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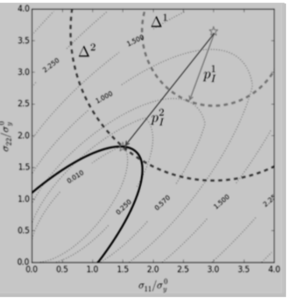

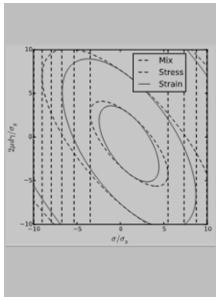

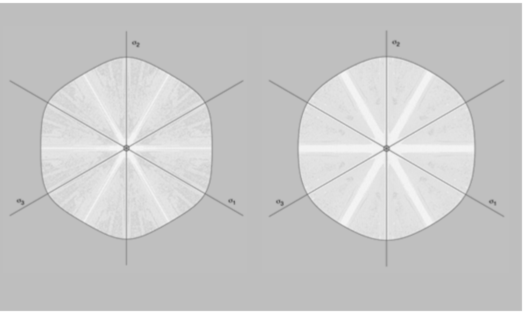

Implicit Integration of Plasticity Models via Trust-Region Methods

Brian T. Lester
William M. Scherzinger

Solid Mechanics Department
Sandia National Laboratories
Albuquerque, NM USA

12th World Congress on Computational Mechanics
Seoul, Korea
July 28, 2016

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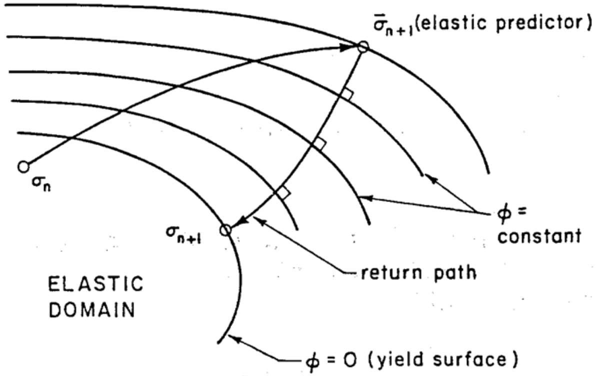
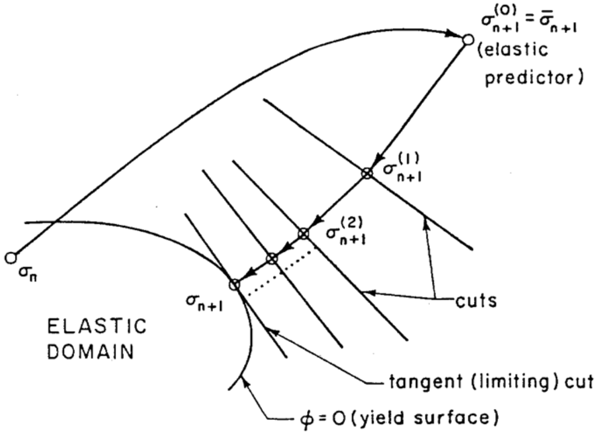
Elastic-Plastic Model Integration

- 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 *robust*

Schematic of CPP-RMA



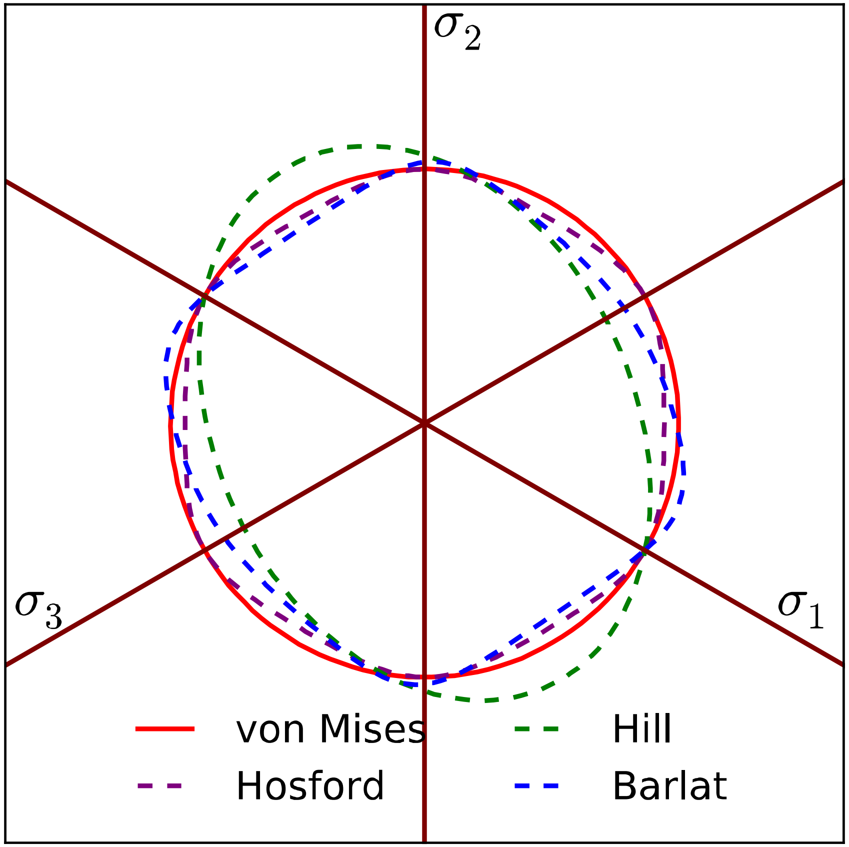
Schematic of CCP-RMA



Ortiz and Simo, 1986 IJNME 23, 353-366

Complex Plasticity Models

- Plasticity models becoming increasingly complex, common
  - Anisotropic and/or non-quadratic yield function forms
  - *e.g.* Hill, Hosford, Kara
- Pose additional challe numerical schemes
  - High curvature
  - Anisotropy
  - Misaligned material di
- Lose guaranteed conv with these implement



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, Sec 1.4.3.2]

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

Proposed Novel RMA Solver

- Numerical methods in non-linear optimization widely studied in recent decades
  - Number of algorithms developed
  - Very few considered for RMA problems

- ***Objective***: Develop a novel trust-region (TR) based integration scheme tailored for constitutive model integration
  - Analyze robustness
  - Address scaling inherit to non-linear optimization schemes
  - Investigate impact of algorithmic parameters on performance

MODELING

Plasticity Models

- Consider two different plasticity models/yield surfaces:
  - Non-quadratic Hosford
  - Anisotropic and non-quadratic Barlat (Yld2004-18P)
  - 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:

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

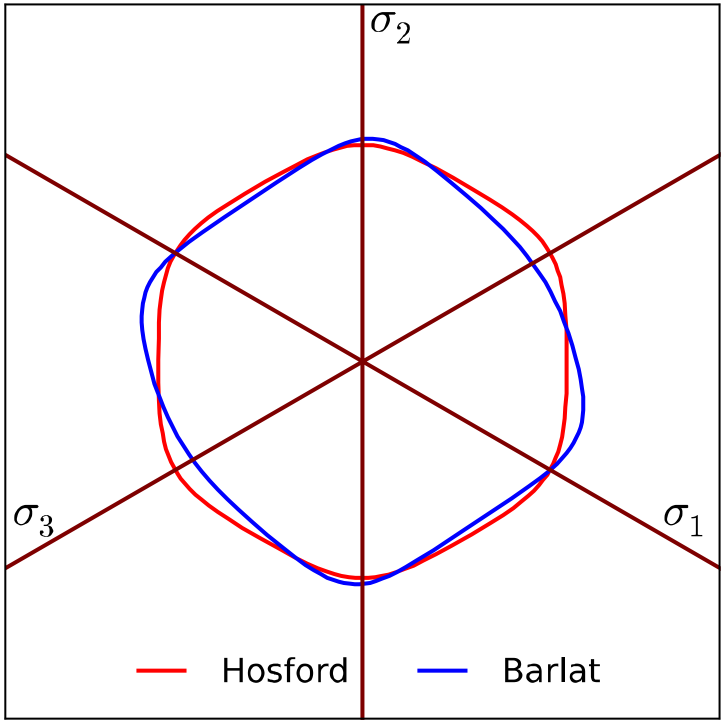
Assoc. Flow Rule:

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

KKT Conditions:

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

Considered Yield Surfaces

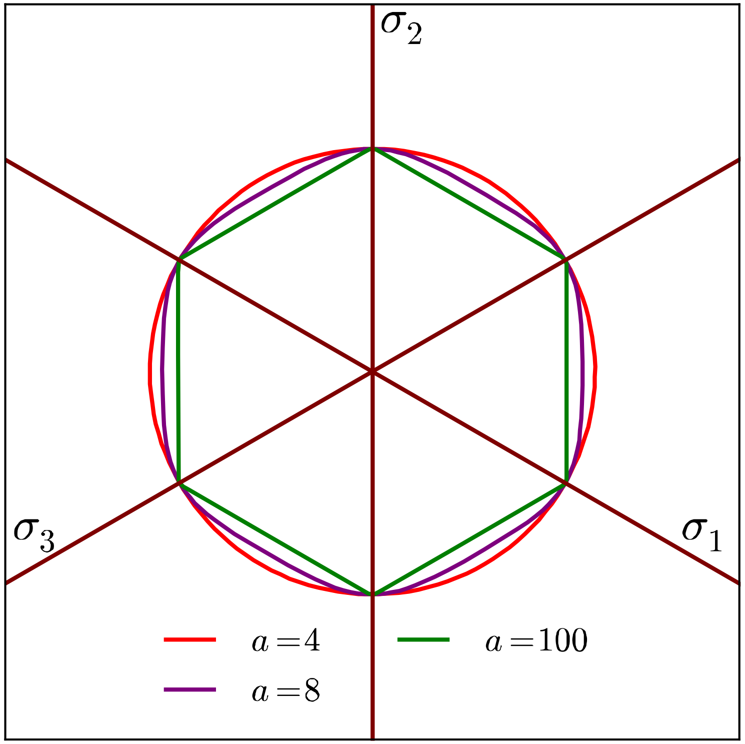


Hosford Yield Surface

- Non-quadratic yield surface requiring only two parameters
  - If $a = 2,\ 4,$ the surface reduces to the von Mises form
  - $a \to \infty$ yields the Tresca condition

Hosford yield surface with different

$$\phi\left(\sigma_{ij}\right) = \left[\frac{1}{2}\left(\left|\sigma_1 - \sigma_2\right|^a \right.\right. \\ \left. + \left|\sigma_2 - \sigma_3\right|^a \right. \\ \left.\left. + \left|\sigma_3 - \sigma_1\right|^a\right)\right]^{1/a}$$



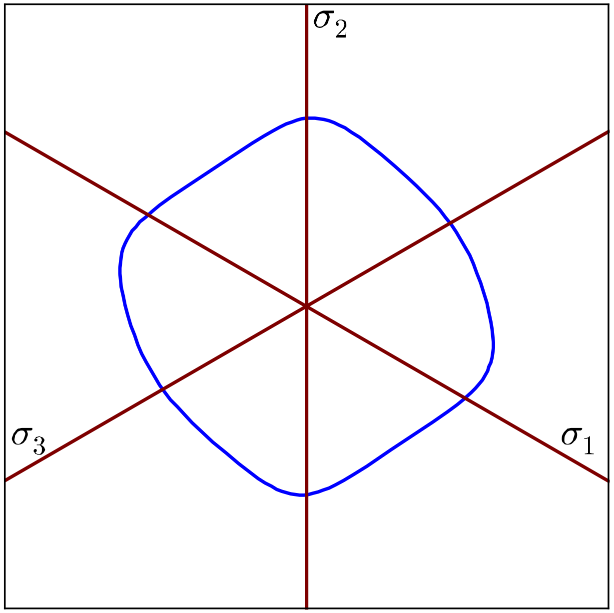
Barlat (Yld2004-18P) Yield Surface

- Anisotropic and non-quadratic yield surface

$$\phi\left(\sigma_{ij}\right) = \left\{ \frac{1}{4} \left[|s'_1 - s''_1|^a + |s'_1 - s''_2|^a + |s'_1 - s''_3|^a \right.\right.$$
$$+ |s'_2 - s''_1|^a + |s'_2 - s''_2|^a + |s'_2 - s''_3|^a$$
$$\left.\left. + |s'_3 - s''_1|^a + |s'_3 - s''_2|^a + |s'_3 - s''_3|^a \right] \right\}^{1/a}$$

$$s'_{ij} = C'_{ijkl} s_{kl} \ ; \ s''_{ij} = C''_{ijkl} s_{kl}$$

$$[C'] = \begin{bmatrix} 0 & -c'_{12} & -c'_{13} & 0 & 0 & 0 \\ -c'_{21} & 0 & -c'_{23} & 0 & 0 & 0 \\ -c'_{31} & -c'_{32} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c'_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c'_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c'_{66} \end{bmatrix}$$



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

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

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

- With a equal weighted, stress normalization:

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

Trust-Region Based Solver

- Step 1: Construct a scaled model problem, $\tilde{m}^{(k)}(\tilde{p}_I)$
- Step 2: With $\alpha^{(k)} = 1$, find $\tilde{p}_I^{(k)}$ minimizing model problem in trusted domain, $\tilde{\Delta}^{(k)}$
- Step 3: Calculate improvement, $\rho^{(k)}$, of a given trial increment, $\tilde{p}_I^{(k)}$
- Step 4: Update variables:
  - If $\rho^{(k)} \geq \mathrm{tol}$:
    - Accept trial solution
    - Keep/increase $\tilde{\Delta}^{(k+1)}$ depending on
  - If $\rho^{(k)} < \mathrm{tol}$:
    - Reject trial solution
    - Decrease $\tilde{\Delta}^{(k+1)}$ for next iteration

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

$$\tilde{\Delta}^{(k)} \geq ||\tilde{p}^{(k)}||$$

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

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

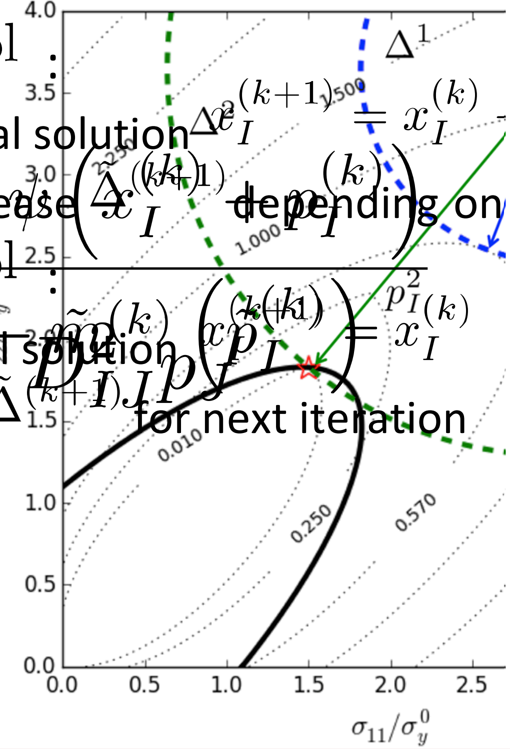
$$\rho^{(k)} = \frac{\psi\left(x_I^{(k)}\right) - \psi\left(x_I^{(k)} + p_I^{(k)}\right)}{\tilde{m}^{(k)}(0) - \tilde{m}^{(k)}\left(\tilde{p}_I^{(k)}\right)}$$

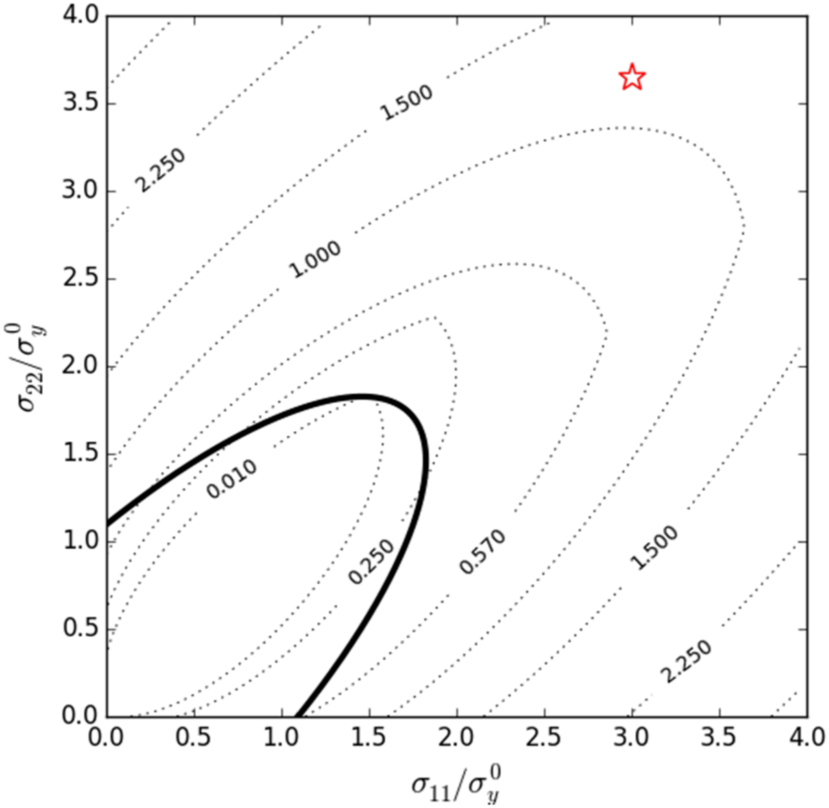
$$x_I^{(k+1)} = x_I^{(k)} +$$

$$x_I^{(k+1)} = x_I^{(k)}$$

$$p_I = D_{IJ}\tilde{p}_J$$

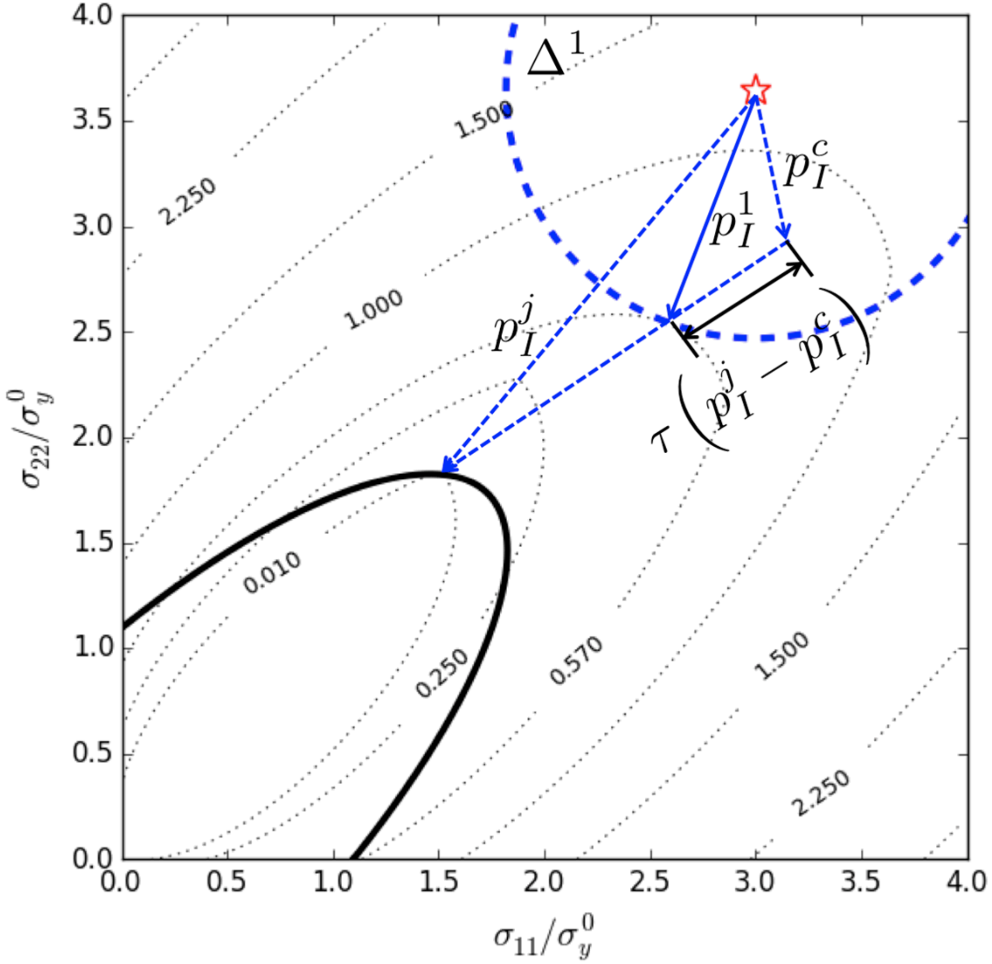
$$D_{IJ}^2 = \Big[$$





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:

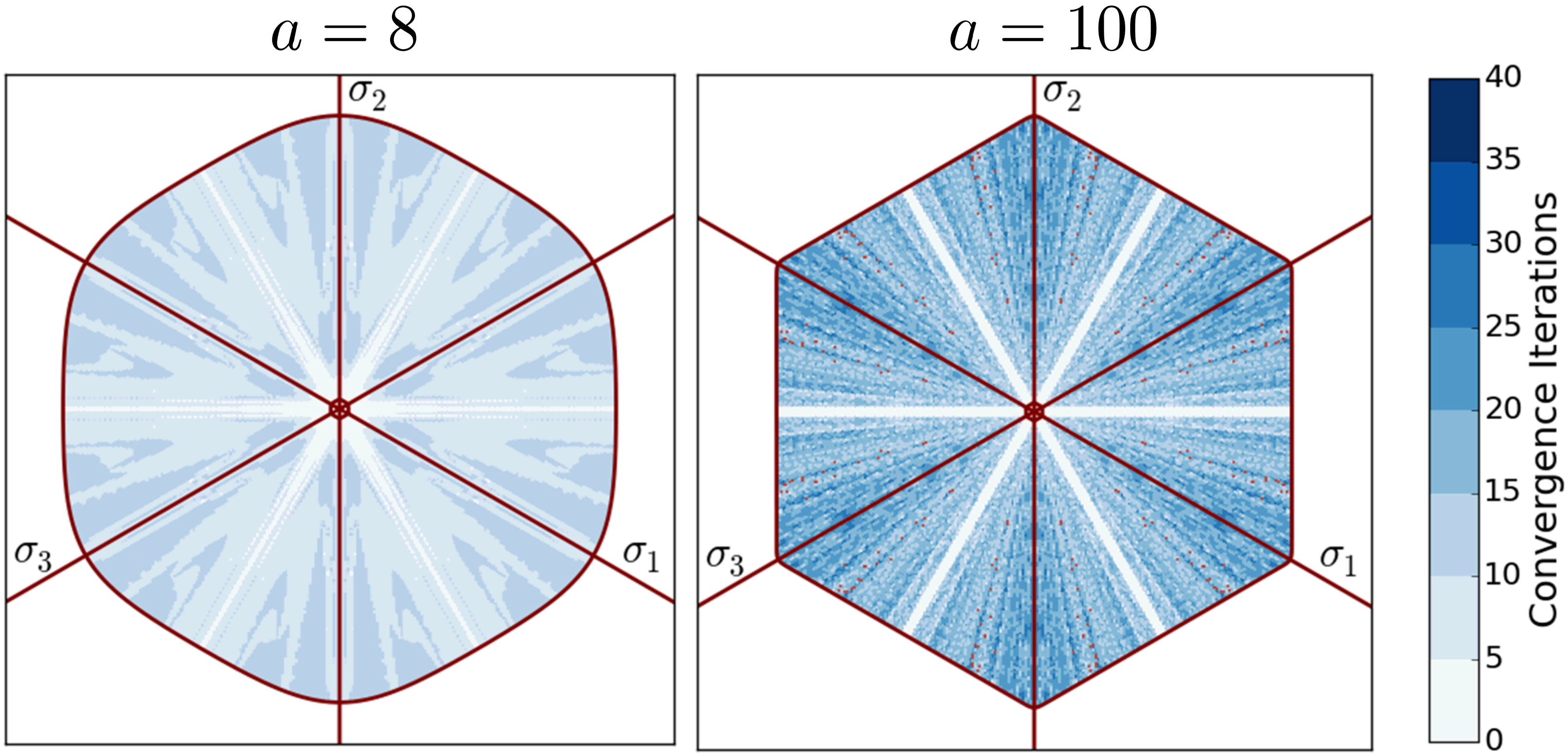
$$\tilde{p}_I^{j(k)} = -\left(\tilde{B}^{(k)}\right)^{-1}_{IJ} \tilde{g}_J^{(k)}$$

Performance of Trust-Region Approach (Hosford)

RESULTS

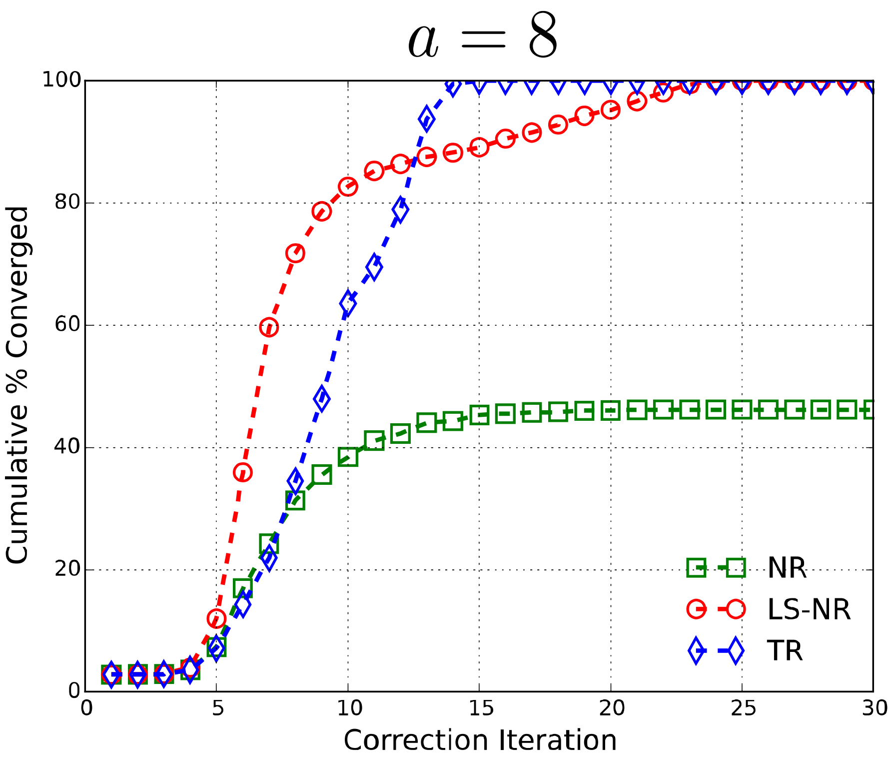
Convergence Maps

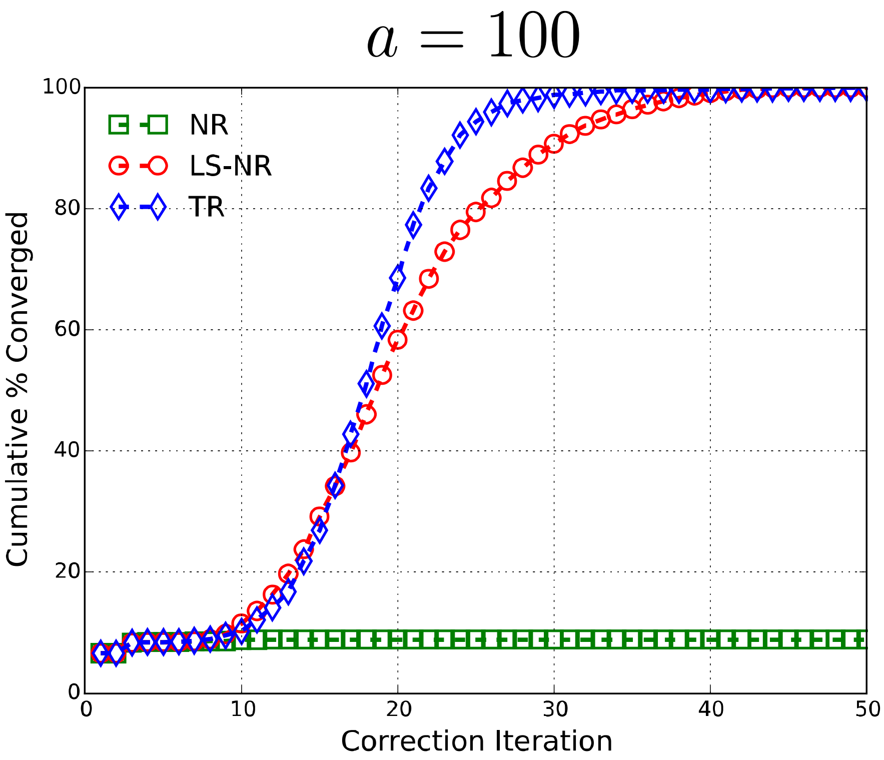
- Determine number of correction iterations needed for TR algorithm at $\phi\left(\sigma_{ij}\right) \leq 30\sigma_y^0$



- Proposed algorithm converges for nearly every trial stress

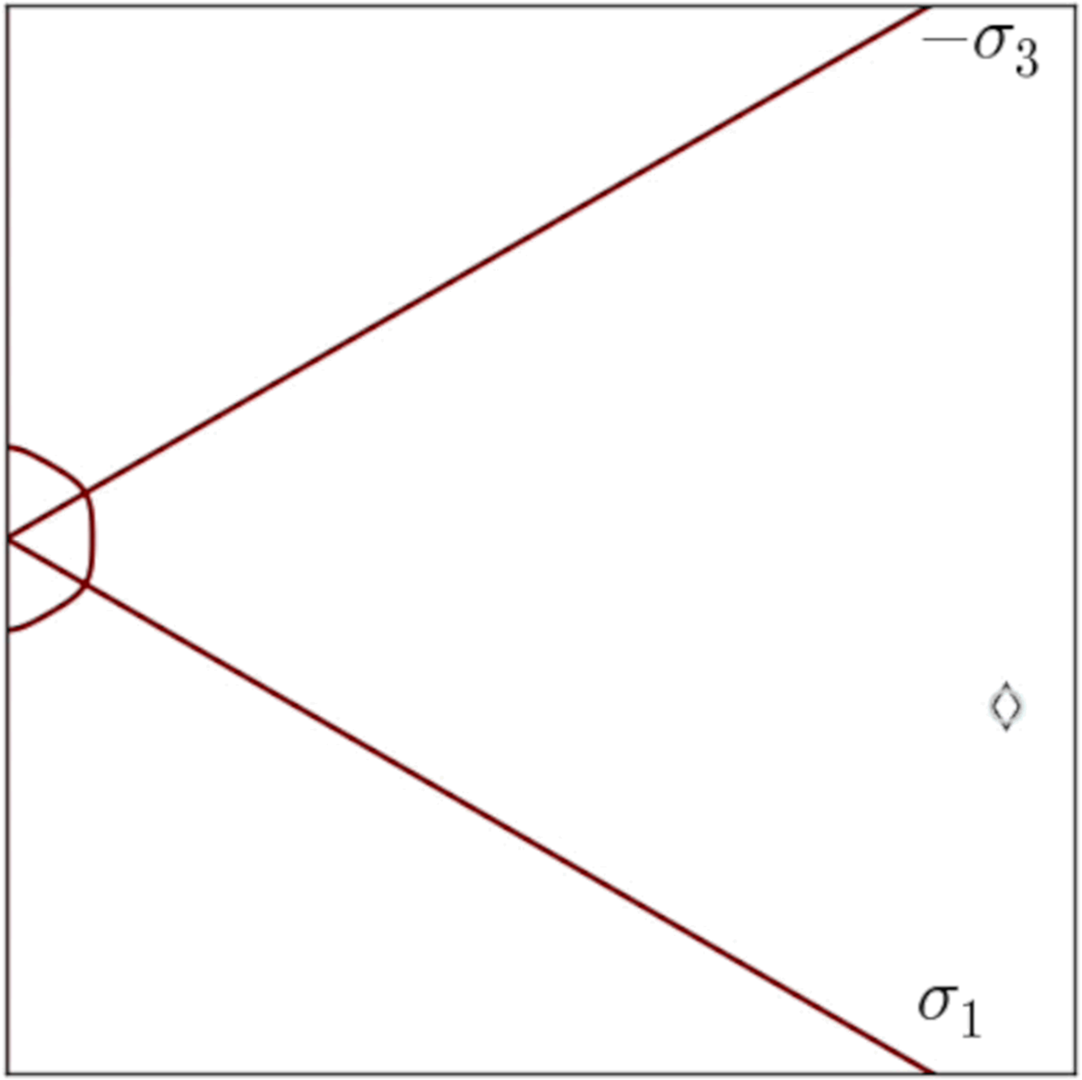
Cumulative Convergence Distributions



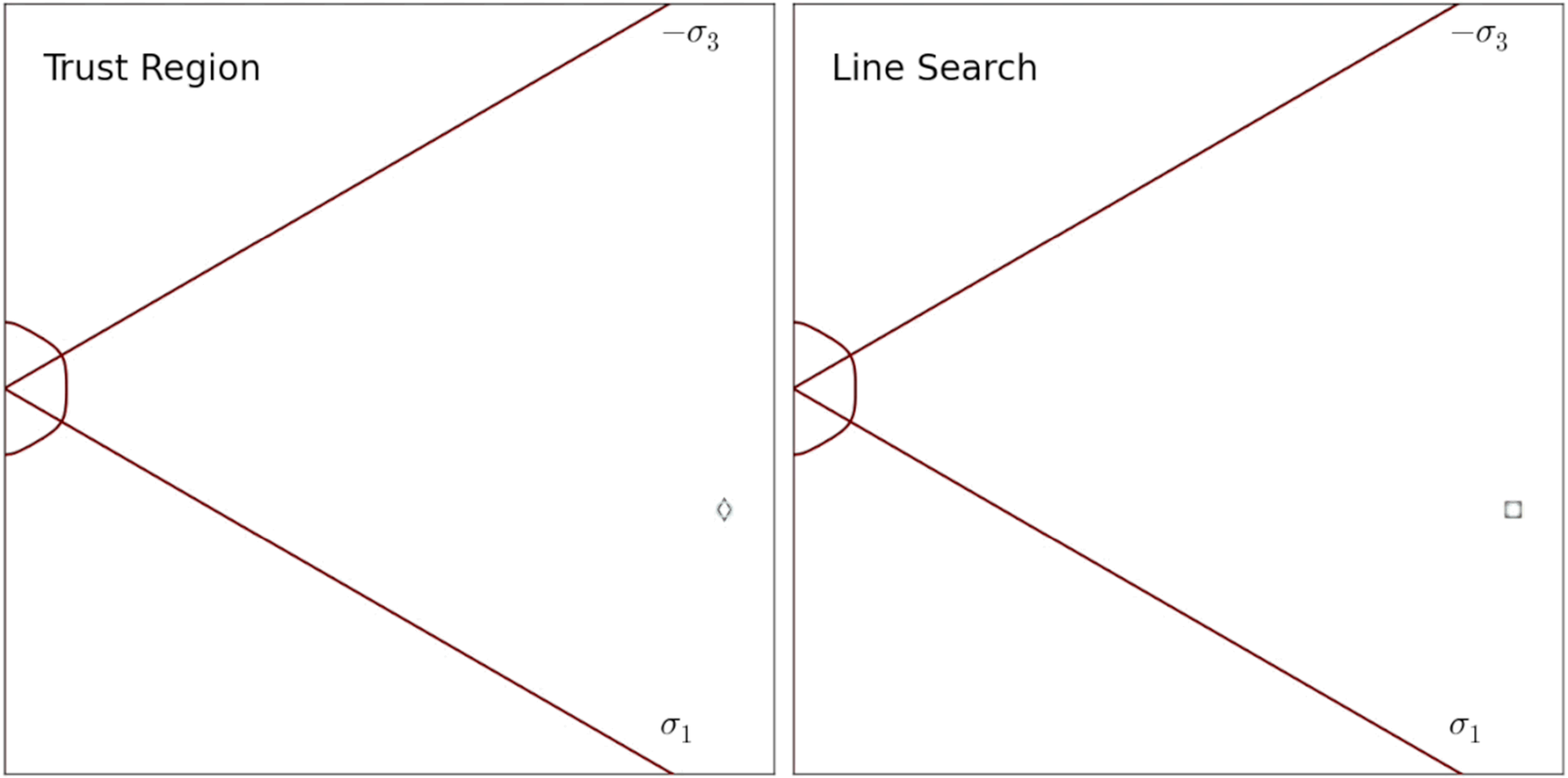


- Convergence of TR method well in excess of traditional NR
  - Comparable with LS-NR
  - TR better at higher iterations

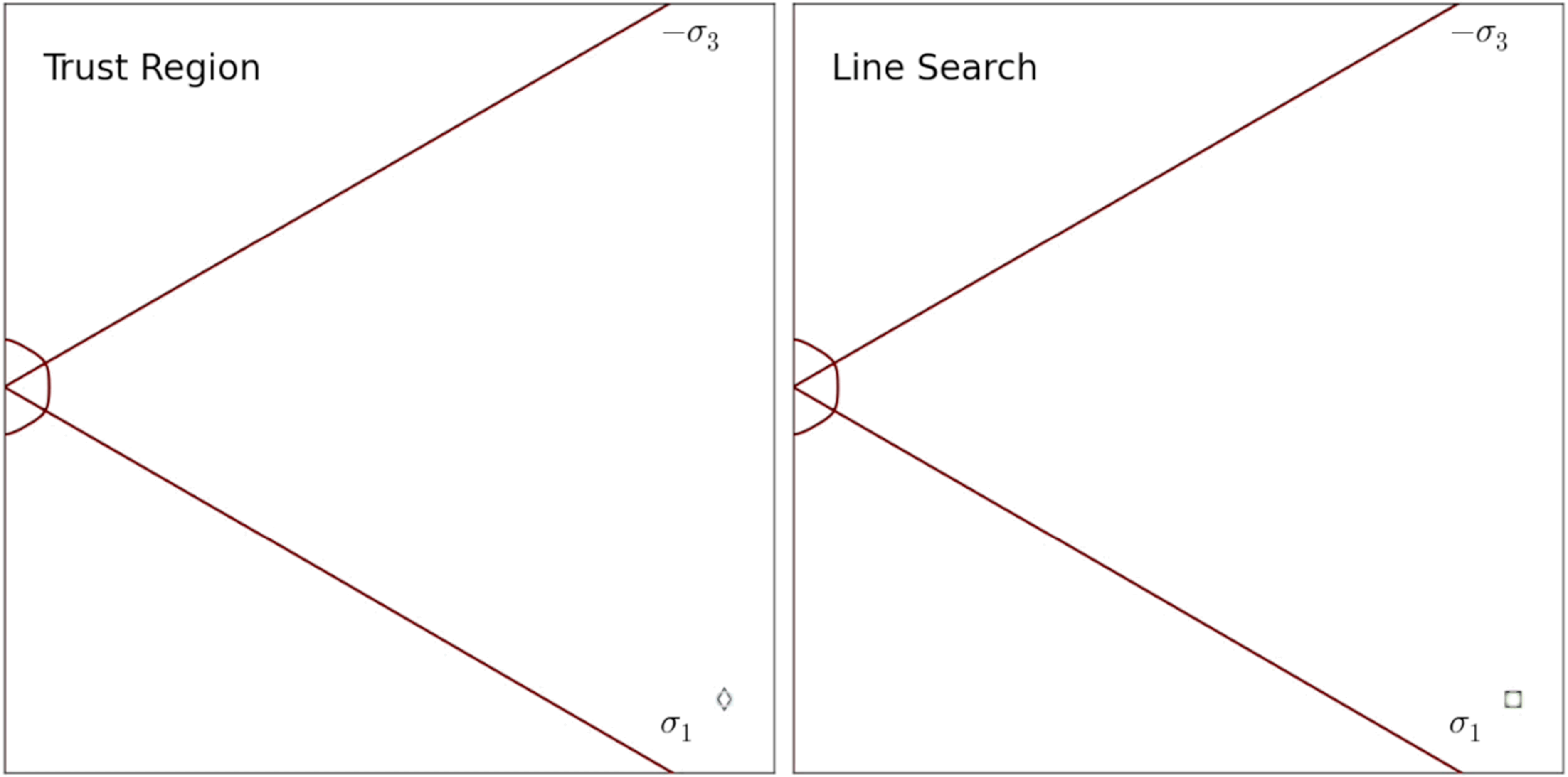
Trust-Region Return Trajectory



Return Trajectory – Comparison (A)

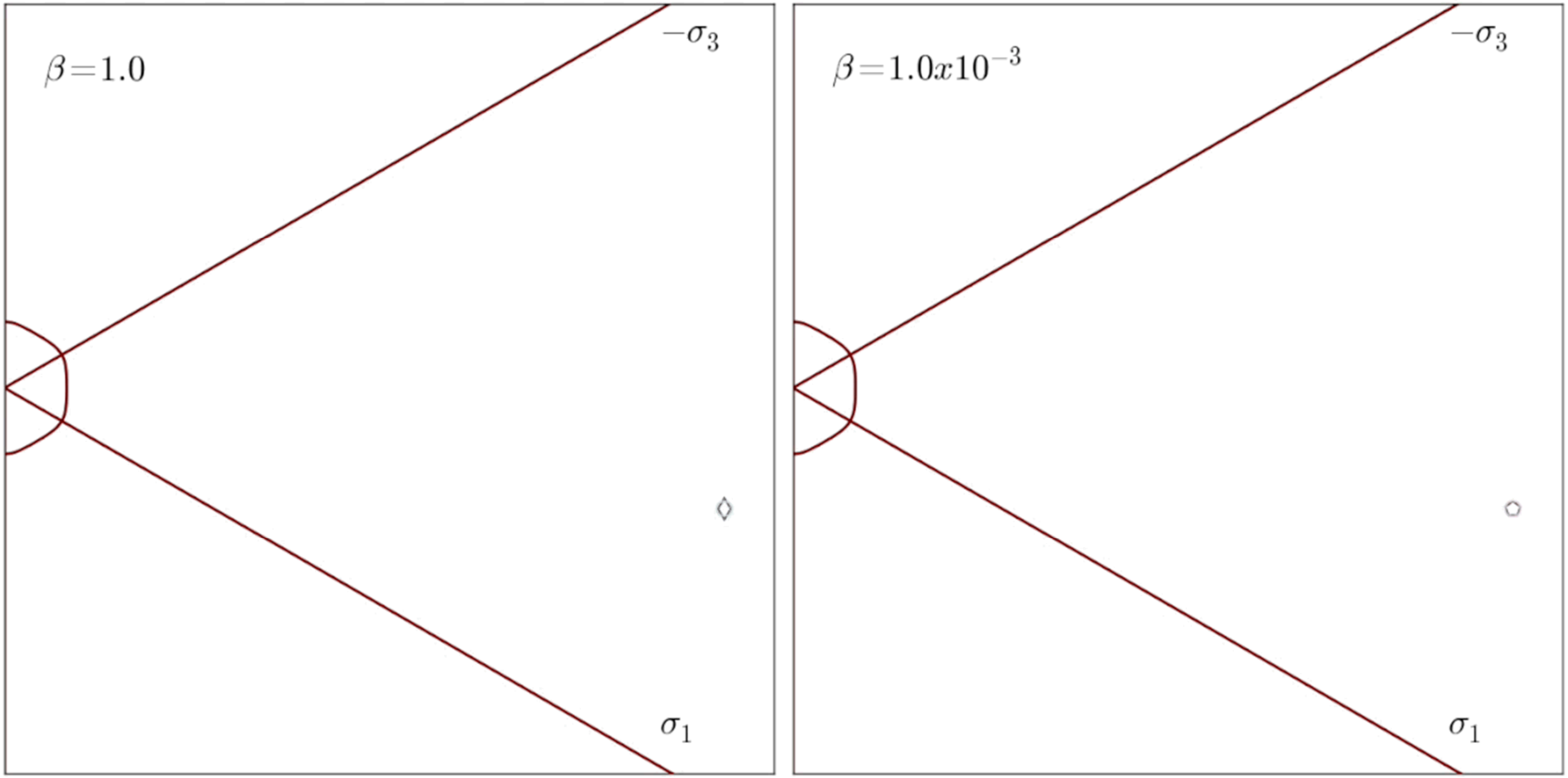


Return Trajectory – Comparison (B)



Scaling in TR

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



Impact of Algorithmic Parameters (Barlat)

RESULTS

Algorithmic Parameters

- Use of non-linear optimization schemes introduces series of algorithmic parameters
  - Scaling in residual, state variables
  - Acceptability conditions
  - Values often taken from optimization literature – not RMA tailored
- How does the choice of these parameters affect performance?
- First look at merit function normalization:

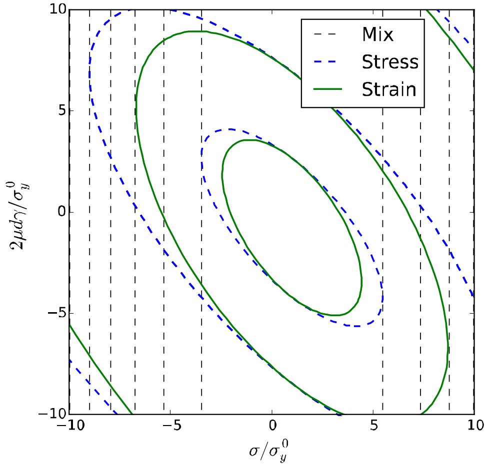
Stress Normalized: $\psi_1^{\sigma}\left(r_I\right) = \frac{1}{2}\left(\left(\frac{E}{\sigma_y^0}\right)^2 r_{ij}^{\varepsilon} r_{ij}^{\varepsilon} + \left(\frac{r^f}{\sigma_y^0}\right)^2\right)$

Strain Normalized: $\psi_2^{\varepsilon}\left(r_I\right) = \frac{1}{2}\left(r_{ij}^{\varepsilon} r_{ij}^{\varepsilon} + \left(\frac{r^f}{2\mu}\right)^2\right)$

Mixed Measure: $\psi_3\left(r_I\right) = \frac{1}{2}\left(r_{ij}^{\varepsilon} r_{ij}^{\varepsilon} + \left(r^f\right)^2\right)$

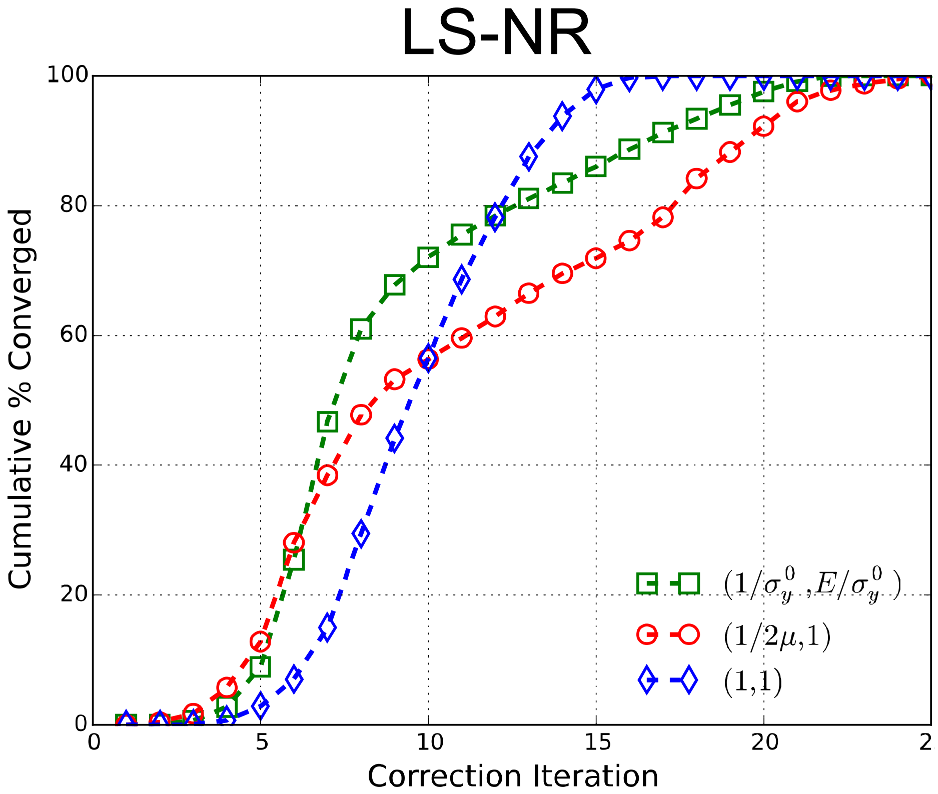
$$c^{W\varepsilon} = c^{Wf} = 1$$

1D Idealization of Different Merit Functions

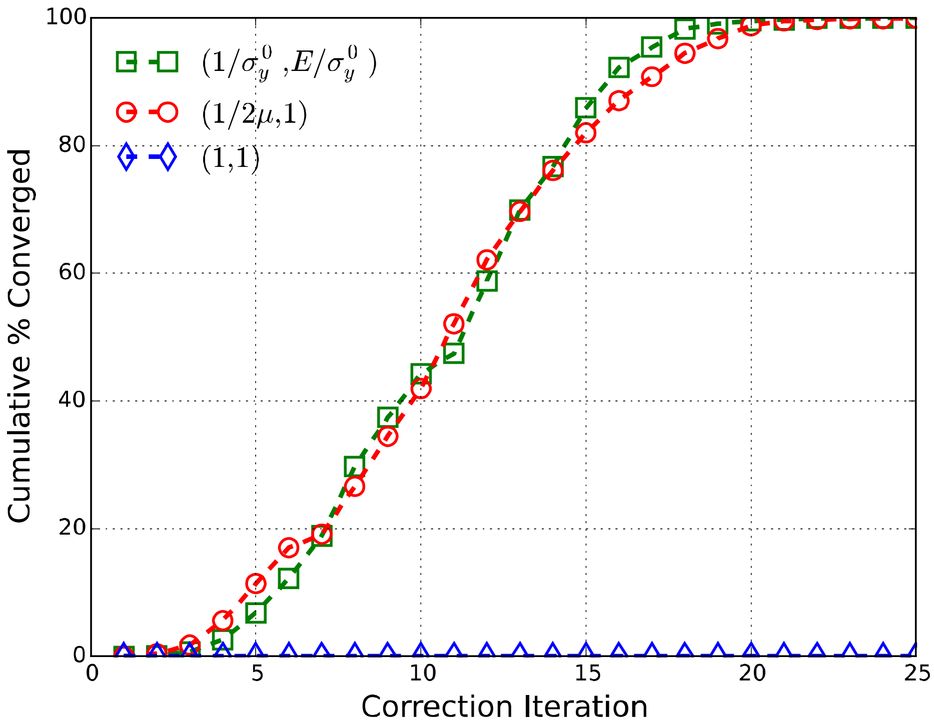


Barlat CCDs -- Normalization

- LS-NR shows stronger dependence on merit function selection
  - Scaled forms do better at lower iterations; Mixed first to hit 100%
- Mixed measure TR converges < 1% of the time

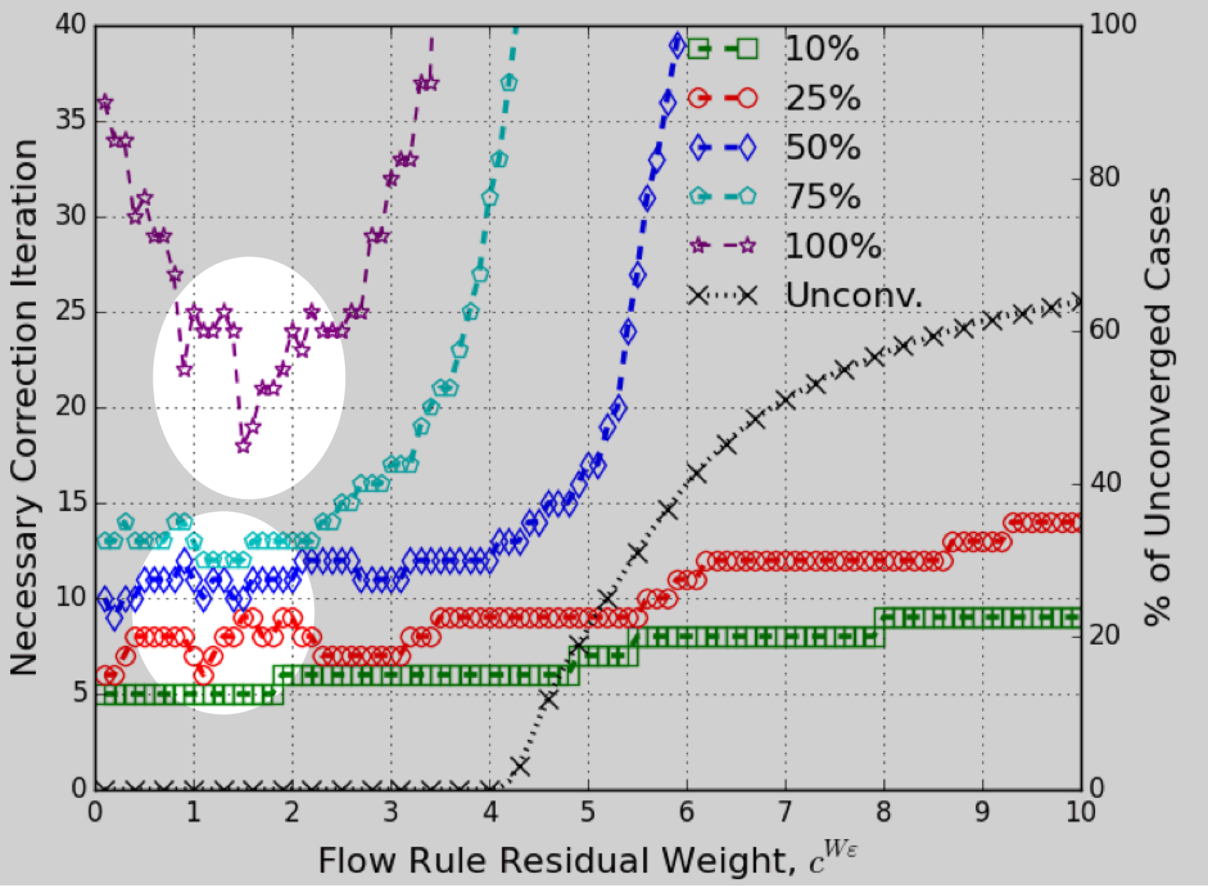


LS-NR



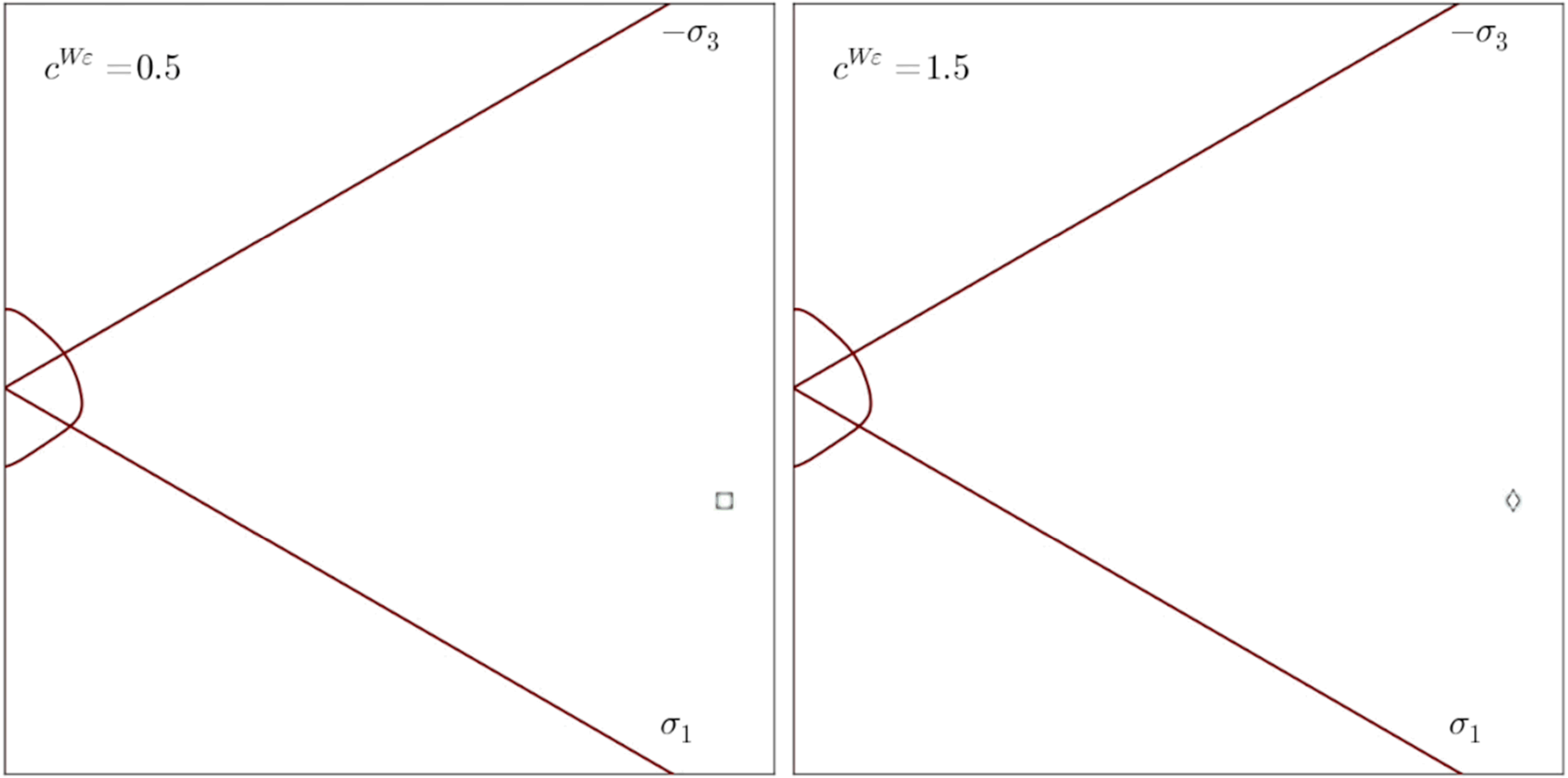
Impact of Weighting

$$\psi_1^\sigma\left(r_I\right)=\frac{1}{2}\left(\left(c^{W\varepsilon}\frac{E}{\sigma_y^0}\right)^2 r_{ij}^\varepsilon r_{ij}^\varepsilon+\left(\frac{r^f}{\sigma_y^0}\right)^2\right)$$



- Weighting can be used aid in selecting appropriate path
- Minimum number of correction iterations **not** at 1

Weighting Return Maps



Conclusions

- Novel implicit integration scheme for CPP-RMA implemented
  - Tailored trust-region approach for complex plasticity models
  - Scales addressed in both state variables and merit functions

- Investigated impact of algorithmic parameters on RMA performance
  - Appropriate selection can aid performance
  - Way to automatically select scaling?

- This algorithm has potential for more complex problems:
  - Multisurface (e.g. Crystal Plasticity; Multiple inelastic mechanisms)
  - More complex mechanisms (Damage)
  - Coupled multiphysics (thermal-mechanical analysis)

Acknowledgements

- Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04- 94AL85000

- Original inspiration and motivation for this work came arose from discussions with Jakob Ostien, Jay Foulk, and Alejandro Mota (SNL-CA)

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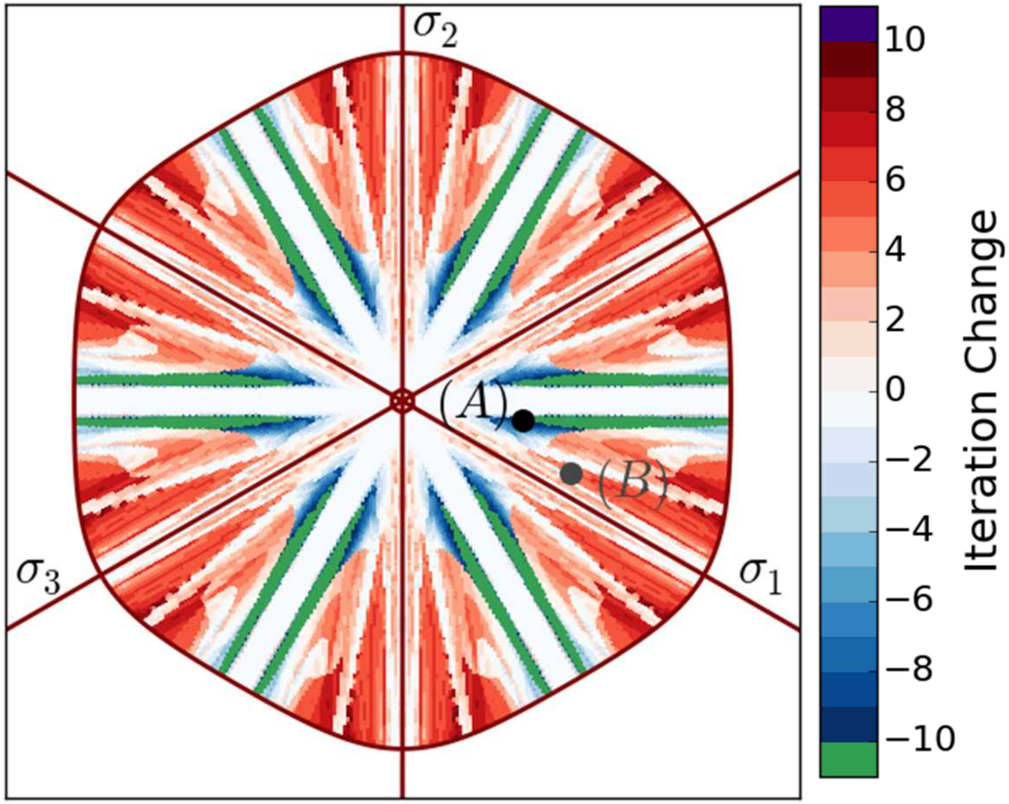
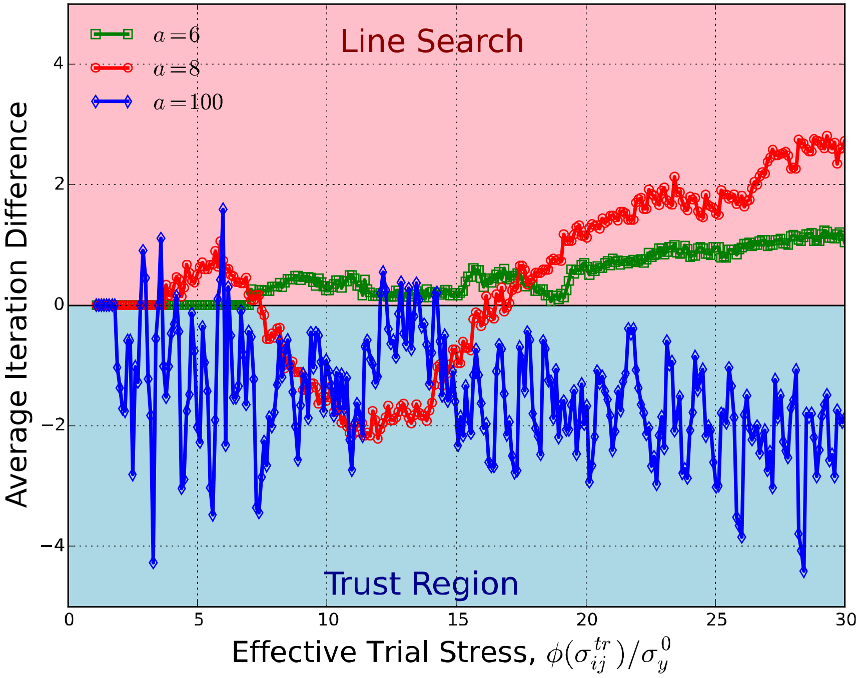
Appendix

Performance: TR vs LS-NR

Iteration change, $a = 8$

$$\mathrm{iter}\,(\mathrm{TR}) - \mathrm{iter}\,(\mathrm{LS})$$

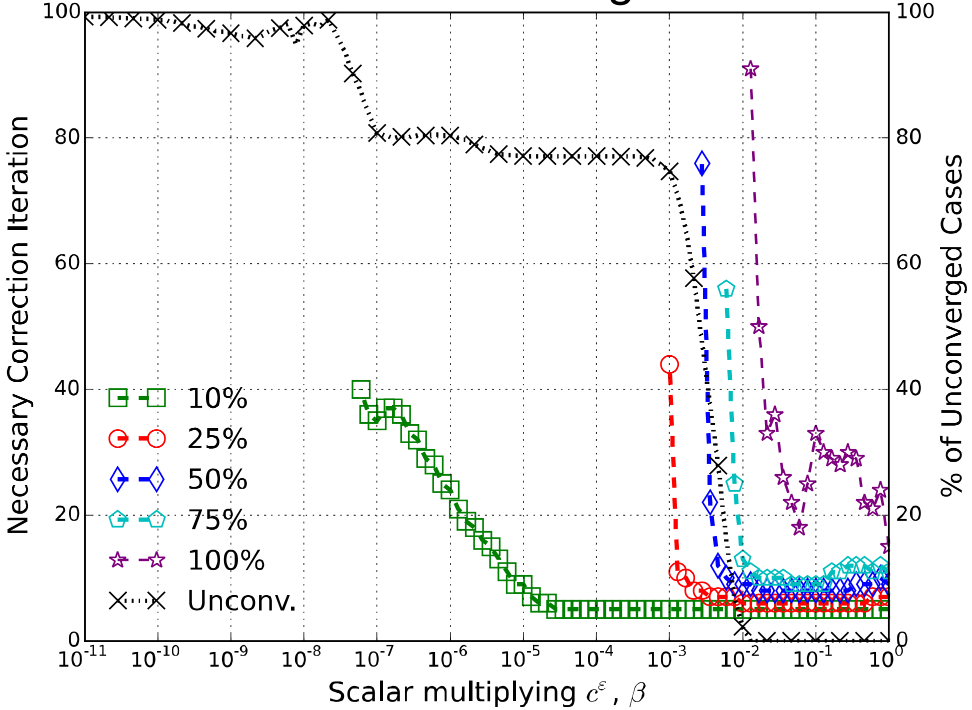




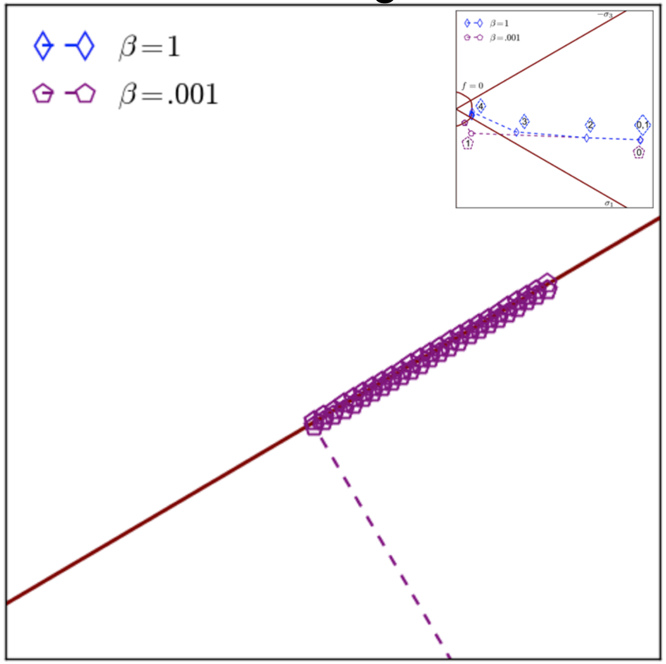
- Regions of large performance increase
- TR seems to do better as (a) increases

Importance of Scaling w/ TR

Convergence Thresholds for Different Scalings



Return Trajectories with Different Scalings

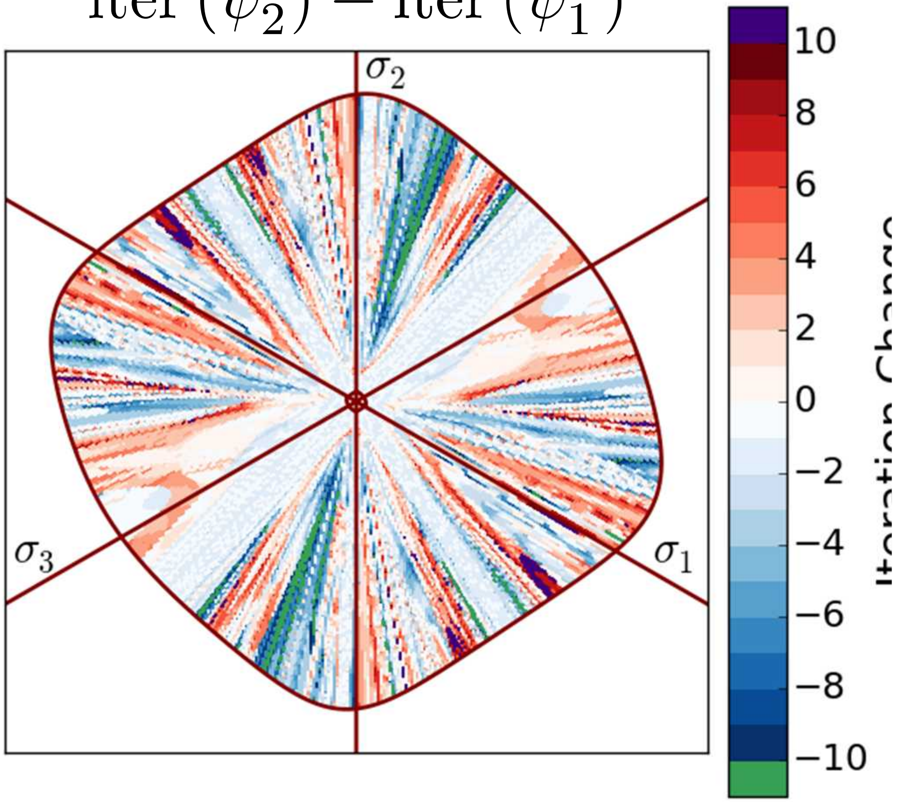


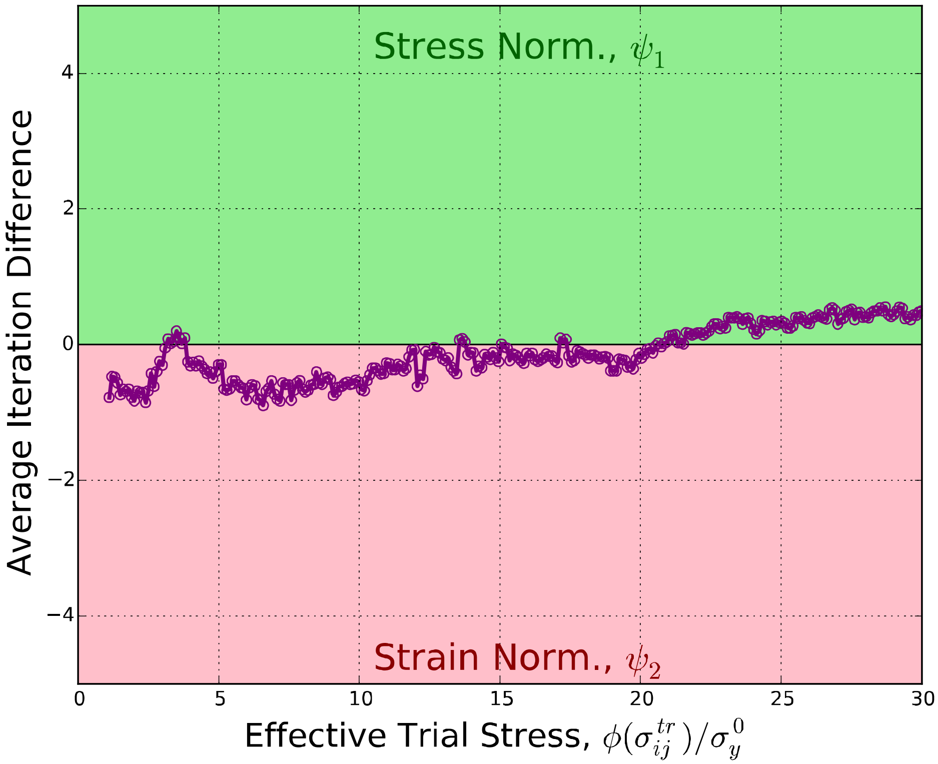
- Appropriately scaling the problem *essential* for TR to converge

Iteration Difference Maps -- Normalization

- Preferable merit function varies with dominant loading
- Limited regions exhibit large differences

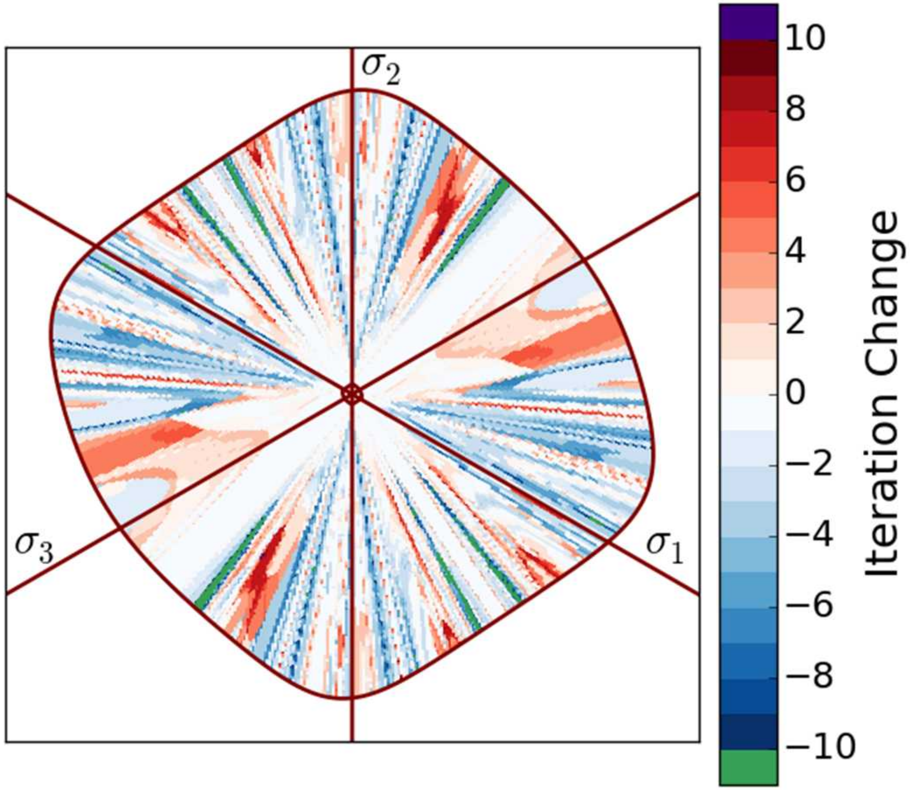
$$\mathrm{iter}\left(\psi_2^{\varepsilon}\right) - \mathrm{iter}\left(\psi_1^{\sigma}\right)$$



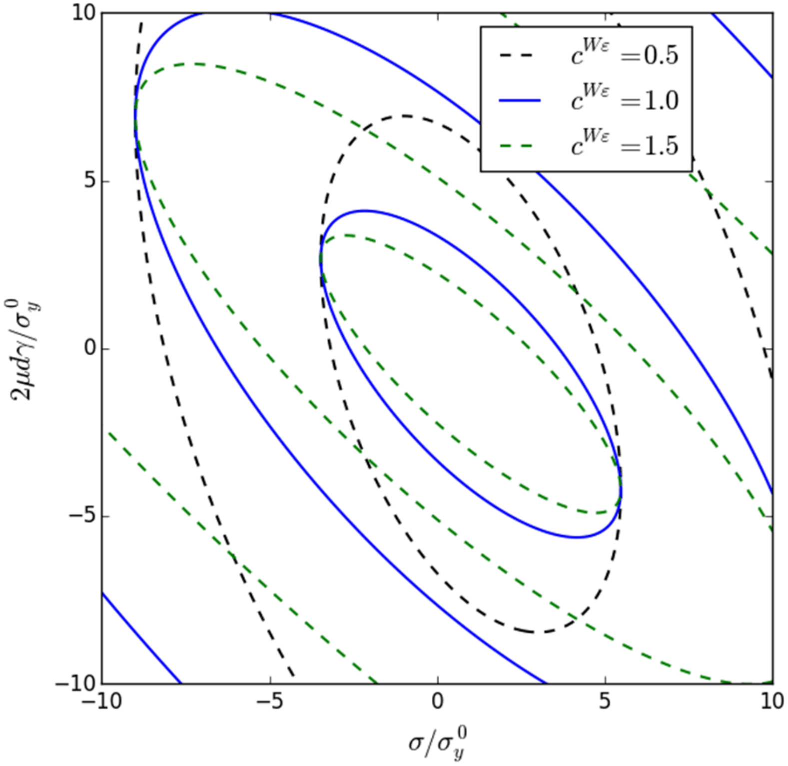


Merit Functions -- Weighting

- Weighting can be used to bias the residual towards either consistency or plastic strain residual
  - Influence return mapping path?



$$\mathrm{iter}\left(c^{W\varepsilon}=1.5\right)-\mathrm{iter}\left(c^{W\varepsilon}=1.0\right)$$



$$\psi_1^{\sigma}$$

Scaled Relations

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

Gradient:

$$\tilde{g}_I^{(k)} = D^1_{LK}r_K^{(k)}D^1_{LJ}J_{JN}^{(k)}\left(D^2\right)^{-1}_{NI}$$

Approximate Hessian:

$$\tilde{B}_{IJ}^{(k)} = \left(D^2\right)^{-1}_{IL}D^1_{MK}J_{KN}^{(k)}D^1_{MA}J_{AL}^{(k)}\left(D^2\right)^{-1}_{NJ}$$

$$\tilde{g}_I^k = \begin{bmatrix} \frac{(c^\varepsilon)^2}{b^\sigma}r_{ij}^{\varepsilon(k)}S_{ijkl}^{ep} + \frac{\left(c^f\right)^2}{b^\gamma}r^{f(k)}\frac{\partial\phi}{\partial\sigma_{ij}^{(k)}}, & \frac{(c^\varepsilon)^2}{b^\gamma}r_{ij}^{\varepsilon(k)}\frac{\partial\phi}{\sigma_{ij}^{(k)}} - \frac{\left(c^f\right)^2}{b^\gamma}r^{f(k)}\frac{\partial\sigma_y}{\partial\bar{\varepsilon}^{p(k)}} \end{bmatrix}^T$$

$$\tilde{B}_{IJ}^k = \begin{bmatrix} \left(\frac{c^\varepsilon}{b^\sigma}\right)^2 S_{ijrs}^{ep}S_{rskl}^{ep} + \left(\frac{c^f}{b^\sigma}\right)^2\frac{\partial\phi}{\partial\sigma_{ij}^{(k)}}\frac{\partial\phi}{\partial\sigma_{kl}^{(k)}}, & \frac{(c^\varepsilon)^2}{b^\sigma b^\gamma}S_{ijrs}^{ep}\frac{\partial\phi}{\partial\sigma_{rs}^{(k)}} - \frac{\left(c^f\right)^2}{b^\sigma b^\gamma}\frac{\partial\sigma_y}{\partial\bar{\varepsilon}^{p(k)}}\frac{\partial\phi}{\partial\sigma_{ij}^{(k)}} \\ \frac{(c^\varepsilon)^2}{b^\sigma b^\gamma}S_{klrs}^{ep}\frac{\partial\phi}{\partial\sigma_{rs}^{(k)}} - \frac{\left(c^f\right)^2}{b^\sigma b^\gamma}\frac{\partial\sigma_y}{\partial\bar{\varepsilon}^{p(k)}}\frac{\partial\phi}{\partial\sigma_{kl}^{(k)}}, & \left(\frac{c^\varepsilon}{b^\gamma}\right)^2\frac{\partial\phi}{\partial\sigma_{rs}^{(k)}}\frac{\partial\phi}{\partial\sigma_{rs}^{(k)}} + \left(\frac{c^f}{b^\gamma}\right)^2\frac{\partial\sigma_y}{\partial\bar{\varepsilon}^{p(k)}}\frac{\partial\sigma_y}{\partial\bar{\varepsilon}^{p(k)}} \end{bmatrix}$$

Selecting TR Size

- For TR, need to set initial, $\tilde{\Delta}^{(0)}$, and maximum, $\bar{\Delta}$, radii
  - Final stress lies between previous converged and trial
  - Maximum plastic strain increment would correspond to input strain
  - Want to enable single step solution

$$\tilde{\Delta}^0 = \bar{\Delta} = b^\sigma \sqrt{\left(\sigma_i^{tr} - \sigma_i^n\right)\left(\sigma_i^{tr} - \sigma_i^n\right)} + b^\gamma d\bar{\varepsilon}$$

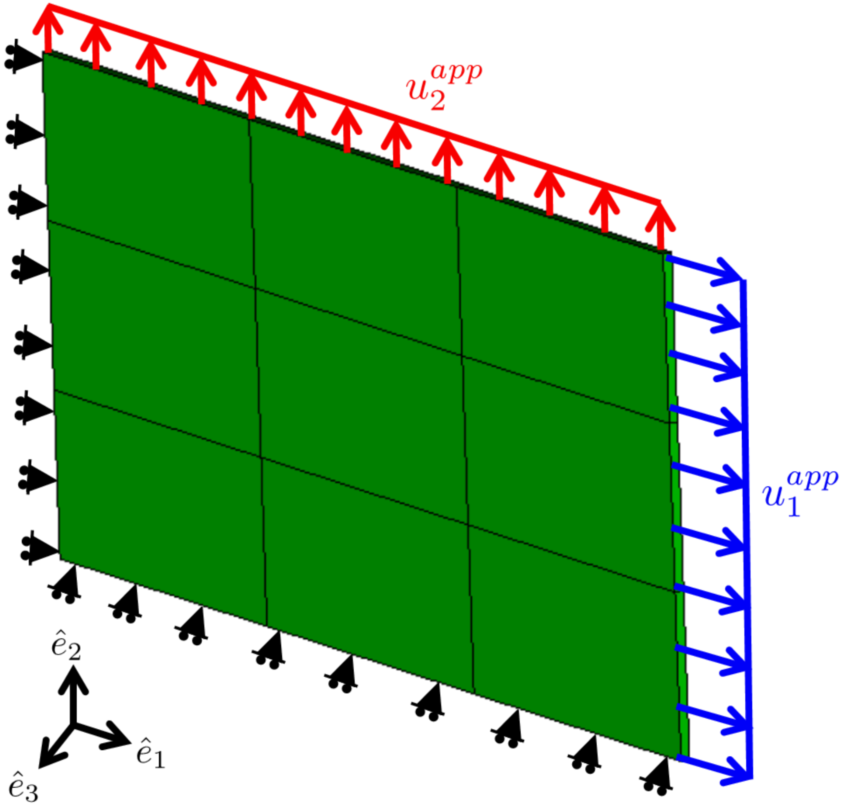
$$d\bar{\varepsilon} = \sqrt{\frac{2}{3} d\varepsilon_{ij}^{n+1} d\varepsilon_{ij}^{n+1}}$$

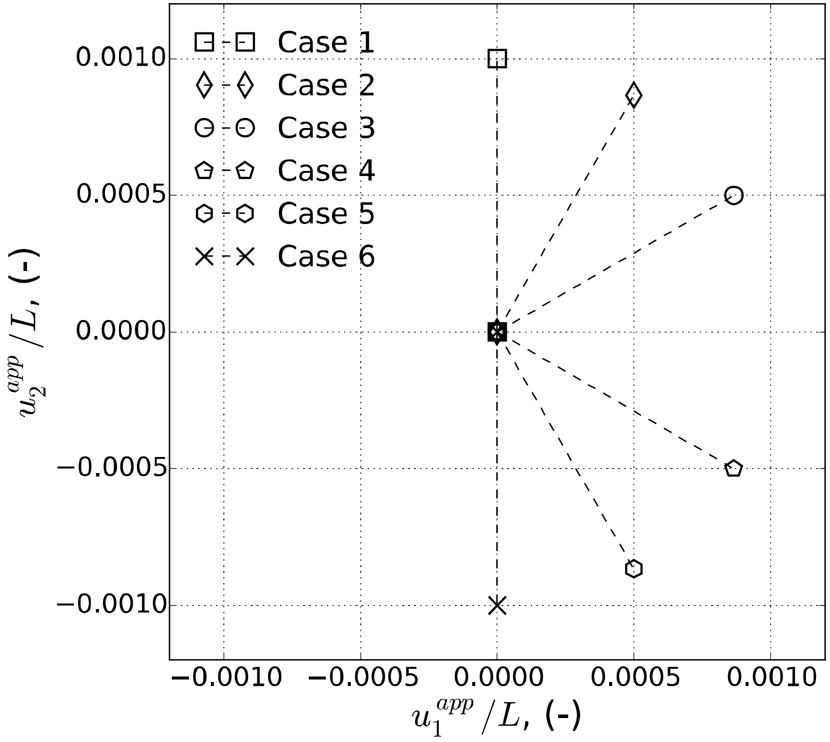
- For robustness analysis

$$\bar{\Delta} = b^\sigma \sqrt{\left(\phi\left(\sigma_{ij}^{tr}\right) - \sigma_y^0\right)\left(\phi\left(\sigma_{ij}^{tr}\right) - \sigma_y^0\right)} + b^\gamma \sqrt{\frac{2}{3} \mathbb{S}_{ijk} \sigma_{kl}^{tr} \mathbb{S}_{ijmn} \sigma_{mn}^{tr}}$$

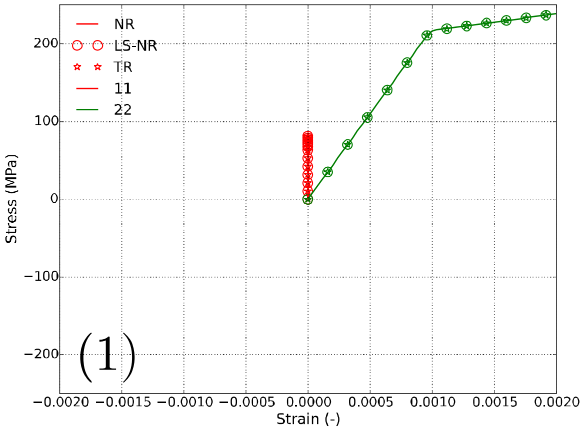
Verification

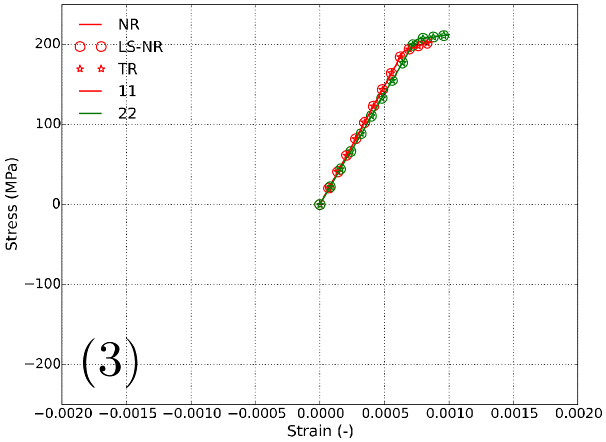
- Verification through Sierra/SM
- Consider series of plane stress, biaxial displacement problems

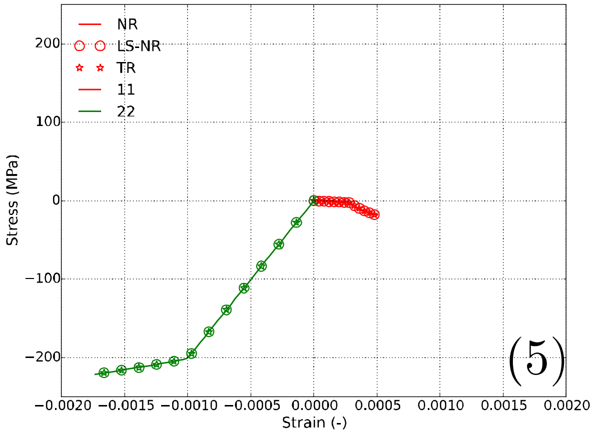


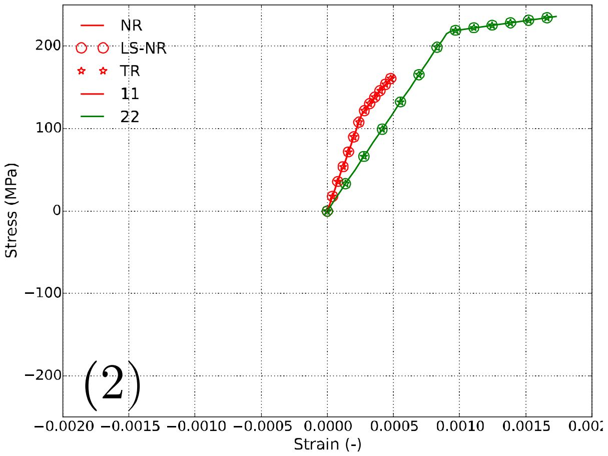


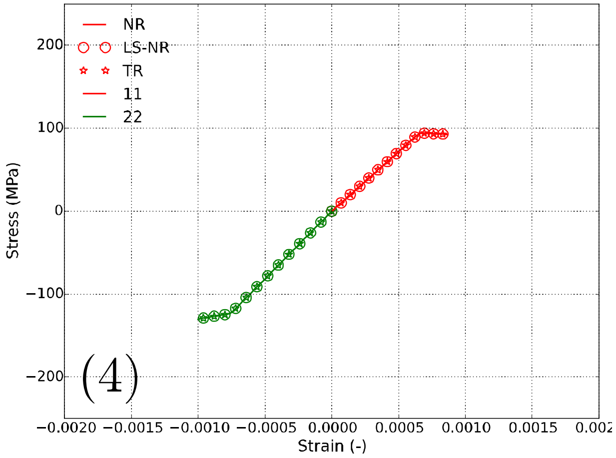
Verification -- Results

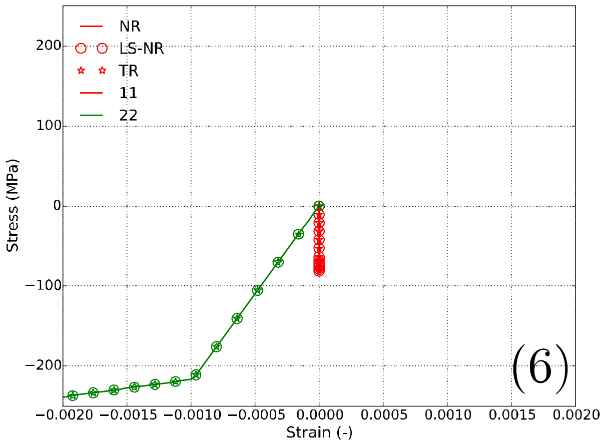






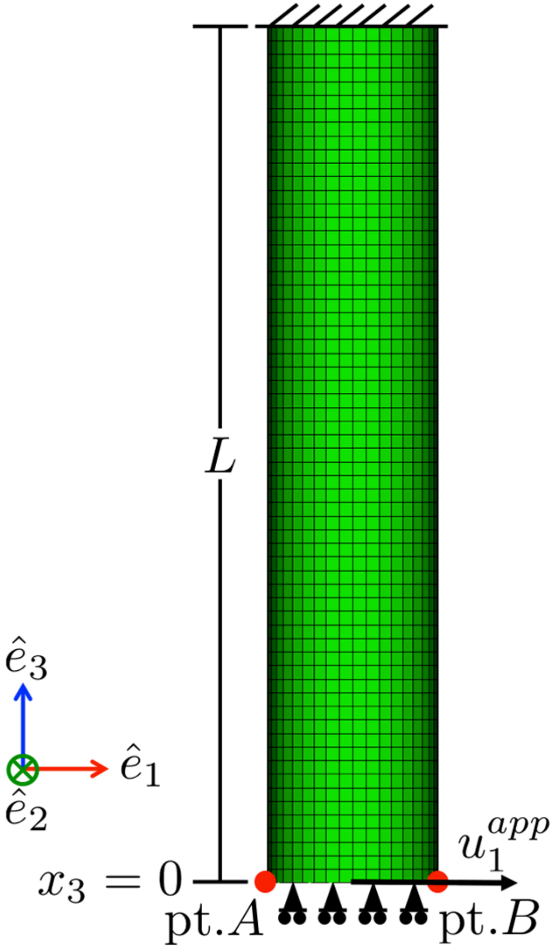


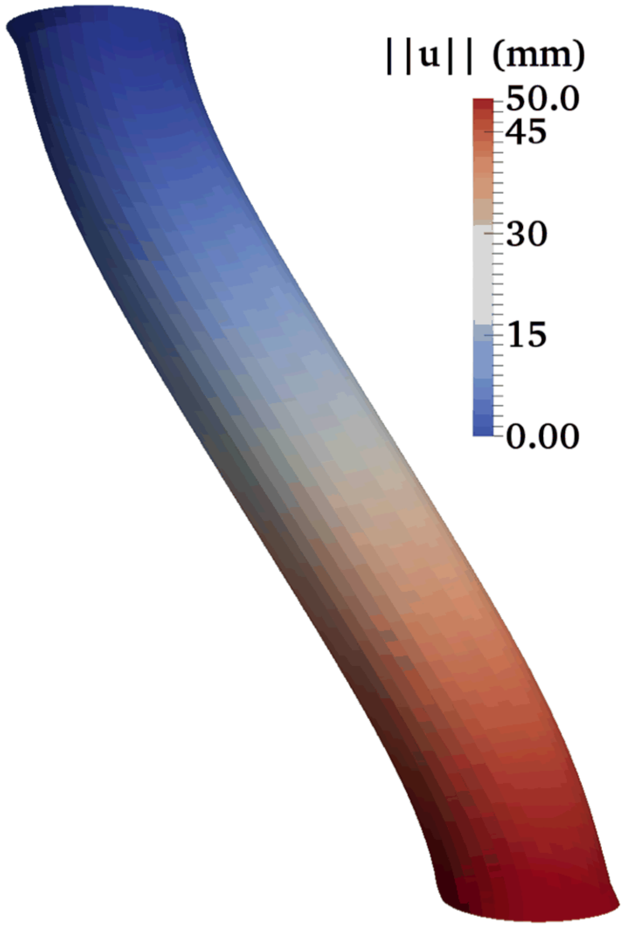




Verification – Large Problem

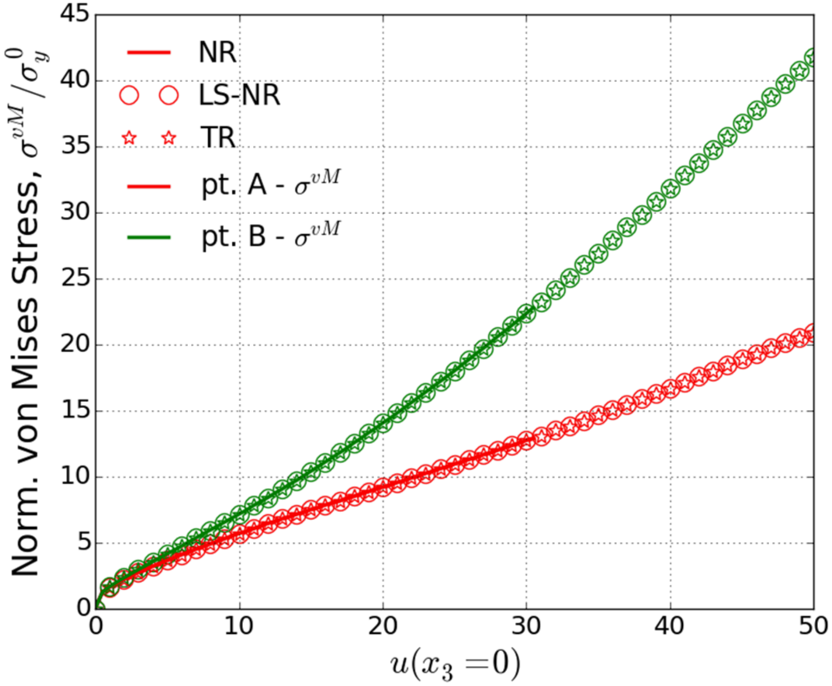
- Rod in Tension and Shear Problem
- Previously considered by Shterenlikht and Alexander

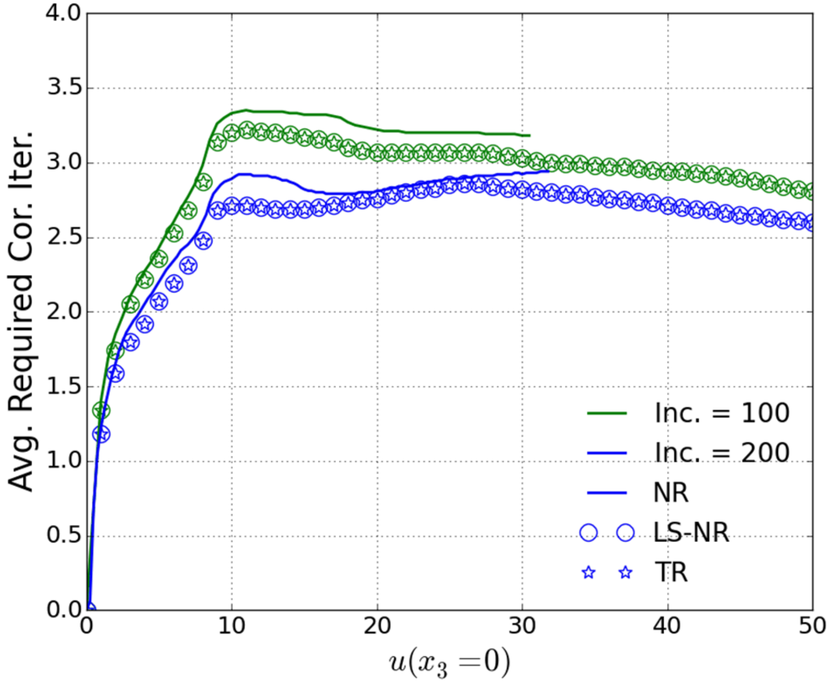




Verification -- Rod Results

- NR Cannot finish simulation





Material Parameters

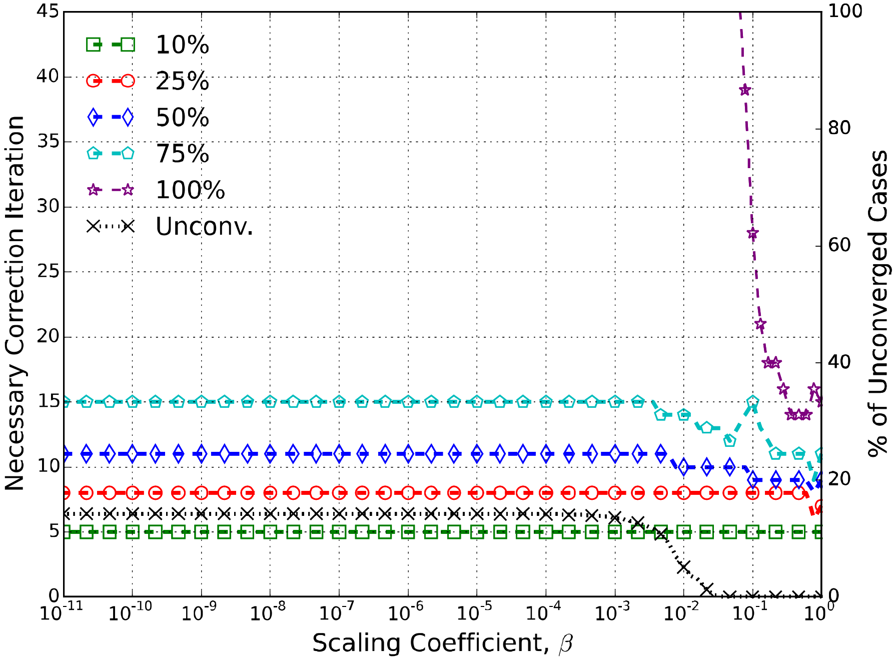
$$E = 200 \text{ GPa} \qquad \sigma_y^0 = 200 \text{ MPa}$$

$$\nu = 0.3 \qquad a = 8$$

c'_{12}	-0.069888	c''_{12}	0.981171
c'_{13}	0.936408	c''_{13}	0.476741
c'_{21}	0.079143	c''_{21}	0.575316
c'_{23}	1.003060	c''_{23}	0.866827
c'_{31}	0.524741	c''_{31}	1.145010
c'_{32}	1.363180	c''_{32}	-0.079294
c'_{44}	1.023770	c''_{44}	1.051660
c'_{55}	1.069060	c''_{55}	1.147100
c'_{66}	0.954322	c''_{66}	1.404620

Scaling Impact

$$b^{\gamma} = \beta 2\mu \text{ and } c^{\varepsilon} = \left(E/\sigma_y^0\right)$$



$$b^{\gamma} = \beta 2\mu \text{ and } c^{\varepsilon} = \beta\left(E/\sigma_y^0\right)$$