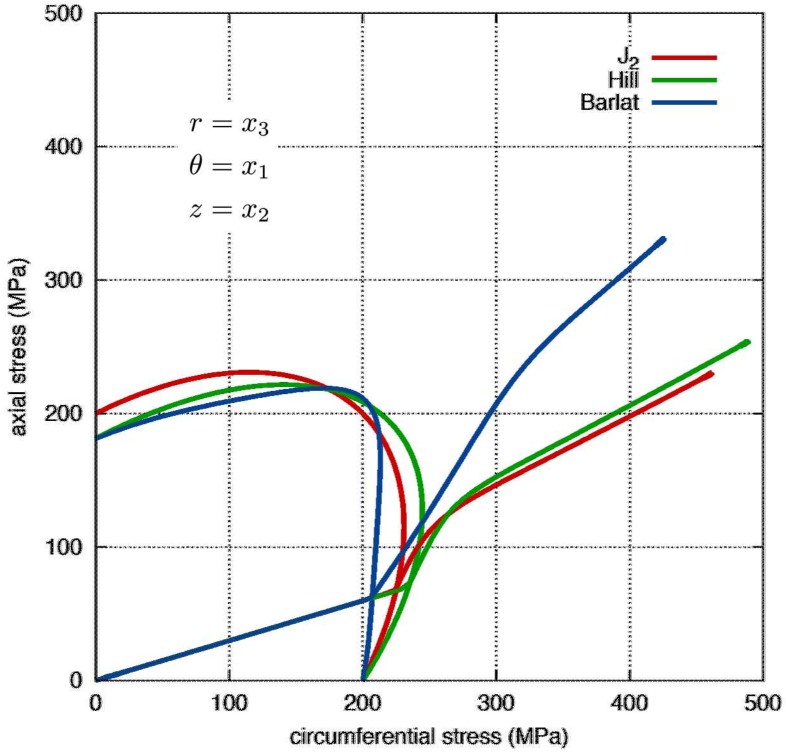
Internal Pressurization of a Cylinder

- Responses exhibit complex stress path evolution
- Requires appropriate numerical implementation

Isotropic Yield Surfaces



Anisotropic Yield Surfaces



Summary So Far…

- Constitutive modeling seeks to develop and implement relationships describing the physics and mechanics of materials
- Goal is to incorporate such models into various analyses (e.g. analytical, FEA)
- Many models exist motivated by different materials and/or mechanics
- Appropriate model depends on needs of modeler and problem

Questions before heading on…

Research Topic: Numerical Integration of Constitutive Models

- Scherzinger, 2017, "A return mapping algorithm for isotropic and anisotropic plasticity models using a line search method", CMAME, 317, p. 526-553
- Lester and Scherzinger, 2017, "Trust-region based return mapping algorithm for implicit integration of elastic-plastic constitutive models", IJNME, 111, p. 257-282

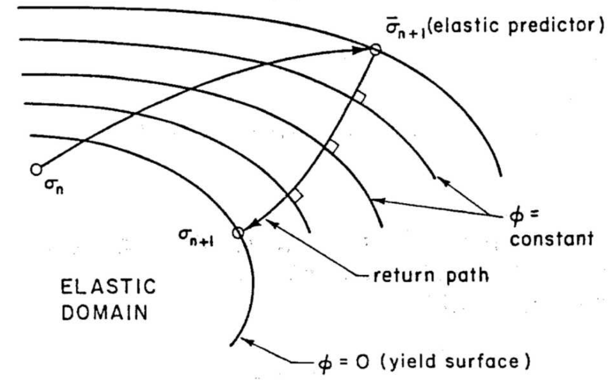
Constitutive Model Integration

- Most stress-updating algorithms still based on Return Mapping Algorithms (RMAs)
  - Fully Implicit Closest Point Projection (CPP)
  - Semi-Implicit Convex Cutting Plane (CCP)

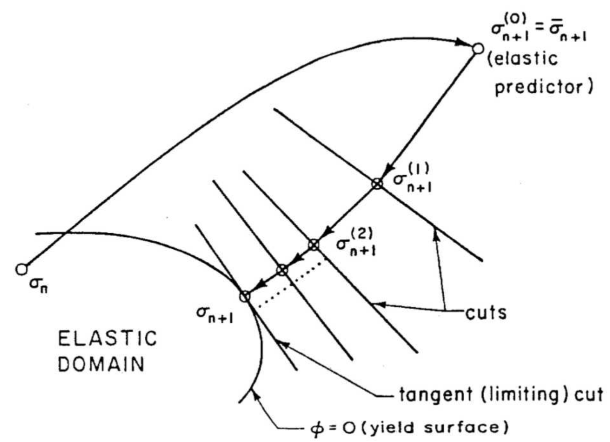
- Implicit integration of constitutive models desirable for
  - Accuracy
  - Speed

- Key requirement of implicit capabilities integration routines must be <u>*robust*</u>

Schematic of CPP-RMA



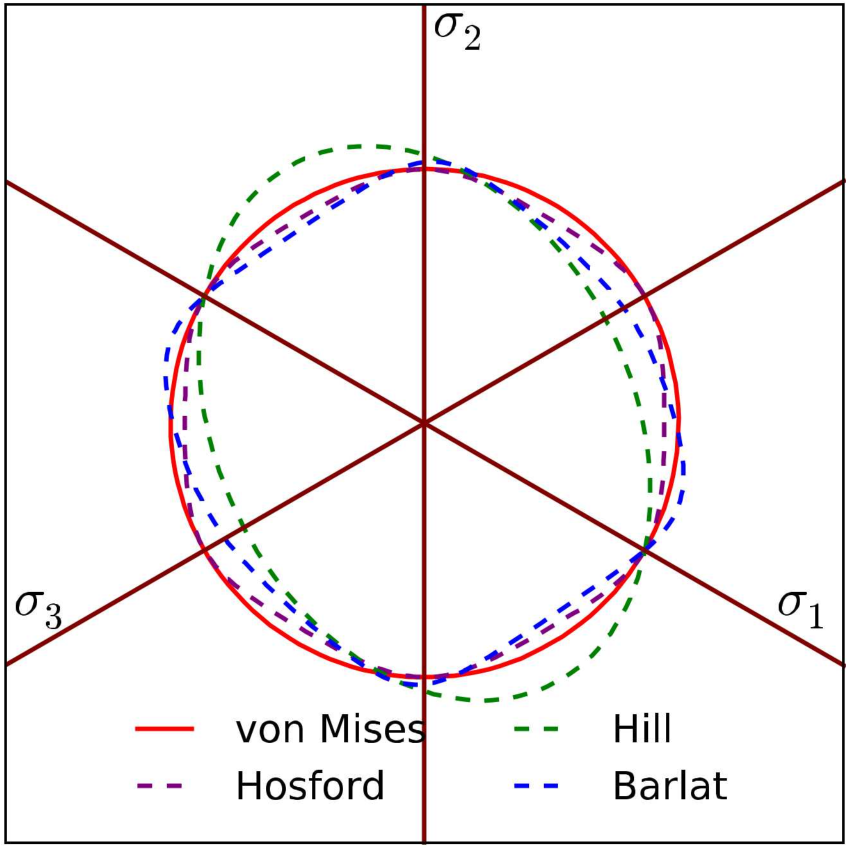
Schematic of CCP-RMA



(Ortiz and Simo, 1986, IJNME **23**, pp. 353-366)

Complex Plasticity Models

- Plasticity models becoming increasingly complex, common
  - Anisotropic and/or non-quadratic yield function forms
  - *e.g.* Hill, Hosford, Karafillis-Boyce, Cazacu, Barlat



- Pose additional challenges for numerical schemes
  - High curvature
  - Anisotropy
  - Misaligned material directions

- Lose guaranteed convergence with these implementations

RMA as Optimization

- "The interpretation of the algorithm… as optimality conditions of a convex minimization problem is of fundamental significance... This interpretation opens the possibility of applying a number of algorithms well developed in convex mathematical programming to solving elastoplastic problems." (Simo and Hughes, 1998, *Computational Inelasticity*, Sec 1.4.3.2)

- Most implementations still based on Newton-Raphson
  - Some line search implementations – not widely adopted
  - Substepping schemes find considerable use

- Want to look at schemes leveraging new optimization schemes

Plasticity Models

- Consider two different plasticity models/yield surfaces:
  - Non-quadratic Hosford
  - Focus on perfect plasticity, $\sigma_y\left(\bar{\varepsilon}^p\right) = \sigma_y^0$

Con. Equation:

$$\dot{\sigma}_{ij} = \mathbb{C}_{ijk}\left(\dot{\varepsilon}_{kl} - \dot{\varepsilon}^{\mathrm{p}}_{kl}\right)$$

Yield Surface:

$$f\left(\sigma_{ij}, \bar{\varepsilon}^p\right) = \phi\left(\sigma_{ij}\right) - \sigma_y\left(\bar{\varepsilon}^p\right)$$

Assoc. Flow Rule:

$$\dot{\varepsilon}^{\mathrm{p}}_{ij} = \dot{\gamma}\frac{\partial f}{\partial \sigma_{ij}}$$

KKT Conditions:

$$\dot{\gamma} \geq 0; \quad \dot{\gamma} f = 0; \quad f \leq 0$$

Return Mapping Problem

- Elastic predictor/inelastic corrector; Fully implicit RMA-CPP
- Solution to non-linear problem $r_I^{(n+1)}(x_I) = 0$

Residual Vector

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

State Vector

$$x_I = \left[\sigma_{ij}, d\gamma\right]^T$$

- Problem solved by iteratively updating the state vector

$$x_I^{(k+1)} = x_I^{(k)} + \alpha^{(k)} p_I^{(k)}$$

Step Size *Step Vector*

Existing Solution Approaches

- Newton-Raphson (NR)

$$\alpha^{(k)} = 1 \;\; \forall k \qquad p_I^{NR(k)} = -\left(J^{(k)}\right)_{IJ}^{-1} r_J^{(k)}$$

$$J_{IJ} = \begin{bmatrix} \left(\mathscr{L}_{ijkl}\right)^{-1} & \dfrac{\partial \phi}{\partial \sigma_{ij}} \\ \dfrac{\partial \phi}{\partial \sigma_{ij}} & -\dfrac{\partial \sigma_y}{\partial \bar{\varepsilon}^p} \end{bmatrix}$$

$$\mathscr{L}_{ijkl} = \left(\mathbb{C}_{ijkl}^{-1} + d\gamma \frac{\partial^2 \phi}{\partial \sigma_{ij} \partial \sigma_{kl}}\right)^{-1}$$

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

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

Merit Function

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

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

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

- 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 Based Solver

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

$$\tilde{m}^{(k)}\left(\tilde{p}_I\right) = \psi^{(k)} + \tilde{g}_I^{(k)}\tilde{p}_I + \frac{1}{2}\tilde{p}_I\tilde{B}_{IJ}^{(k)}\tilde{p}_J$$

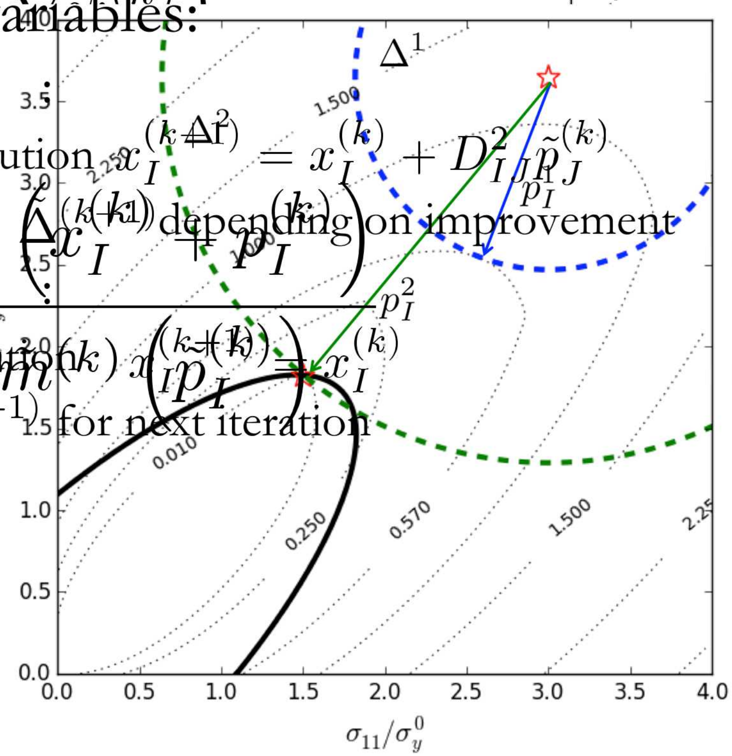
- Step 3: Calculate improvement, $\rho^{(k)}$, of a given trial increment, $\tilde{p}_I^{(k)}$
- Step 4: Update variables:
  - If $\rho^{(k)} \geq$ tol:
    - Accept trial solution $x_I^{(k+1)} = x_I^{(k)} + D^2_{IJ}\tilde{p}_J^{(k)}$
    - Keep/increase $\Delta^{(k+1)}$ depending on improvement
  - If $\rho^{(k)} <$ tol:
    - Reject trial solution $x_I^{(k+1)} = x_I^{(k)}$
    - Decrease $\Delta^{(k+1)}$ for next iteration

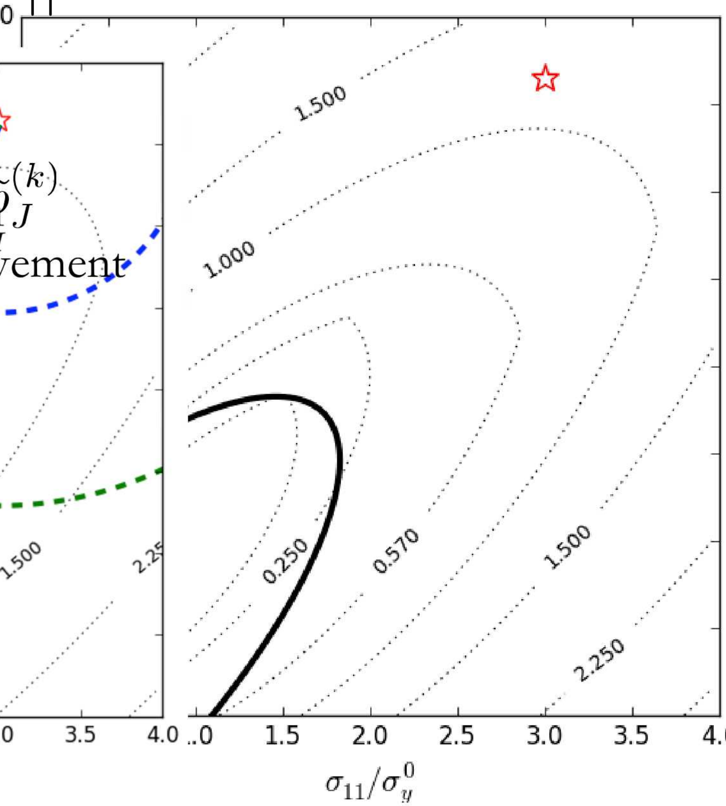
$$\tilde{g}_I^{(k)} = \left(\Sigma \ldots\right)$$

$$\tilde{B}_{IJ}^{(k)}$$

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

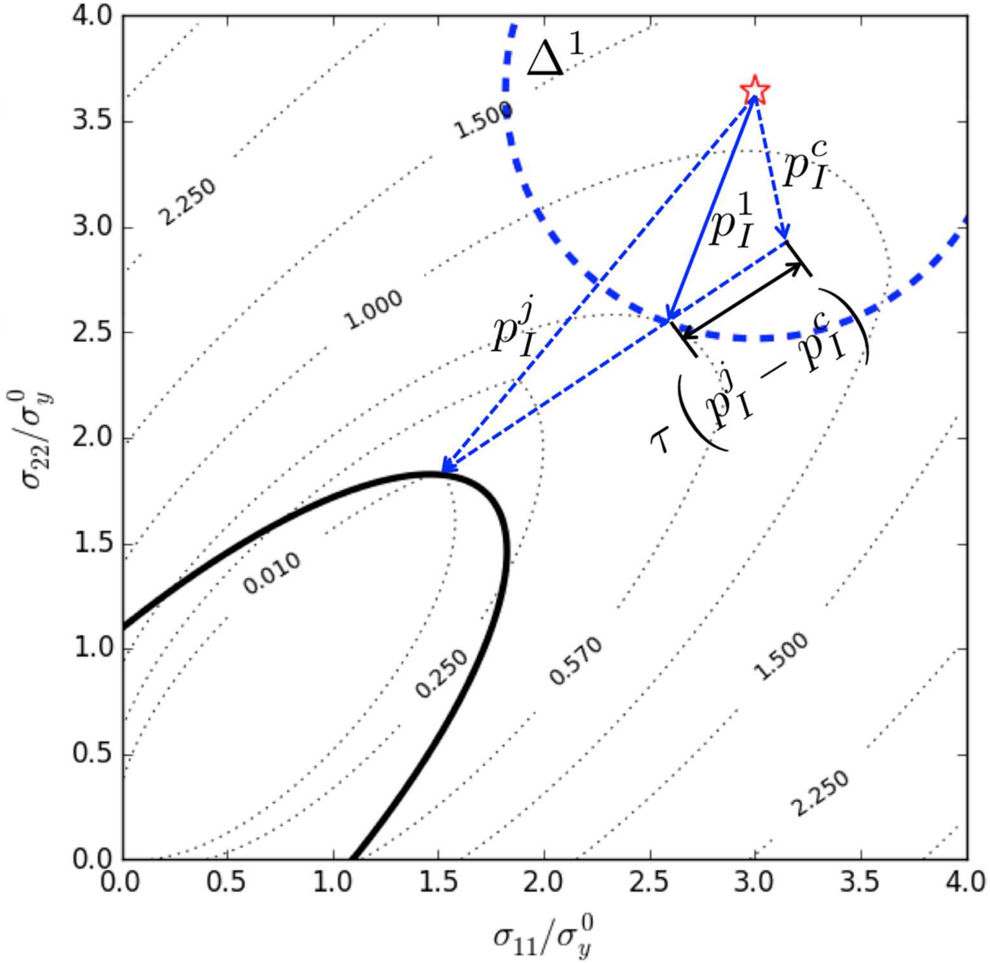
$$D^2_{IJ} = \left[\ b \ \ldots\right.$$





Determination of Step Vector

- To find the step vector, use the dogleg method



Cauchy Point:

$$\tilde{p}_I^{c(k)} = -\tau^{(k)} \left(\frac{\tilde{\Delta}^{(k)}}{||\tilde{g}_I^{(k)}||} \right) \tilde{g}_I^{(k)}$$

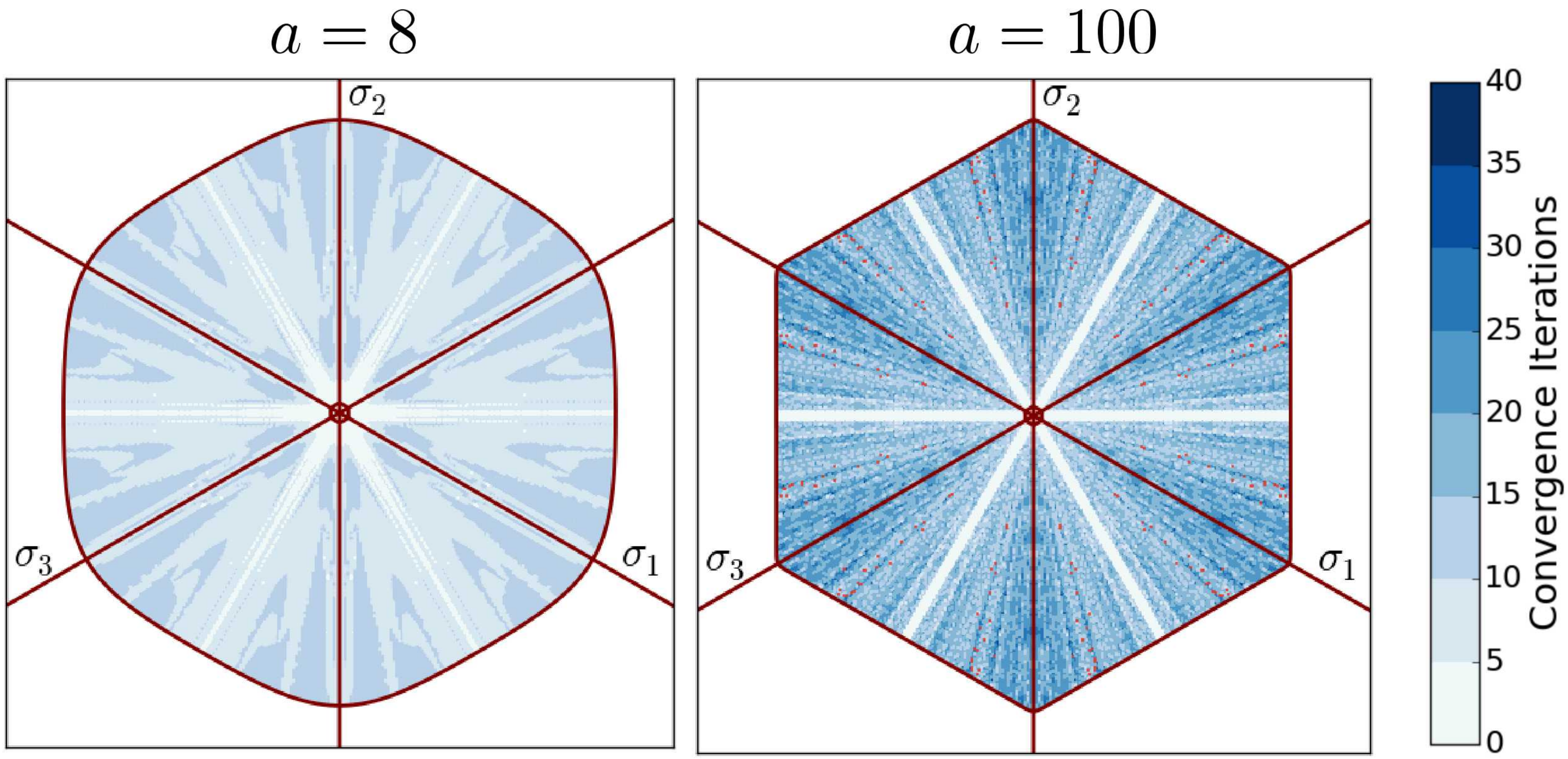
$$\tau^{(k)} = \min \left[1, \frac{||\tilde{g}_I^{(k)}||^3}{\tilde{\Delta}^{(k)} \tilde{g}_I^{(k)} \tilde{B}_{IJ}^{(k)} \tilde{g}_J^{(k)}} \right]$$

Fullstep:

$$\tilde{p}_I^{j(k)} = -\left(\tilde{B}^{(k)} \right)_{IJ}^{-1} \tilde{g}_J^{(k)}$$

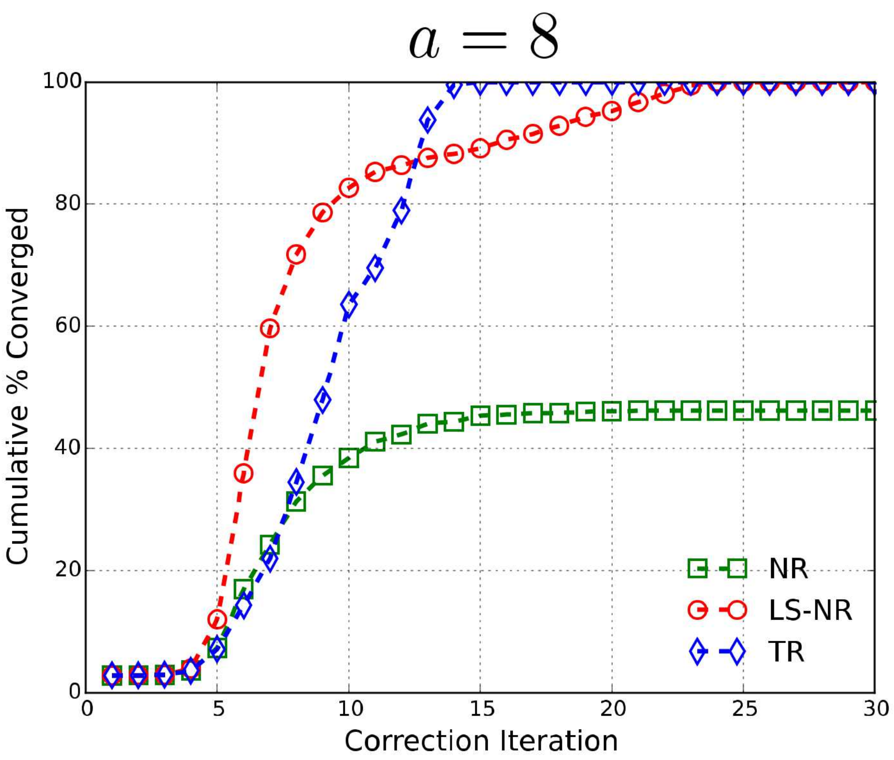
Convergence Maps

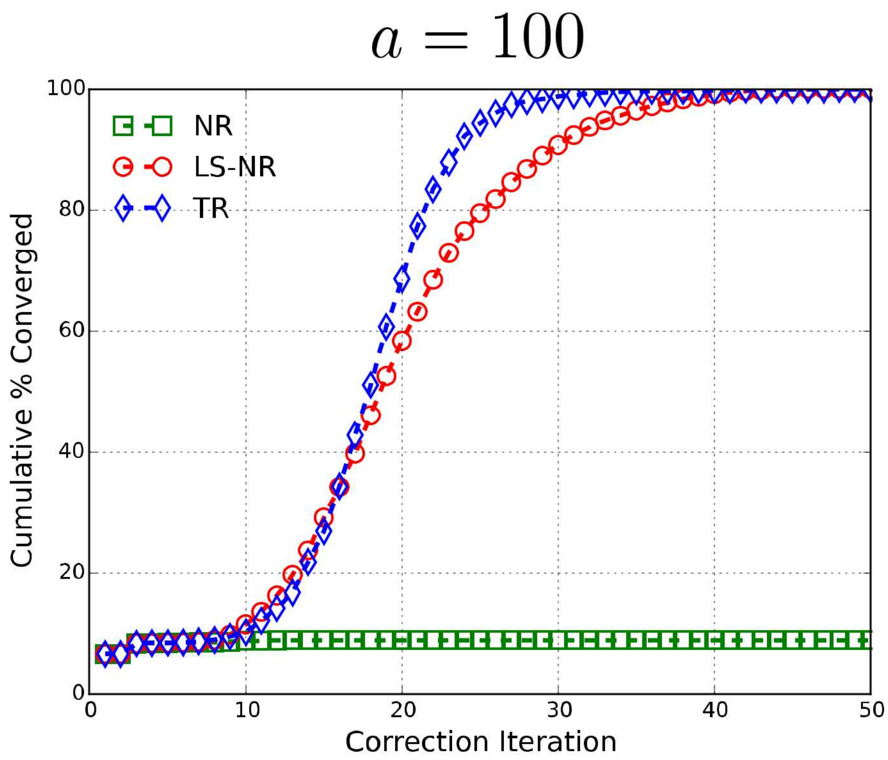
- Determine number of correction iterations needed for TR algorithm at $\phi(\sigma_{ij}) \leq 30\sigma_y^0$



- Proposed algorithm converges for nearly every trial stress

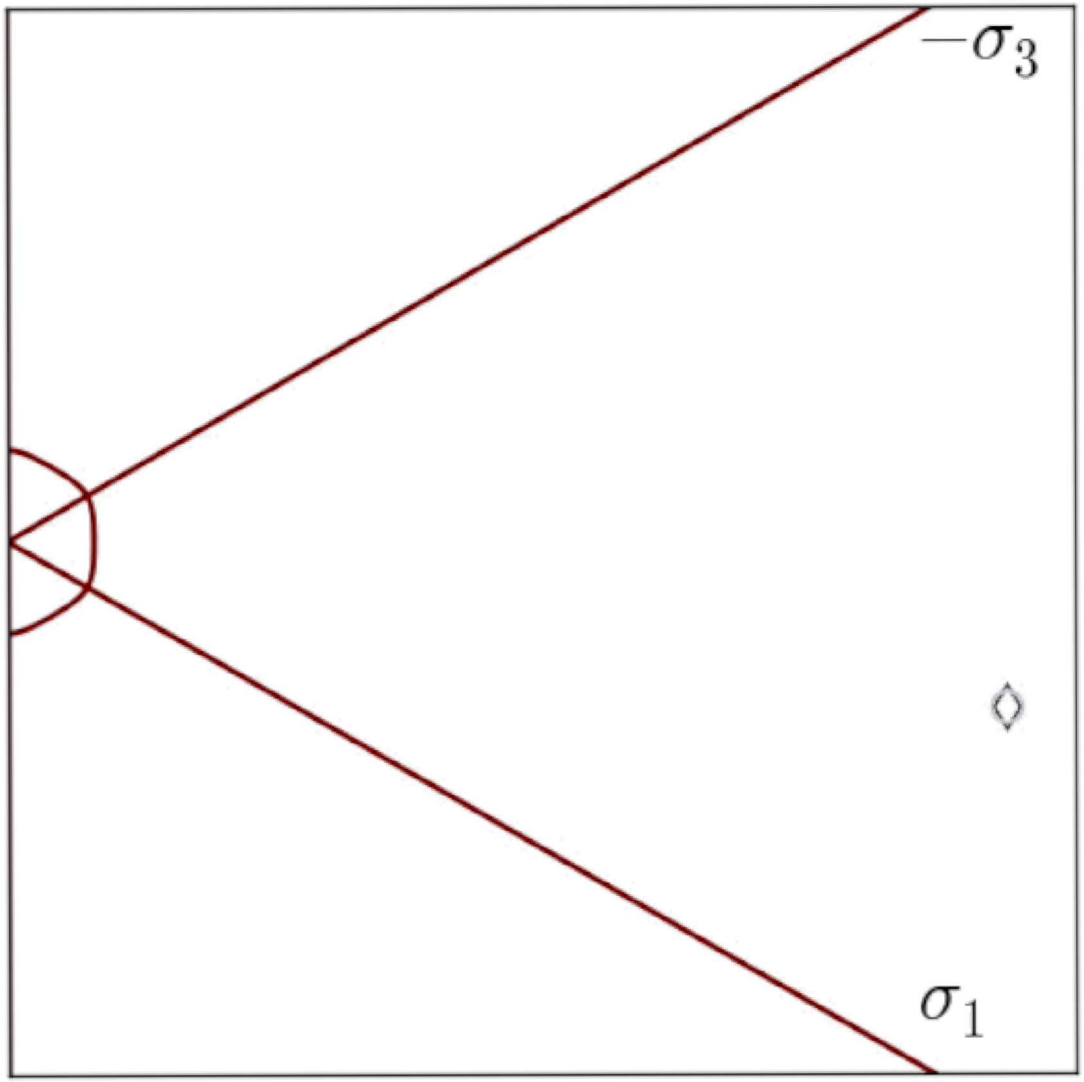
Cumulative Convergence Distributions



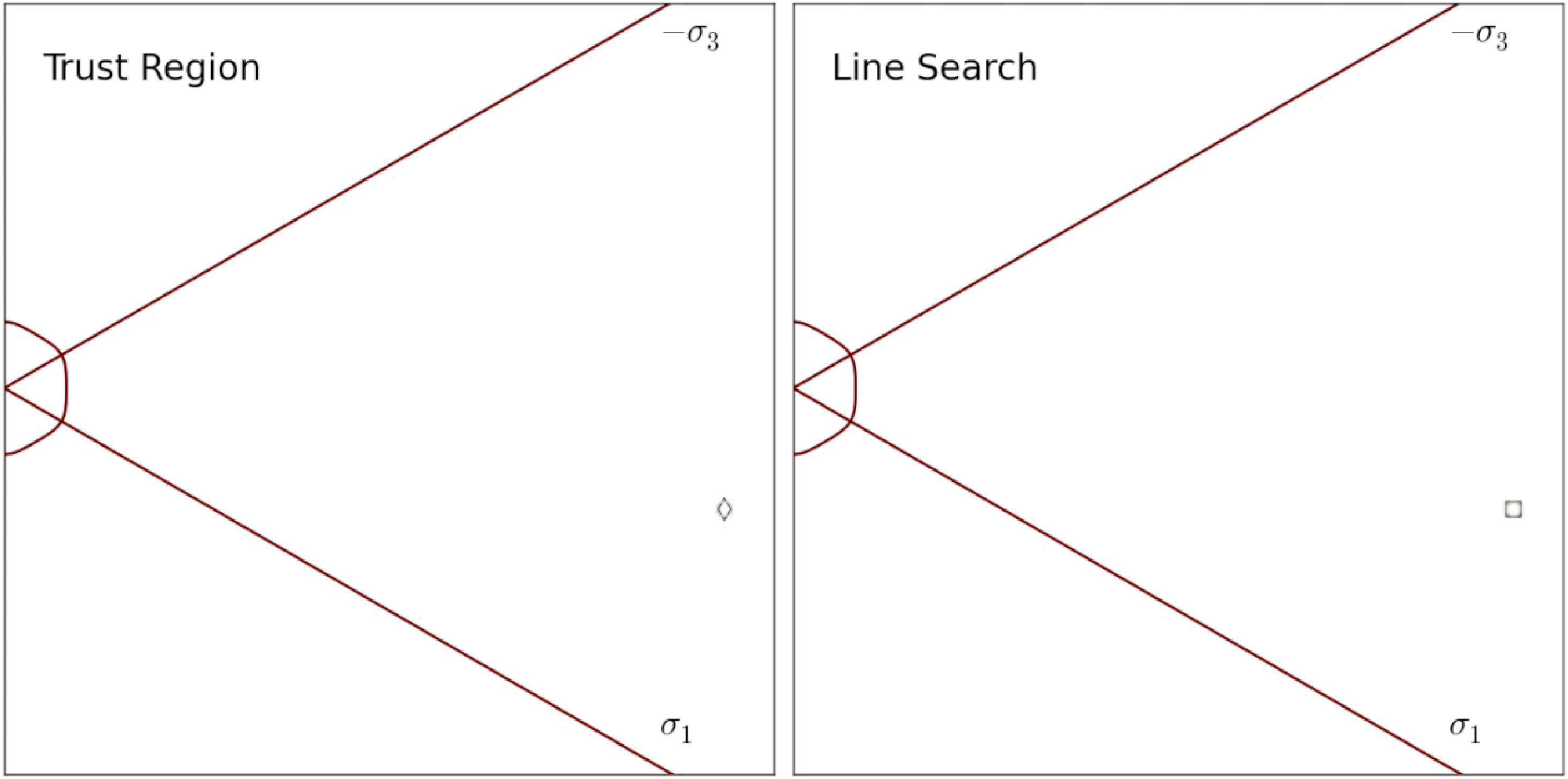


- Convergence of TR method well in excess of traditional NR
  - Comparable with LS-NR
  - TR better at higher iterations

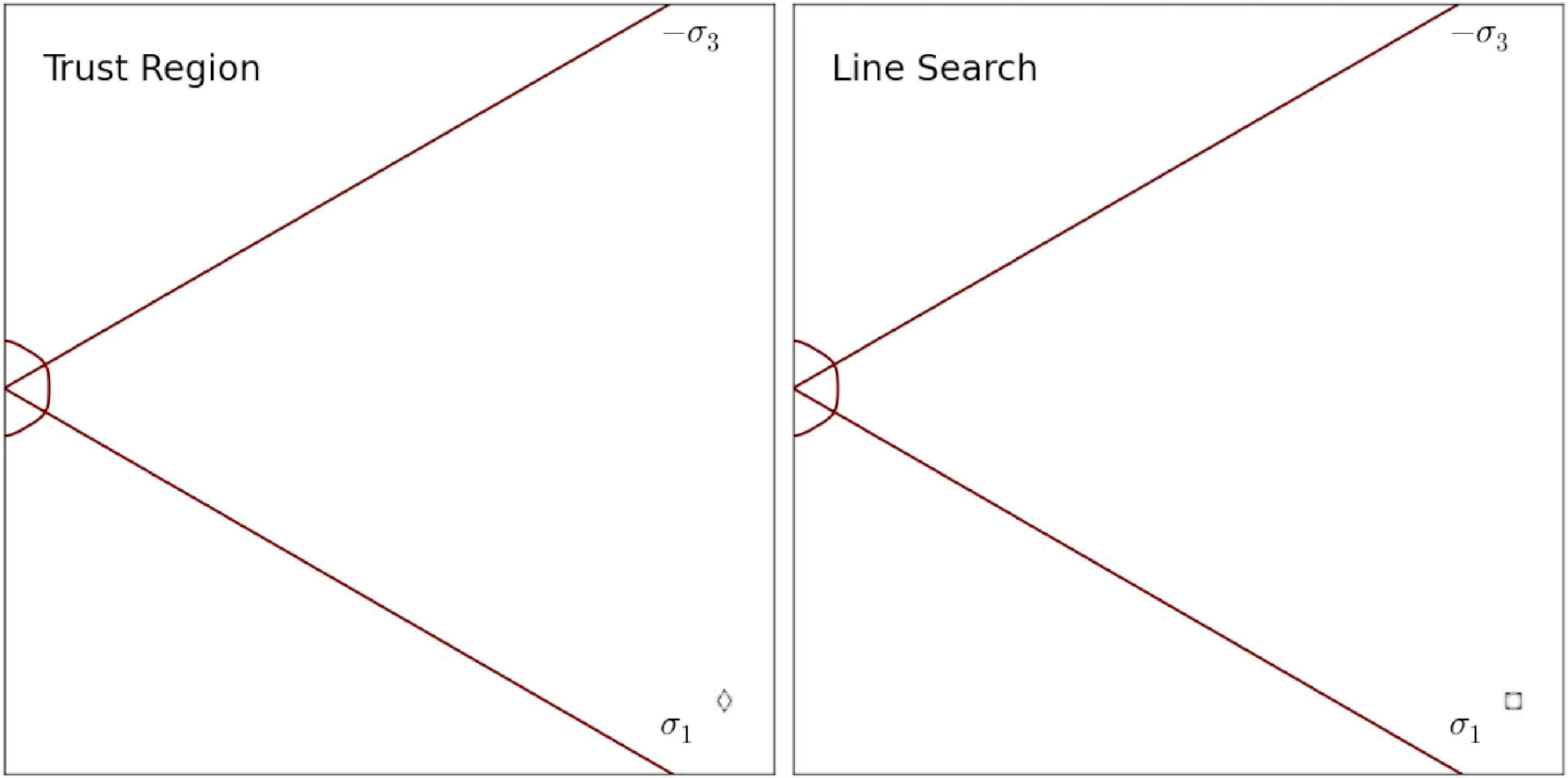
Trust-Region Return Trajectory



Return Trajectory Comparison (A)

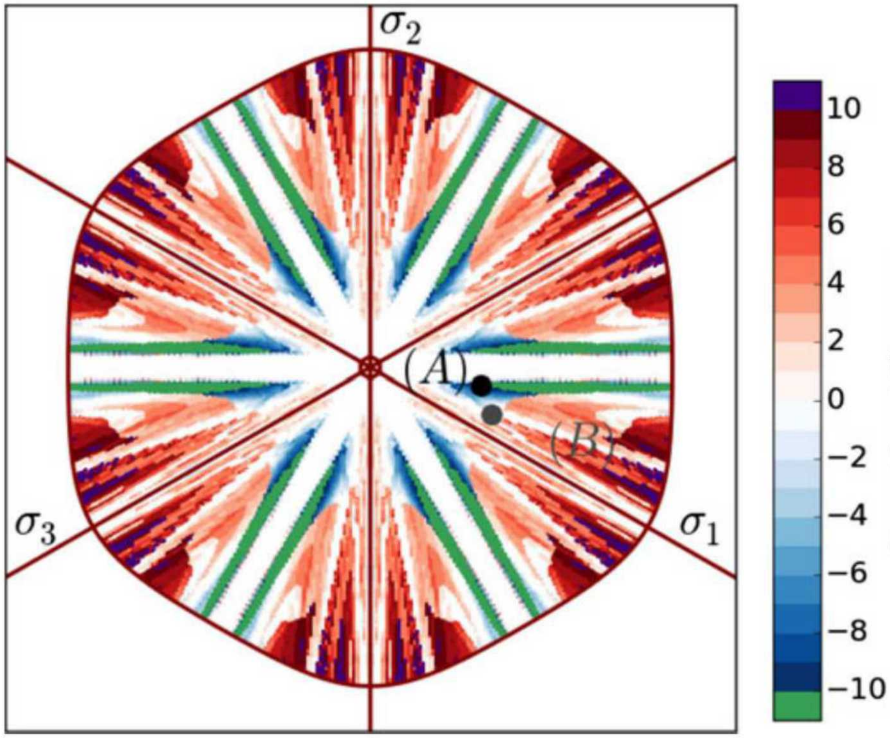


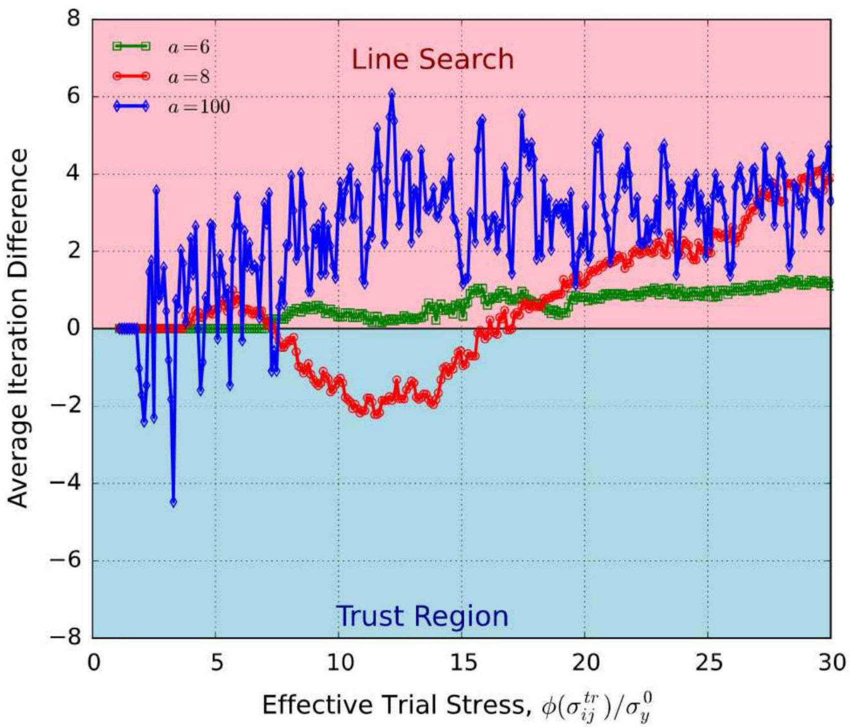
Return Trajectory Comparison (B)



Method Comparison

Iter(TR) – iter(LS-NR)





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

Research Topic: Develop of a Distortional Hardening Plasticity Model

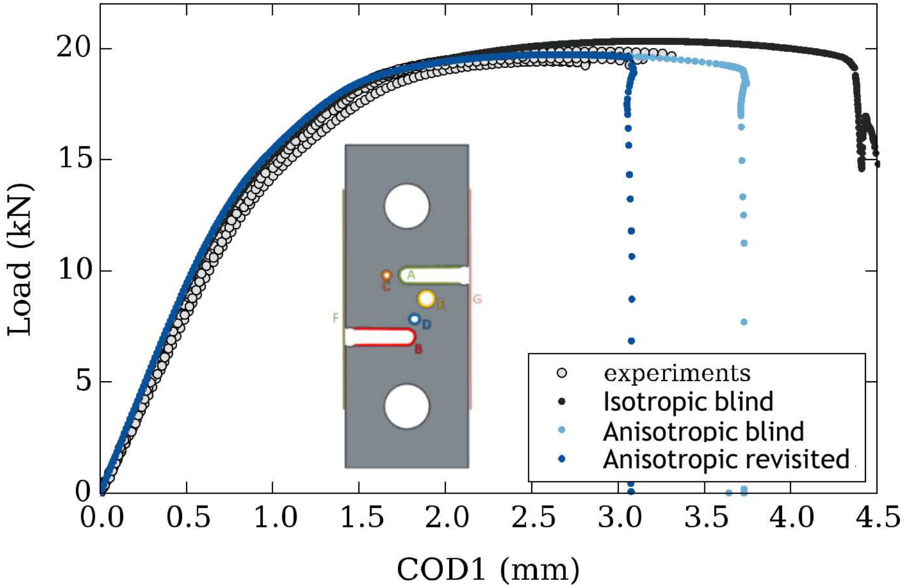
- Lester and Scherzinger, 2018, “An evolving effective stress approach to anisotropic distortional hardening”, IJSS, 143, p. 194-208

Anisotropic Plasticity

- Plastic anisotropy needed for modeling complex multiaxial loadings
  - Manufacturing processes (e.g. sheet metal forming)
  - Ductile Failure

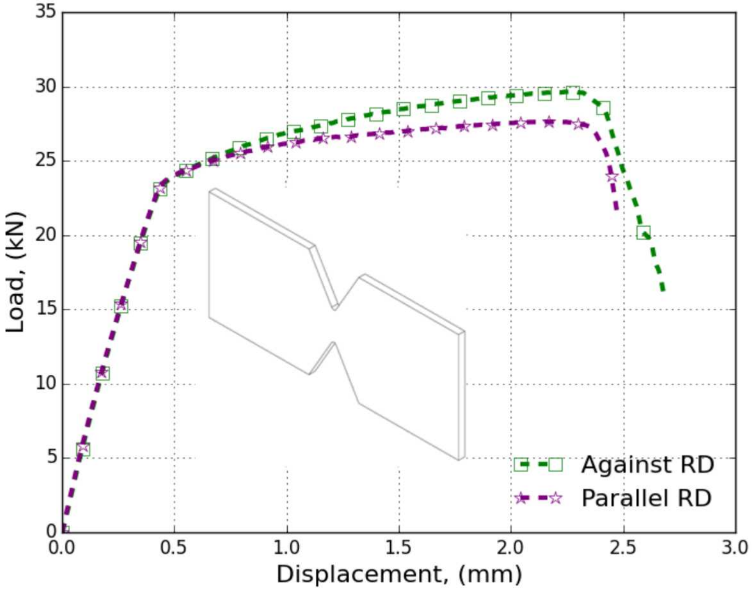
2nd Sandia Fracture Challenge (SFC2) (Ti-6Al-4V)

Isotropic and Anisotropic Failure Predictions



Karlson et al., 2016, *Int. Jrnl. Frac.*, 198: 179-195

Notched Shear Calibration Data for SFC2

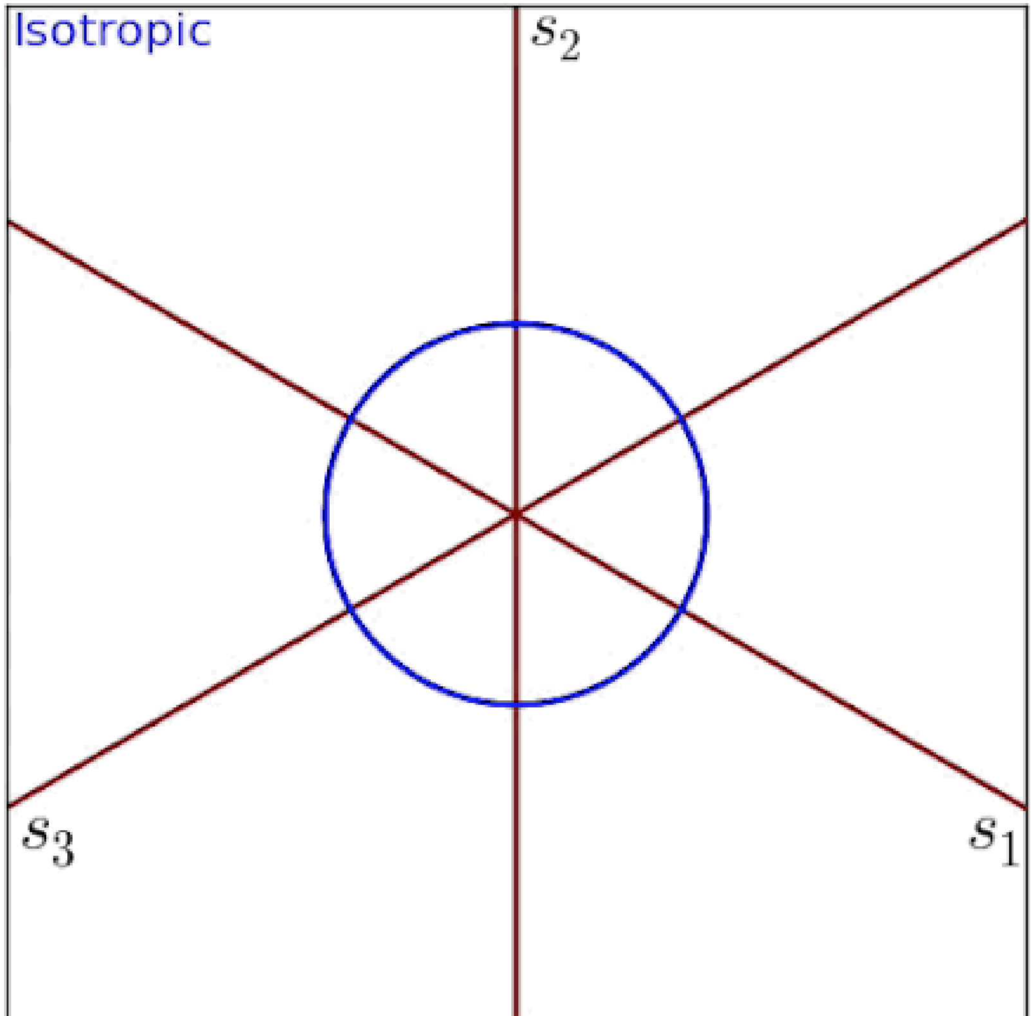


Boyce et al., 2016, *Int. Jrnl. Frac.*, 198: 5-100

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

Plastic Hardening

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



Free Energy

State Variables

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

Free Energy

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

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

Constitutive Behavior

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

Dissipation Inequality

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

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

- 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

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)

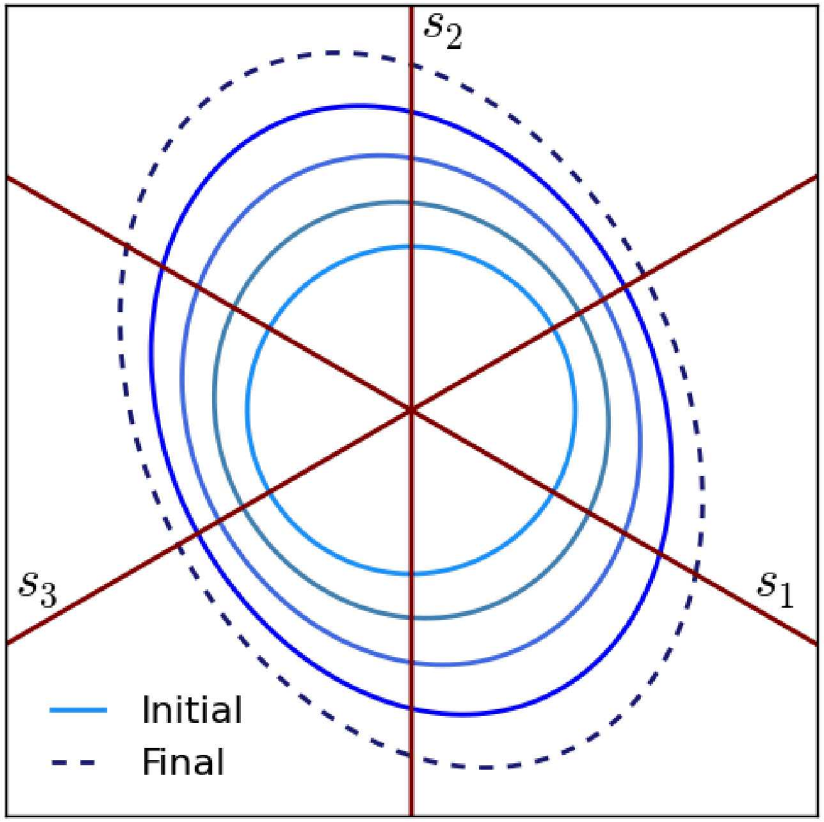
$$\phi\left(\sigma_{ij}, N\right) = \sum_{k=1}^{n_{\mathrm{es}}} \zeta^{(k)}\left(N\right)\phi^{(k)}\left(\sigma_{ij}\right)$$

- 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

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

Numerical Implementation

- Use Line-Search Augmented Newton-Raphson (LS-NR) approach

$$\text{Minimize} \qquad \psi = \frac{1}{2}\left[\left(\frac{E}{\sigma_y^0}\right)^2 r^{\varepsilon}_{ij} r^{\varepsilon}_{ij} + \left(\frac{r^f}{\sigma_y^0}\right)^2 + \left(\frac{P^{\mathrm{mod}} r^{\eta}}{\sigma_y^0}\right)^2\right]$$

Residuals

$$-r^{f(k)} = f(\sigma_{ij}, \kappa, \eta) \qquad \text{Consistency}$$

$$-r^{\varepsilon(k)}_{ij} = -d\varepsilon^{p}_{ij} + d\kappa \frac{\partial \phi}{\partial \sigma_{ij}} \qquad \text{Plastic Strain Flow Rule}$$

$$-r^{\eta(k)} = d\eta - d\kappa \frac{\partial \phi}{\partial N} \qquad \text{DHV Flow Rule}$$

System of Linearized Residuals

$$-r^{f} = \frac{\partial \phi}{\partial \sigma_{ij}} \Delta\sigma_{ij} - \frac{\partial \sigma_y}{\partial \kappa}\Delta\kappa + \frac{\partial \phi}{\partial \eta}\Delta\eta$$

$$-r^{\varepsilon}_{ij} = \mathscr{L}^{-1}_{ijkl}\Delta\sigma_{kl} + \frac{\partial \phi}{\partial \sigma_{ij}}\Delta\kappa + d\kappa \frac{\partial^2 \phi}{\partial \sigma_{ij}\partial \eta}\Delta\eta$$

$$-r^{\eta} = d\kappa \frac{\partial^2 \phi}{\partial N \partial \sigma_{ij}}\Delta\sigma_{ij} + \frac{\partial \phi}{\partial N}\Delta\kappa + \left(-1 + d\kappa \frac{\partial^2 \phi}{\partial N \partial \eta}\right)\Delta\eta$$

$$\Delta\kappa = \frac{-\frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl} r^{\varepsilon}_{kl} + r^f}{\frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl}\frac{\partial \phi}{\partial \sigma_{kl}} + \frac{\partial \sigma_y}{\partial \kappa}}$$

"Classical" solution for isotropic hardening plasticity

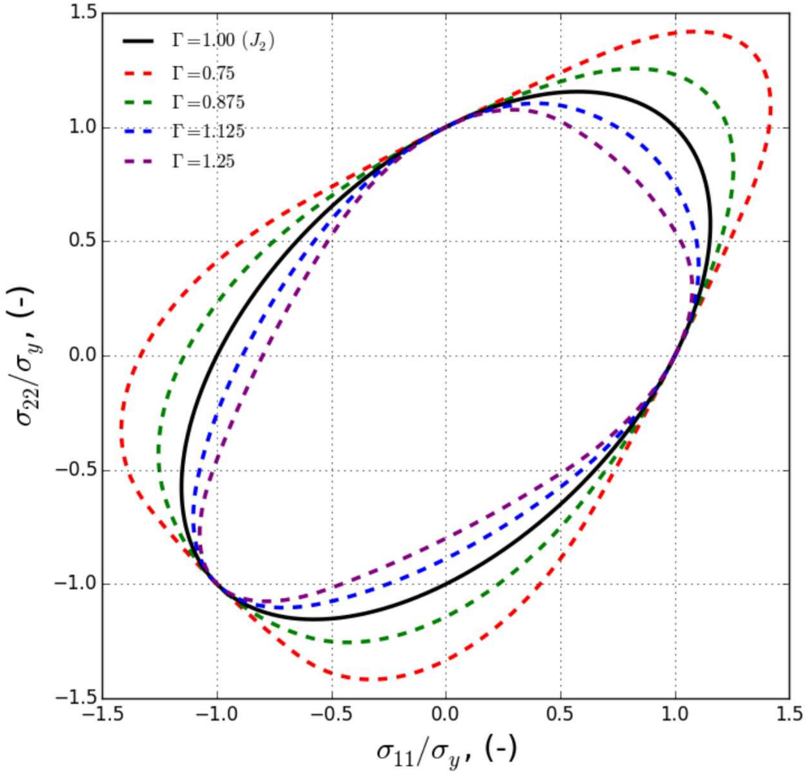
$$\Delta\kappa = \frac{-\frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl} r^{\varepsilon}_{kl} + r^f + \frac{1}{\omega}\left(\frac{\partial \phi}{\partial \eta} - d\kappa \frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl}\frac{\partial^2 \phi}{\partial \sigma_{kl}\partial \eta}\right)\left(r^{\eta} - d\kappa \frac{\partial^2 \phi}{\partial N \partial \sigma_{ij}}\mathscr{L}_{ijkl} r^{\varepsilon}_{kl}\right)}{\frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl}\frac{\partial \phi}{\partial \sigma_{kl}} + \frac{\partial \sigma_y}{\partial \kappa} + \frac{1}{\omega}\left(\frac{\partial \phi}{\partial \eta} - d\kappa \frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl}\frac{\partial^2 \phi}{\partial \sigma_{kl}\partial \eta}\right)\left(\frac{\partial \phi}{\partial N} - d\kappa \frac{\partial \phi}{\partial \sigma_{ij}}\mathscr{L}_{ijkl}\frac{\partial^2 \phi}{\partial \sigma_{kl}\partial N}\right)}$$

(Scherzinger, 2017, CMAME, 317, pp.526-553; Lester and Scherzinger, 2017, IJNME, 112, pp. 257-282)

Strength-Differential Evolution

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

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



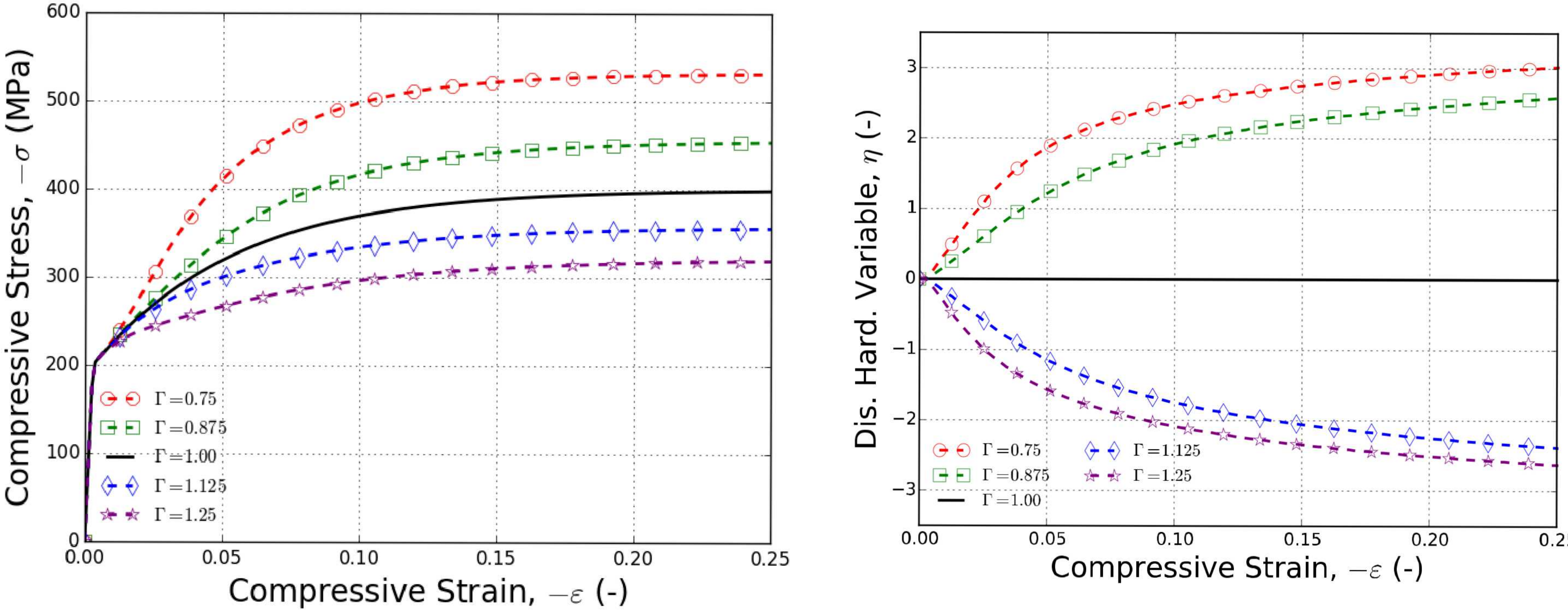
$$\Gamma = \frac{\sigma_y^{0(t)}}{\sigma_y^{0(c)}}$$

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

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

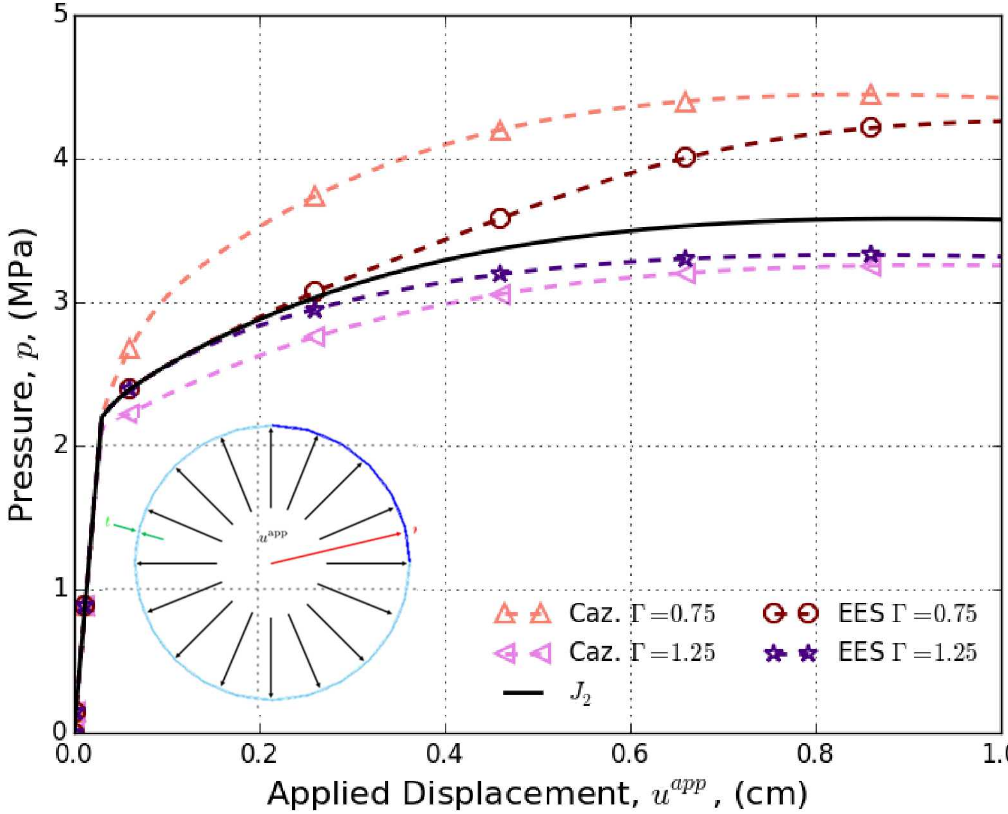
(Cazacu *et al.*, 2006, IJP, 22, pp.1171-1194)

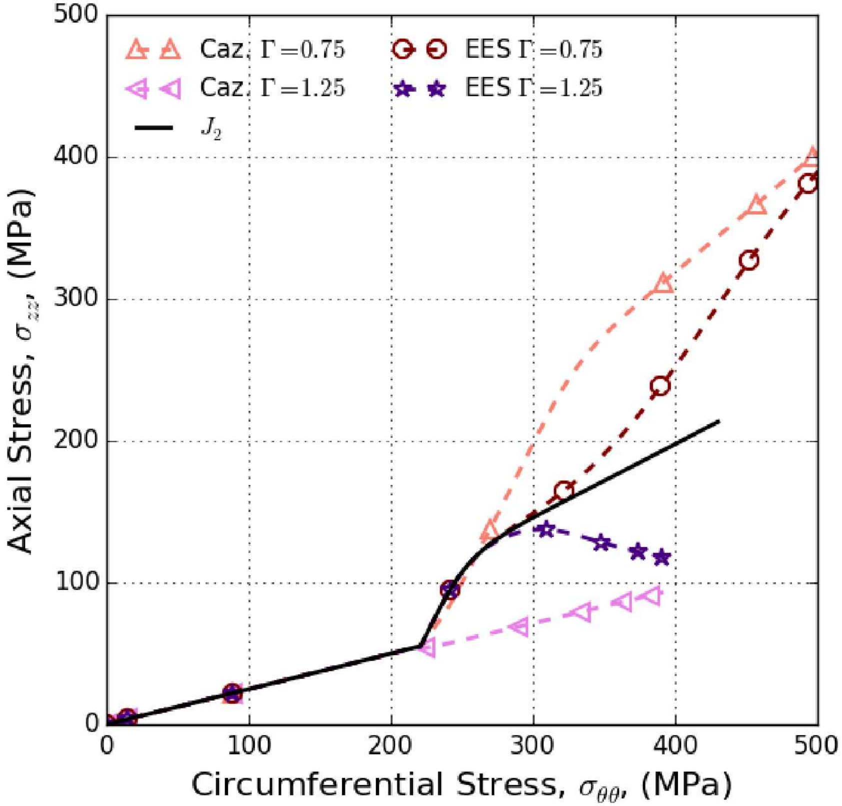
Constitutive Behavior



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

Pressurized Cylinder



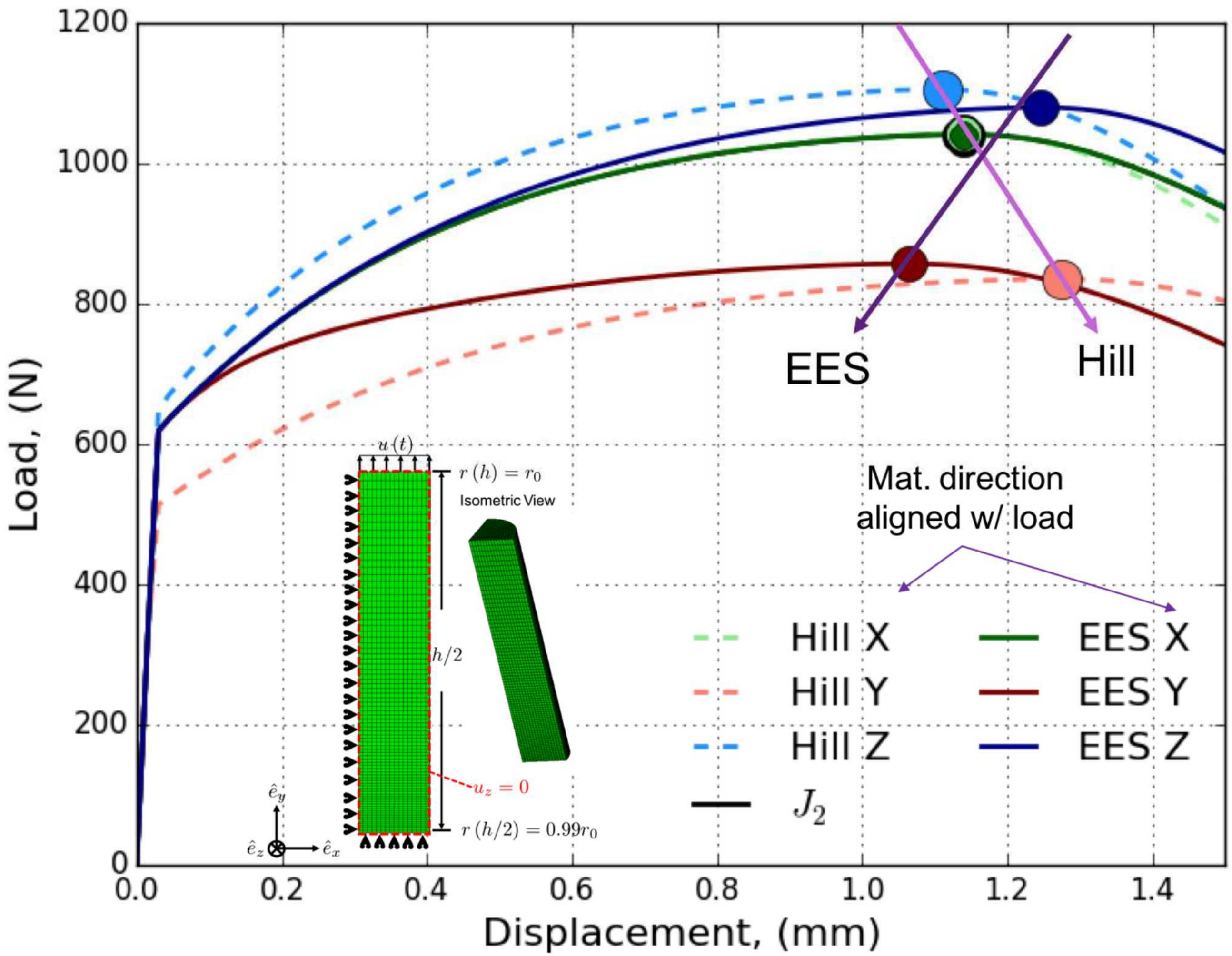


$$p = \frac{F}{(r + \bar{u}_r)\, h}$$

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

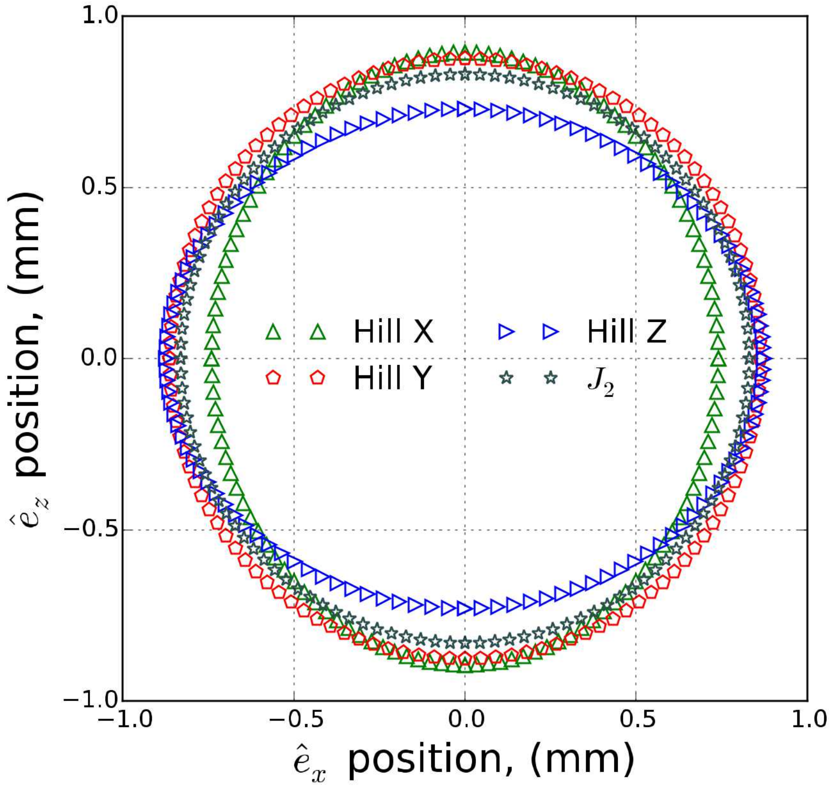
Tensile Cylinder

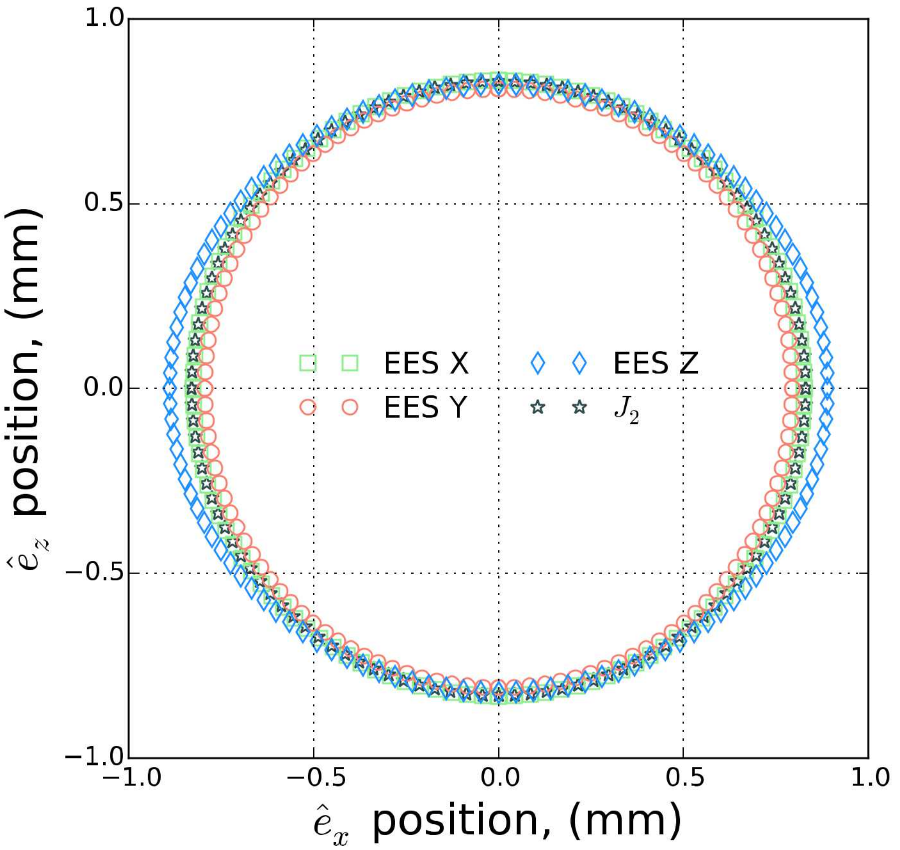
- Consider loading of a uniaxial tensile bar with the classic Hill'48 yield surface



Tensile Cylinder Cross-Sections

- Can also see the impact of the hardening choices on cross-section shapes of the bars





Conclusions

- Constitutive modeling is a complex subject
  - Decades of existing work; yet still more to do
  - Robust numerical implementations
  - Development of new models

- Here, provided but a brief introduction…

Acknowledgements

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Questions?