DESIGN SENSITIVITY ANALYSIS: APPLICATIONS

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January 2003

Introduction

- Overview
- Tangent matrix
- Multi-level Newton method: Coupled analyses
- Multi-level Newton method: Domain decomposition
- Optimization environment

Optimization problem

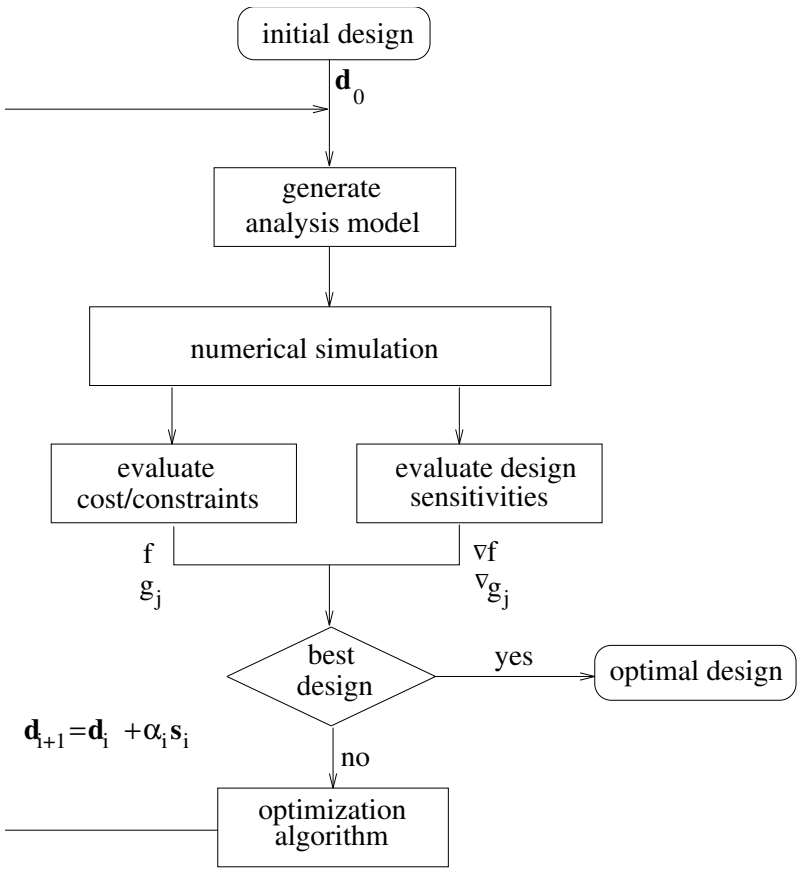
$$\begin{array}{ll} \min\limits_{\mathbf{d}} & F(\mathbf{d}) \\ \text{such that} & G_i(\mathbf{d}) \leq 0, \;\; i = 1, 2, \cdots, n_g \end{array}$$

- $\mathbf{d}$ design parameters
- F cost function
- G_i inequality constraint

Nonlinear Programming Caveats

- Continuous design space
- Deterministic analyses
- Smooth cost and constraint functions
- Local minima

Optimization algorithm

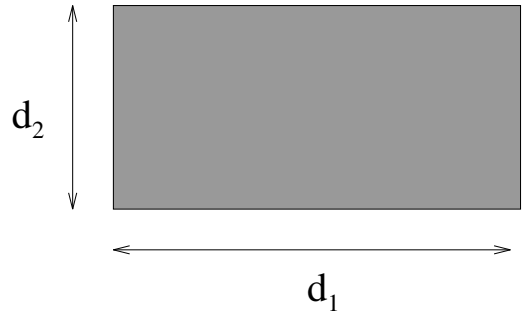


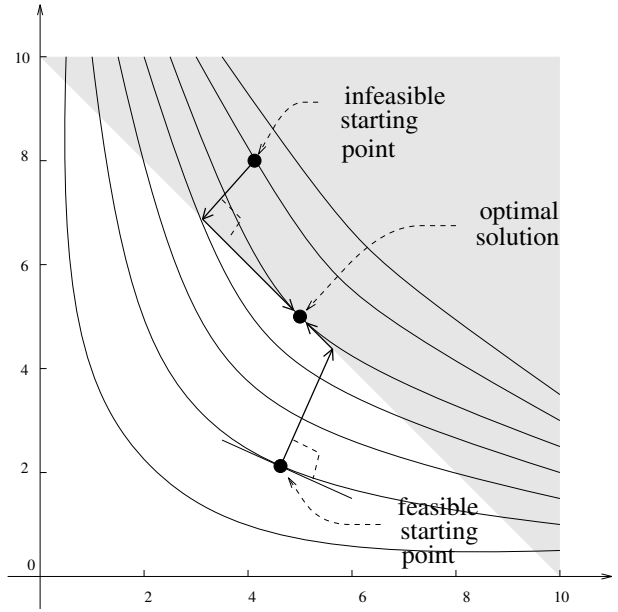
Example: sheet design

- Maximize objective function (surface area)
  $F = d_1\, d_2$

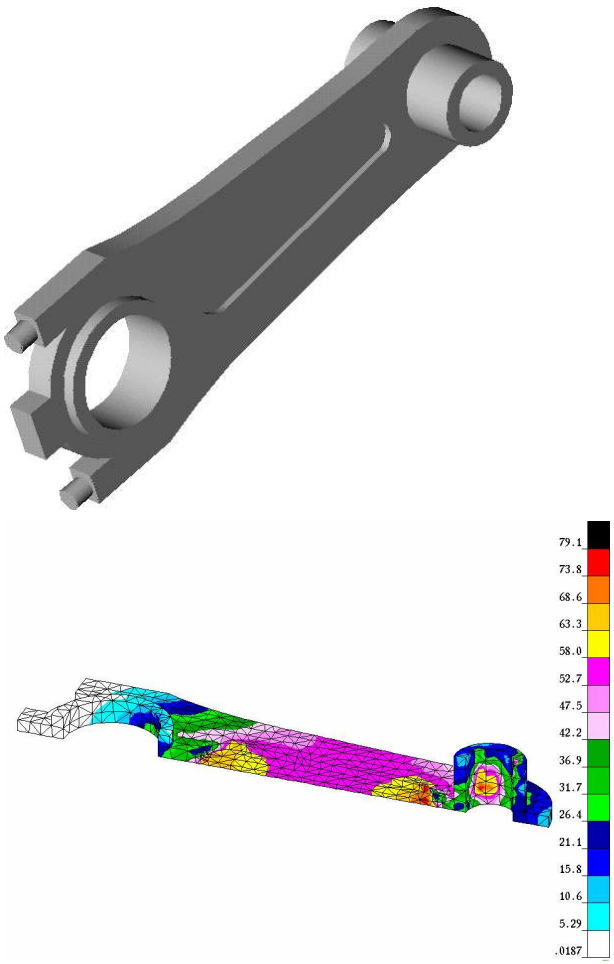
- Constraints (on perimeter)
  $G = 2\,(d_1 + d_2) - 20 \leq 0$

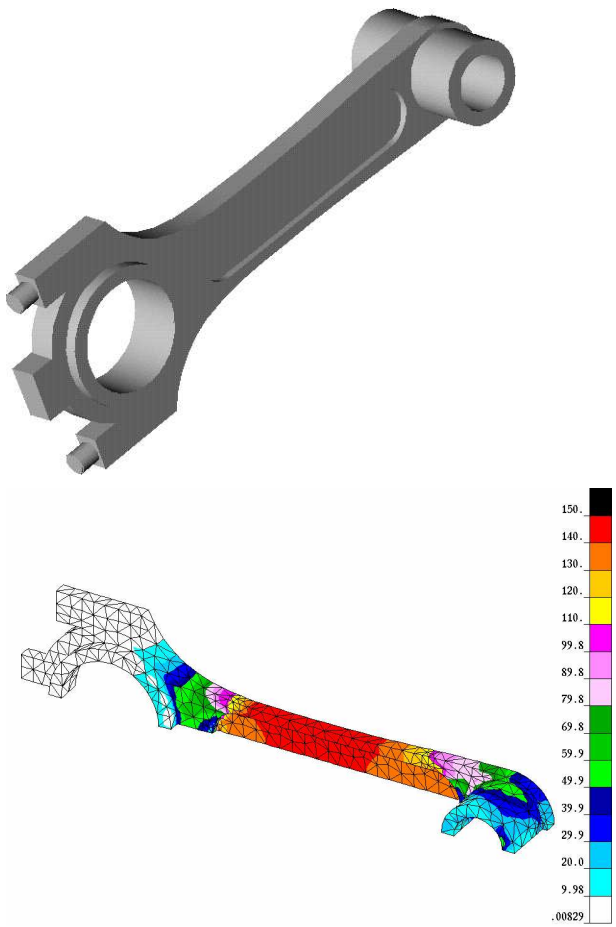
- Side Constraints
  $d_i \geq 0$





Connecting rod shape optimization

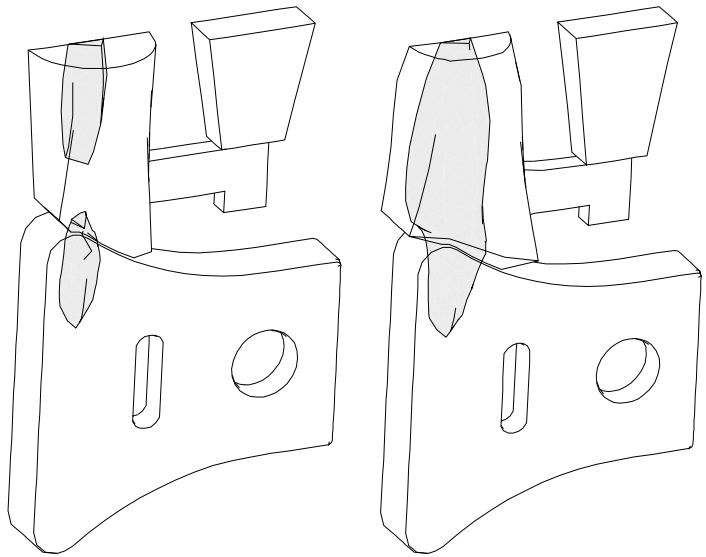




w/ S. Chen

Casting optimization

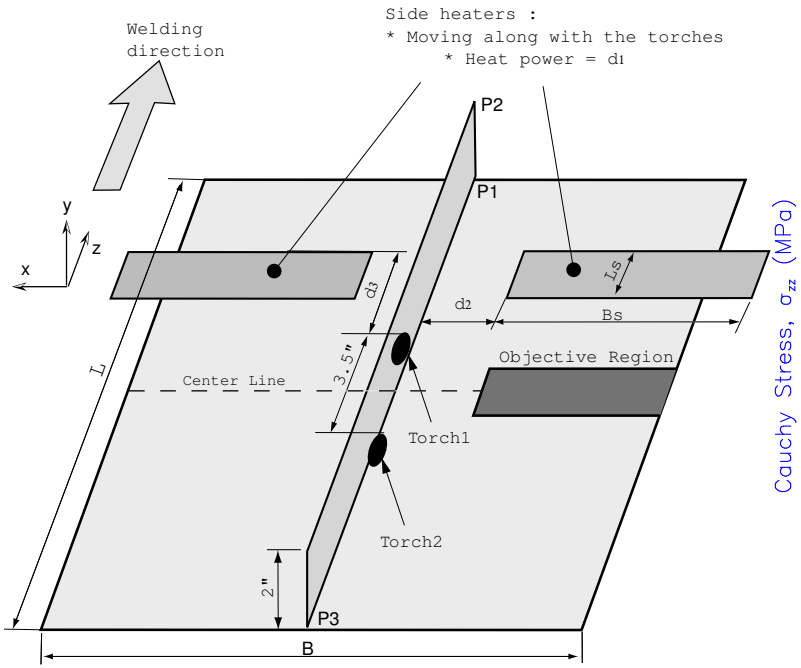
- Minimize riser volume
- Enforce directional solidification
- Thermal conduction

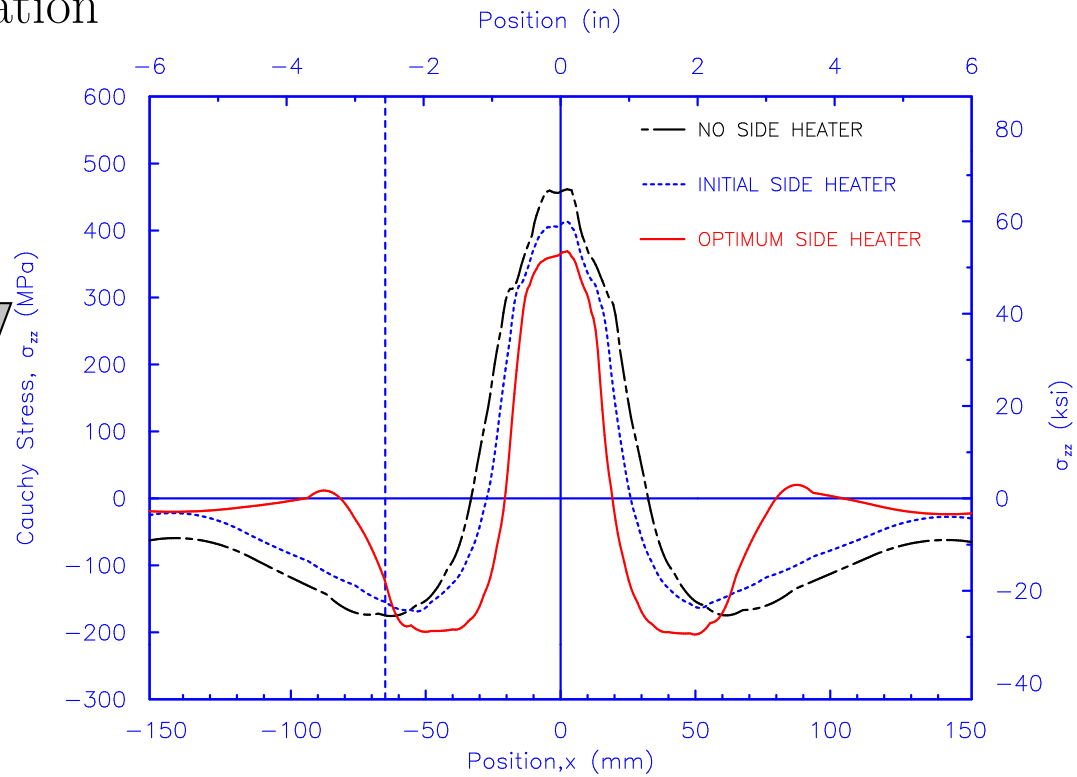


w/ J.A. Dantzig and P.E. Byrne

Weld optimization

- Design thermal tensioning process
- Minimize longitudinal residual stress away from heat effected zone
- Optimize heater power and location

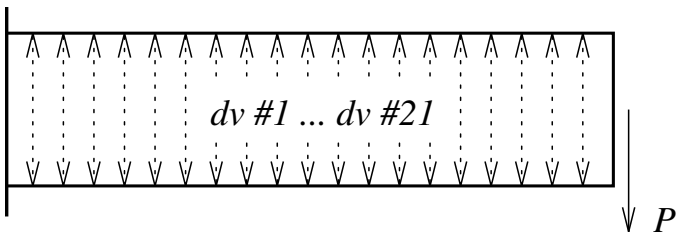


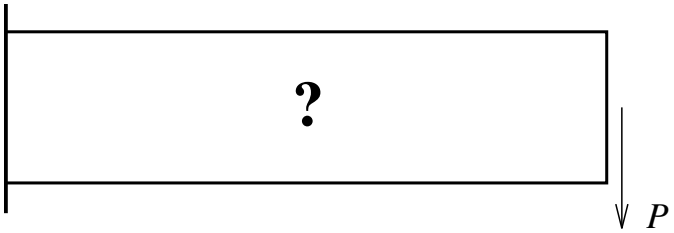


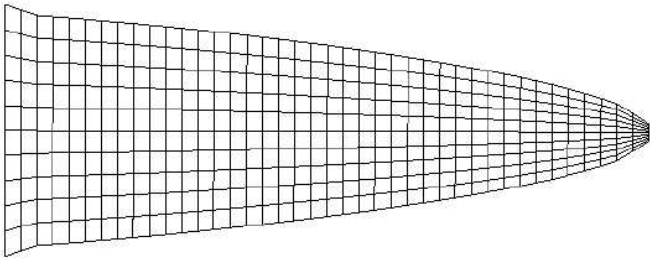
w/ P. Michaleris

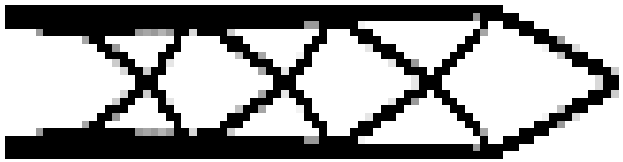
Topology optimization

- Distribute material
- Many design parameters



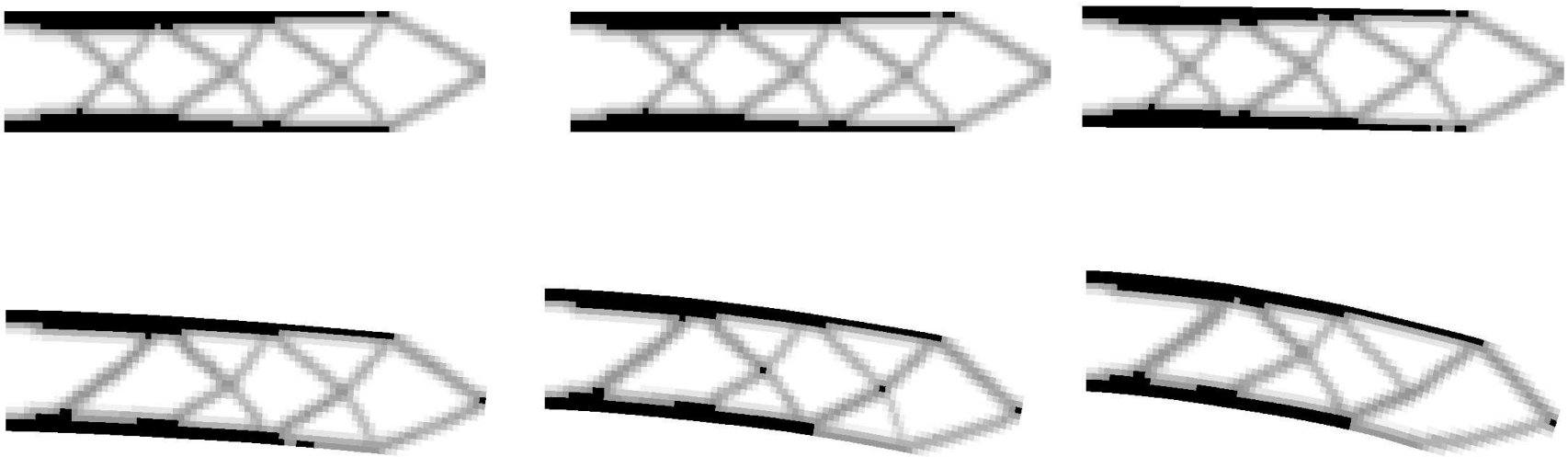




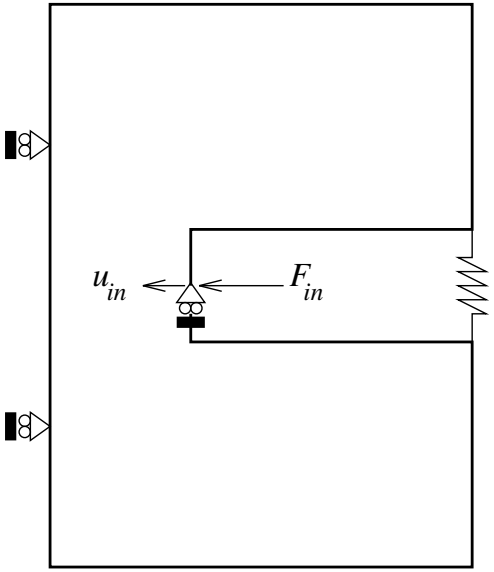


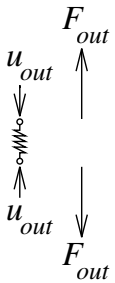
w/ T.E. Bruns

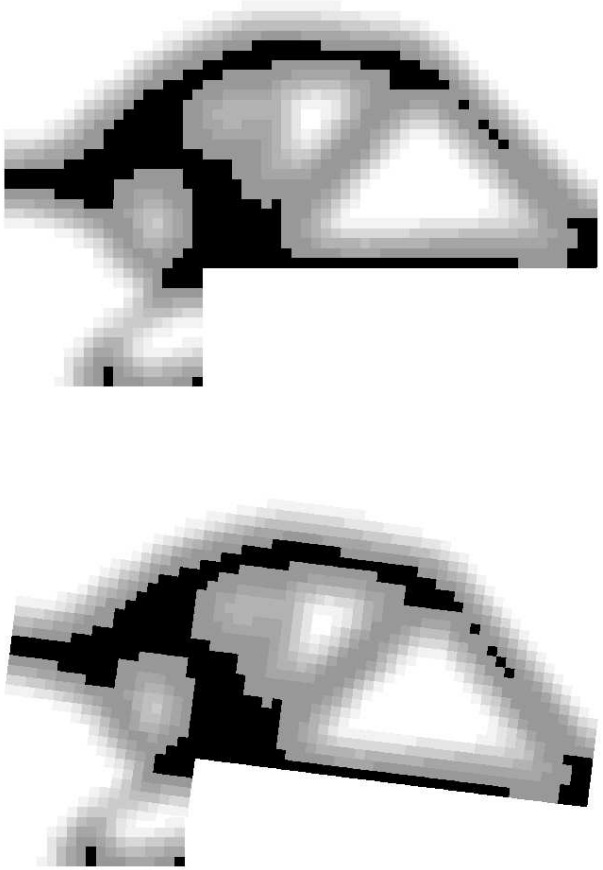
Topology optimization: Load dependent designs



Topology optimization: Compliant mechanisms

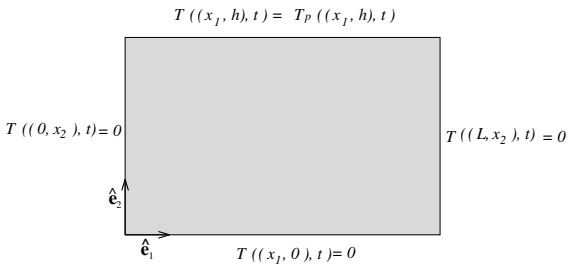




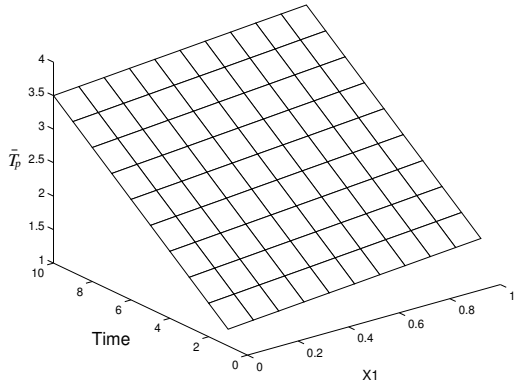


Identification problem: example

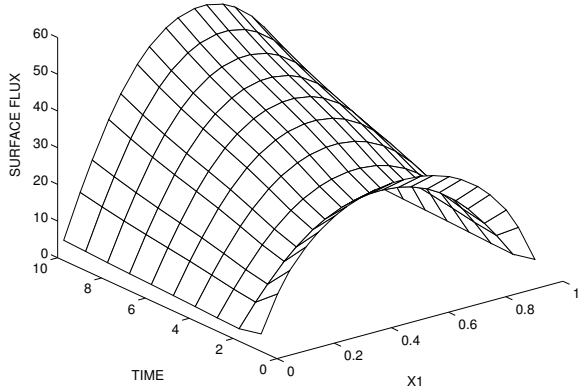
- Find T_p
- Minimize Error, $F = \int \frac{1}{2}(q^n - q_{data})^2 dx$
- 81 variables
- Ill-posed $\Rightarrow$ Need regularization



Plate

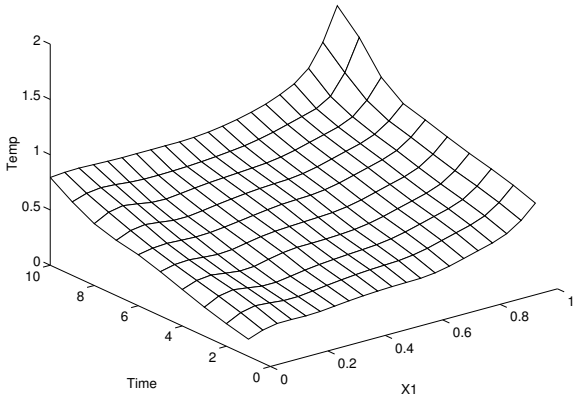


Target distribution

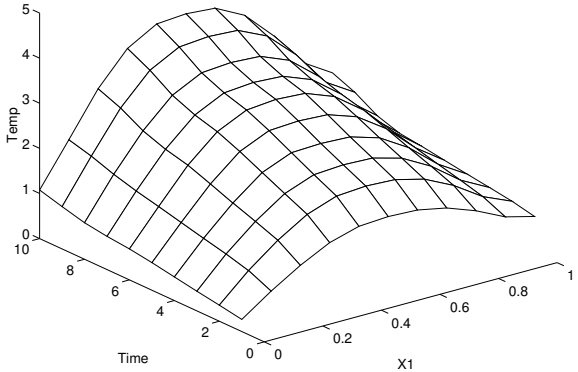


Experimental flux

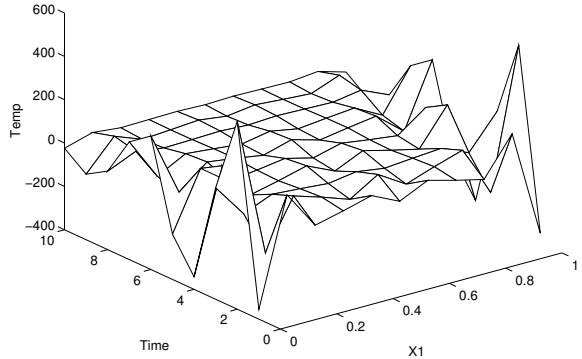
w/ G. Dorai



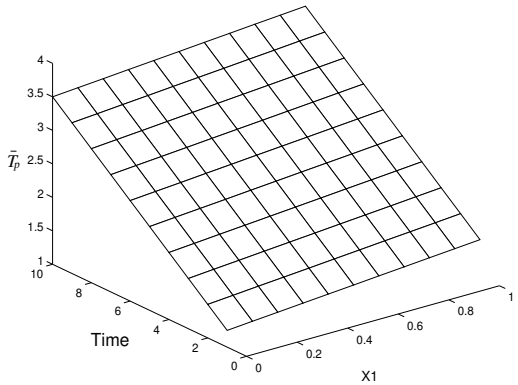
Initial distribution



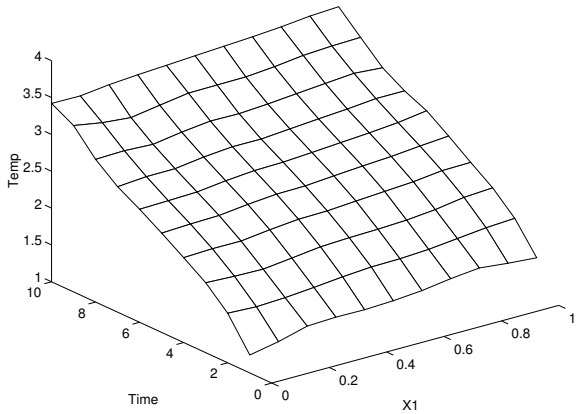
BFGS



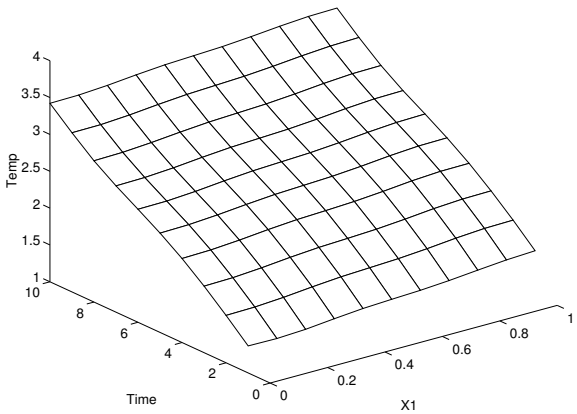
Newton's



Target distribution



w/ regularization
$\approx$ 40 iterations



w/ regularization
1 iteration

Sensitivity analysis

- Analysis
  - Evaluate residual, $\mathbf{R}(\mathbf{u}^I) \stackrel{?}{=} \mathbf{0}$
  - Newton update, $\left[\frac{D\mathbf{R}}{D\mathbf{u}}(\mathbf{u}^I)\right] \Delta\mathbf{u} = -\mathbf{R}(\mathbf{u}^I)$

- Generalized response functional $F(d) = G(\mathbf{u}(d), d)$

- Sensitivity $\frac{DF}{Dd} = \frac{\partial G}{\partial \mathbf{u}} \frac{D\mathbf{u}}{Dd} + \frac{\partial G}{\partial d}$
  - Finite difference: $\frac{DF}{Dd} \approx \frac{G(\mathbf{u}(d+\triangle d), d+\triangle d) - G(\mathbf{u}(d), d)}{\triangle d}$
  - Direct: $\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{Dd} + \frac{\partial \mathbf{R}}{\partial d} = \mathbf{0}$
  - Adjoint: $\frac{DF}{Dd} = \frac{\partial G}{\partial d} - \boldsymbol{\lambda}^T \frac{\partial \mathbf{R}}{\partial d} + \frac{D\mathbf{u}^T}{Dd} \overbrace{\left\{ \frac{\partial G^T}{\partial \mathbf{u}} - \frac{\partial \mathbf{R}^T}{\partial \mathbf{u}} \boldsymbol{\lambda} \right\}}^{\mathbf{0}}$

Sensitivity analysis: Notes

- Direct solvers preferred
- n linear pseudo or m linear adjoint problems
- Eliminate truncation & round-off errors
- Transient analyses: Implicit time integration preferred
- Coupled analyses: OK
- Use automatic differentiation, symbolic algebra or finite difference: $\frac{\partial \mathbf{R}}{\partial d}$

Nonlinear transient sensitivity analysis

Incremental Form:

- Residual at time t_n

$$ {}^{n}\mathbf{R}({}^{n}\mathbf{u}, {}^{n-1}\mathbf{u}) = \mathbf{0} $$

- Newton-Raphson

$$ \frac{\partial\, {}^{n}\mathbf{R}}{\partial\, {}^{n}\mathbf{u}}({}^{n}\mathbf{u}^{I}, {}^{n-1}\mathbf{u})\Delta\mathbf{u} = -\,{}^{n}\mathbf{R}({}^{n}\mathbf{u}^{I}, {}^{n-1}\mathbf{u}) $$

- Sensitivity Analysis:

$$ F(d) = G({}^{n}\mathbf{u}(d), d) $$

$$ \frac{DF}{Dd} = \frac{\partial G}{\partial\, {}^{n}\mathbf{u}}\frac{D\, {}^{n}\mathbf{u}}{Dd} + \frac{\partial G}{\partial d} $$

Direct differentiation:

- Residual at time t_n

$$ {}^{n}\mathbf{R}({}^{n}\mathbf{u}(d),\, {}^{n-1}\mathbf{u}(d), d) = \mathbf{0} $$

- Differentiate

$$ \frac{\partial\, {}^{n}\mathbf{R}}{\partial\, {}^{n}\mathbf{u}} \frac{D\, {}^{n}\mathbf{u}}{Dd} + \frac{\partial\, {}^{n}\mathbf{R}}{\partial\, {}^{n-1}\mathbf{u}} \frac{D\, {}^{n-1}\mathbf{u}}{Dd} + \frac{\partial\, {}^{n}\mathbf{R}}{\partial d} = \mathbf{0} $$

- Pseudo problem: $\frac{D\, {}^{n}\mathbf{u}}{Dd}$

$$ \frac{\partial\, {}^{n}\mathbf{R}}{\partial\, {}^{n}\mathbf{u}} \frac{D\, {}^{n}\mathbf{u}}{Dd} = - \left(\frac{\partial\, {}^{n}\mathbf{R}}{\partial\, {}^{n-1}\mathbf{u}} \frac{D\, {}^{n-1}\mathbf{u}}{Dd} + \frac{\partial\, {}^{n}\mathbf{R}}{\partial d} \right) $$

- Compute $\frac{D\, {}^{n}\mathbf{u}}{Dd}$ simultaneously with ${}^{n}\mathbf{u}$.

Adjoint method:

- Augment functional

$$\frac{DF}{Dd} = \frac{\partial G}{\partial\, {}^n\mathbf{u}} \frac{D\, {}^n\mathbf{u}}{Dd} + \frac{\partial G}{\partial d} -$$

$$\sum_{j=1}^{n} {}^j\boldsymbol{\lambda}^T \left(\frac{\partial\, {}^j\mathbf{R}}{\partial\, {}^j\mathbf{u}} \frac{D\, {}^j\mathbf{u}}{Dd} + \frac{\partial\, {}^j\mathbf{R}}{\partial\, {}^{j-1}\mathbf{u}} \frac{D\, {}^{j-1}\mathbf{u}}{Dd} + \frac{\partial\, {}^j\mathbf{R}}{\partial d} \right)$$

- Explicit component

$$\frac{D\hat{F}_E}{Dd} \equiv \frac{\partial G}{\partial d} - \sum_{j=1}^{n} {}^j\boldsymbol{\lambda}^T \frac{\partial\, {}^j\mathbf{R}}{\partial d} - {}^1\boldsymbol{\lambda}^T \frac{\partial\, {}^1\mathbf{R}}{\partial\, {}^0\mathbf{u}} \frac{D\, {}^0\mathbf{u}}{Dd}$$

Adjoint method (cont):

- Implicit component

$$\frac{D\hat{F}_I}{Dd} = -\left({}^1\boldsymbol{\lambda}^T \frac{\partial\, {}^1\mathbf{R}}{\partial\, {}^1\mathbf{u}} \frac{D\, {}^1\mathbf{u}}{Dd} + {}^2\boldsymbol{\lambda}^T \frac{\partial\, {}^2\mathbf{R}}{\partial\, {}^1\mathbf{u}} \frac{D\, {}^1\mathbf{u}}{Dd} \right)$$

$$-\left({}^2\boldsymbol{\lambda}^T \frac{\partial\, {}^2\mathbf{R}}{\partial\, {}^2\mathbf{u}} \frac{D\, {}^2\mathbf{u}}{Dd} + {}^3\boldsymbol{\lambda}^T \frac{\partial\, {}^3\mathbf{R}}{\partial\, {}^2\mathbf{u}} \frac{D\, {}^2\mathbf{u}}{Dd} \right)$$

$$\ldots$$

$$-\left({}^{n-1}\boldsymbol{\lambda}^T \frac{\partial\, {}^{n-1}\mathbf{R}}{\partial\, {}^{n-1}\mathbf{u}} \frac{D\, {}^{n-1}\mathbf{u}}{Dd} + {}^n\boldsymbol{\lambda}^T \frac{\partial\, {}^n\mathbf{R}}{\partial\, {}^{n-1}\mathbf{u}} \frac{D\, {}^{n-1}\mathbf{u}}{Dd} \right)$$

$$-\left({}^n\boldsymbol{\lambda}^T \frac{\partial\, {}^n\mathbf{R}}{\partial\, {}^n\mathbf{u}} \frac{D\, {}^n\mathbf{u}}{Dd} \frac{\partial G}{\partial\, {}^n\mathbf{u}} \frac{D\, {}^n\mathbf{u}}{Dd} \right)$$

Adjoint method (cont):

- Solve adjoint problems

$$n: \qquad \left(\frac{\partial\, {}^n\mathbf{R}}{\partial\, {}^n\mathbf{u}}\right)^T {}^n\boldsymbol{\lambda} = \frac{\partial G}{\partial\, {}^n\mathbf{u}}$$

$$n-1: \quad \left(\frac{\partial\, {}^{n-1}\mathbf{R}}{\partial\, {}^{n-1}\mathbf{u}}\right)^T {}^{n-1}\boldsymbol{\lambda} = -\left(\frac{\partial\, {}^n\mathbf{R}}{\partial\, {}^{n-1}\mathbf{u}}\right)^T {}^n\boldsymbol{\lambda}$$

$$\ldots$$

$$2: \qquad \left(\frac{\partial\, {}^2\mathbf{R}}{\partial\, {}^2\mathbf{u}}\right)^T {}^2\boldsymbol{\lambda} = -\left(\frac{\partial\, {}^3\mathbf{R}}{\partial\, {}^2\mathbf{u}}\right)^T {}^3\boldsymbol{\lambda}$$

$$1: \qquad \left(\frac{\partial\, {}^1\mathbf{R}}{\partial\, {}^1\mathbf{u}}\right)^T {}^1\boldsymbol{\lambda} = -\left(\frac{\partial\, {}^2\mathbf{R}}{\partial\, {}^1\mathbf{u}}\right)^T {}^2\boldsymbol{\lambda}$$

- Requires much storage or recomputation

Tangent matrix

- Subiterations required to compute $\mathbf{R}$

- Secondary response is an implicit function of primary response

- E.g. stress and yield stress are implicit functions of displacement
  - Given $\mathbf{u}_n$, $\boldsymbol{\sigma}_{n-1}$ and $\boldsymbol{\alpha}_{n-1}$ compute $\boldsymbol{\sigma}_n$, $\boldsymbol{\alpha}_n$ and $\partial\boldsymbol{\sigma}_n/\partial\mathbf{u}_n$
  - Solve the residual equation

$$\mathbf{r}((\boldsymbol{\sigma}_n, \boldsymbol{\alpha}_n); (\mathbf{u}_n, \boldsymbol{\sigma}_{n-1}, \boldsymbol{\alpha}_{n-1})) = \mathbf{0}$$

  - Differentiate to obtain

$$\frac{\partial\,\mathbf{r}}{\partial(\boldsymbol{\sigma}_n, \boldsymbol{\alpha}_n)} \left\{ \begin{array}{c} \frac{\partial\boldsymbol{\sigma}_n}{\partial\mathbf{u}_n} \\ \\ \frac{\partial\boldsymbol{\alpha}_n}{\partial\mathbf{u}_n} \end{array} \right\} = -\frac{\partial\mathbf{r}}{\partial\mathbf{u}_n}$$

Phase change analysis

- Primary response: enthalpy H
- Secondary response: solid volume fraction ϵ_s and temperature T
- Mushy zone relations: Scheil assumption

$$\mathbf{r}((T,\epsilon_s);H) = \left\{ \begin{array}{c} \epsilon_s - 1 + \left(\frac{T_f - T_l}{T_f - T}\right)^{-(1-k)} \\ c_p\,T + (1-\epsilon_s)\,L - H \end{array} \right\} \qquad \frac{\partial\,\mathbf{r}}{\partial H} = \left\{ \begin{array}{c} 0 \\ -1 \end{array} \right\}$$

$$\frac{\partial\,\mathbf{r}}{\partial(\epsilon_s,T)} = \left[\begin{array}{cc} 1 & \frac{(-1+k)\left(\frac{T_f-T_l}{T_f-T}\right)^{k}}{T_f-T_l} \\ -L & c_p \end{array} \right] \text{ and } \left[\frac{\partial\,\mathbf{r}}{\partial(\epsilon_s,T)}\right] \left\{ \begin{array}{c} \frac{\partial\,\epsilon_s}{\partial H} \\ \frac{\partial\,T}{\partial H} \end{array} \right\} = -\frac{\partial\,\mathbf{r}}{\partial H}$$

- Symbolic algebra, automatic differentiation
- Finite difference

Stage IV hardening w/ two state variable hybrid model

- Crystal flow stress: $\tau - \hat{\tau}_a = \frac{S_\varepsilon(\dot{\varepsilon},T)}{S_\varepsilon(\dot{\varepsilon}_r,T_r)} \frac{\mu}{\mu_r} \hat{\tau}_\varepsilon$
- Strength evolution: $\frac{d\hat{\tau}_\varepsilon}{d\Gamma} = \theta_o \left[1 - \frac{\hat{\tau}_\varepsilon}{\hat{\tau}_{\varepsilon s}} + \frac{\alpha\, \mu_r\, k_o\, b}{k_1\, \hat{\tau}_\varepsilon\, \overline{L}_g}\right]$
- Second evolutionary state variable $\hat{\tau}_\lambda$: $\hat{\tau}_\lambda = \frac{\alpha\, \mu_r\, k_o\, b}{k_1\, \overline{L}_g}$ and $\frac{d\hat{\tau}_\lambda}{d\Gamma} = a''\, \hat{\tau}_\lambda^{1-\frac{1}{r}}$
- Large strain compression and torsion of HY100 Martensitic steel

Parameter identification

- Identify material parameters and initial conditions

$$\underset{\boldsymbol{d} = [\boldsymbol{d}_p,\, \boldsymbol{d}_i]}{\text{Minimize}} \qquad E(\boldsymbol{d}) = \sqrt{\sum_{p=1}^{P} \left(1 - \frac{T_{ij}^p}{\tilde{T}_{ij}^p}\right)^2}$$

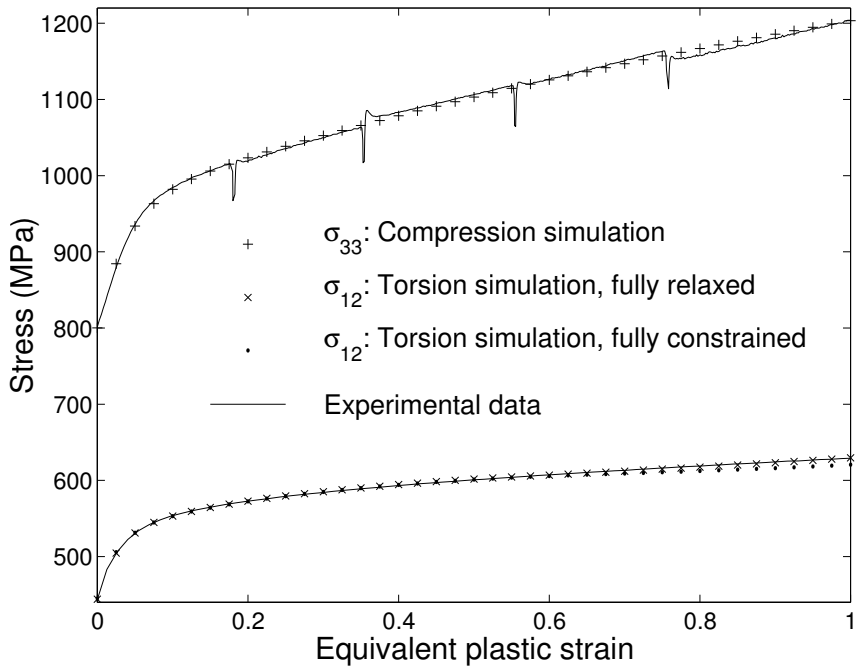
Material parameters

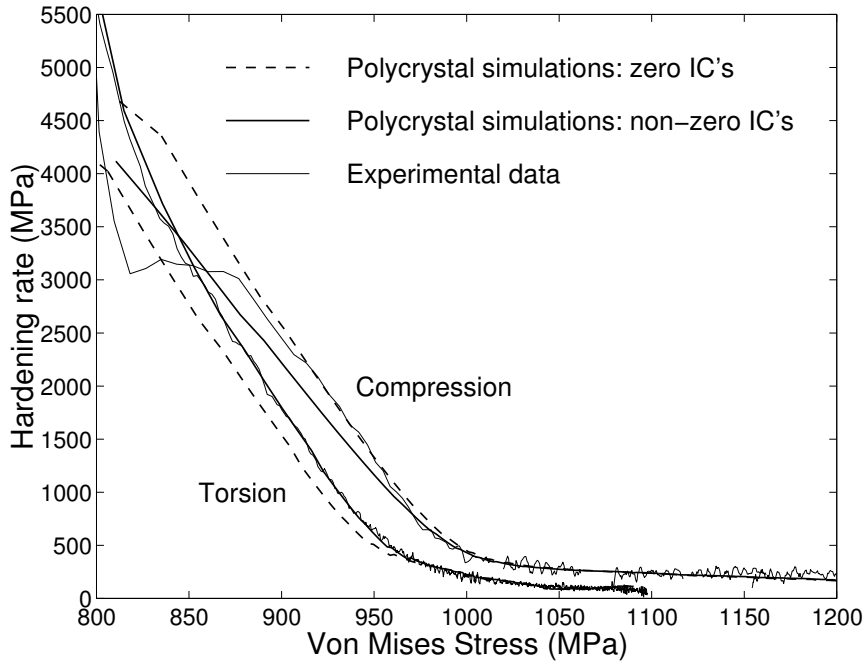
$$\boldsymbol{d}_p = [g_o, g_{o\varepsilon s}, \theta_o, c, \eta, \hat{\tau}_a, \hat{\tau}_{\varepsilon so}, \dot{\varepsilon}_{so}, \dot{\varepsilon}_o]$$

Initial conditions

$$\boldsymbol{d}_i = [\hat{\tau}_\varepsilon^1 \,|_{\Gamma=0}; \hat{\tau}_\lambda^1 \,|_{\Gamma=0}; \ldots; \hat{\tau}_\varepsilon^k \,|_{\Gamma=0}; \hat{\tau}_\lambda^k \,|_{\Gamma=0}]$$

HY100 Steel





w/ A.J. Beaudoin and S. Kok

Multi-level Newton method: Coupled analyses

- Coupled analyses: $f(\hat{x}(y); y) = 0$ and $g(\hat{y}(x); x) = 0$
- Form a "self consistent" residual

$$\boldsymbol{\mathcal{R}}(x, y) = \left\{ \begin{array}{c} x - \hat{x}(y) \\ y - \hat{y}(x) \end{array} \right\} = \mathbf{0}$$

- Solve by Newton's method

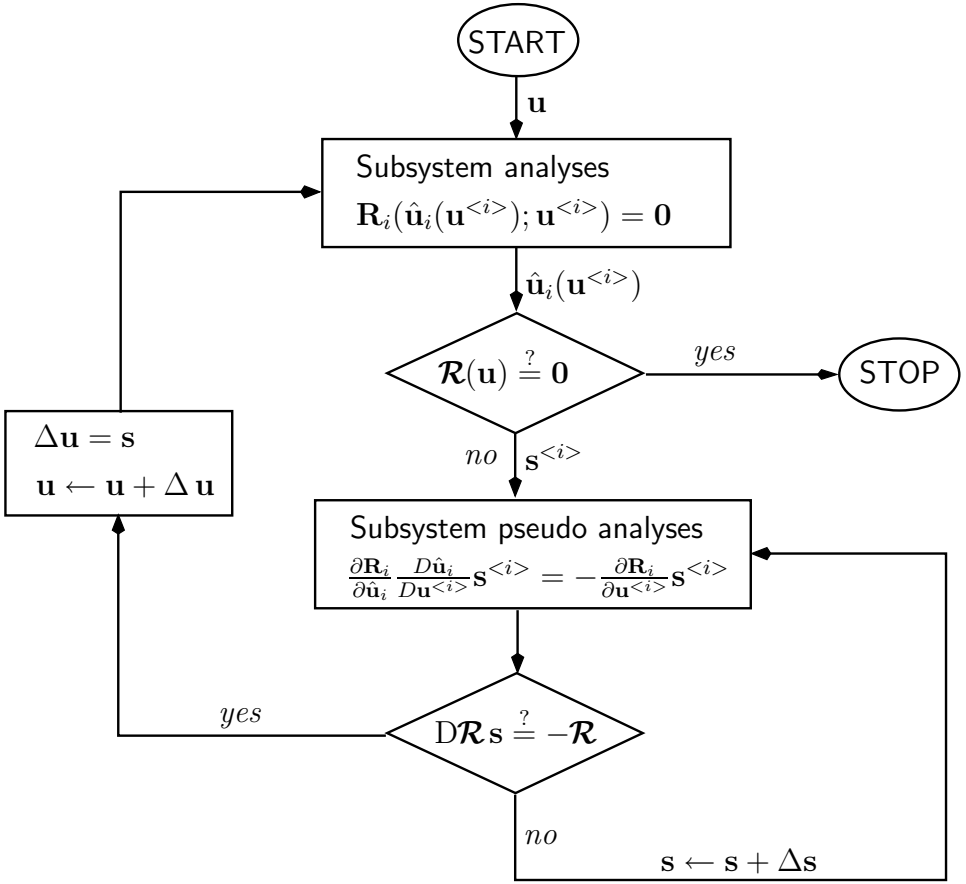
$$\mathrm{D}\boldsymbol{\mathcal{R}}(x, y)\, \boldsymbol{\Delta} = -\boldsymbol{\mathcal{R}}(x, y) = \left[\begin{array}{cc} 1 & -\hat{x}'(y) \\ -\hat{y}'(x) & 1 \end{array} \right] \left\{ \begin{array}{c} \Delta x \\ \Delta y \end{array} \right\} = - \left\{ \begin{array}{c} x - \hat{x}(y) \\ y - \hat{y}(x) \end{array} \right\}$$

- Iteratively solve Newton update (GMRES, Ubik Solve)

$$\mathrm{D}\boldsymbol{\mathcal{R}}(x, y)\, \mathbf{s} = \left\{ \begin{array}{c} s_x - \hat{x}'(y)\, s_y \\ -\hat{y}'(x)\, s_x + s_y \end{array} \right\} = \left\{ \begin{array}{c} s_x - \frac{1}{\epsilon}[\hat{x}(y + \epsilon s_y) - \hat{x}(y)] \\ \\ -\frac{1}{\epsilon}[\hat{y}(x + \epsilon s_x) - \hat{y}(x)] + s_y \end{array} \right\}$$

- Matrix free parallelization
- Linear analyses

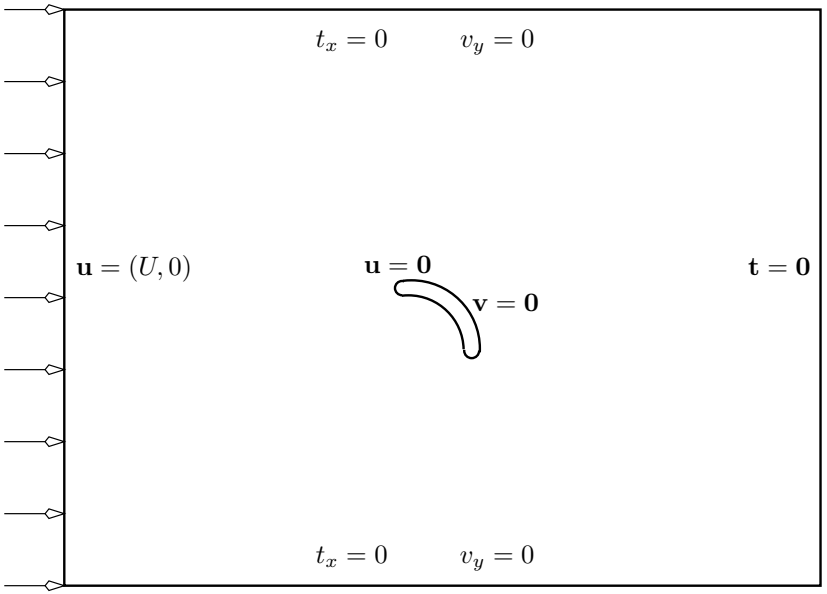
Multi-level Newton method



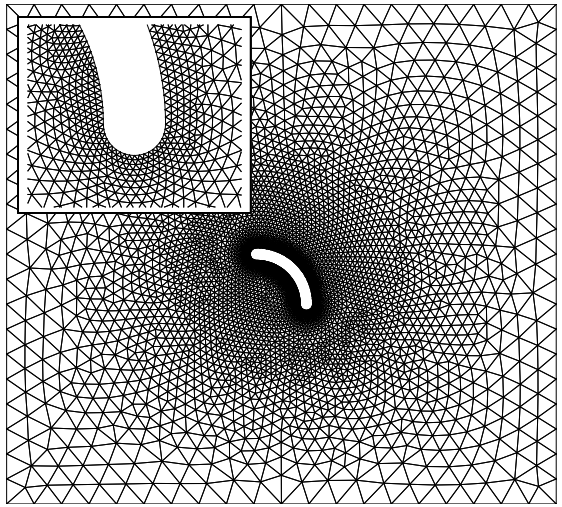
Aeroelasticity

- Coupled fluids, structure, and mesh motion analyses
- Low speed flow $Re = 50$
- $\approx$ 4500 nodes and $\approx$ 8800 elements
- Iterations and CPU
  - MLN: 5 Newton $\times$ 15 GMRES iterations $\Longrightarrow$ 161 CPU
  - Semi-analytical MLN: 8 Newton $\times$ 15 GMRES iterations $\Longrightarrow$ 215 CPU
  - Finite difference MLN: 8 Newton $\times$ 15 GMRES iterations $\Longrightarrow$ 2134 CPU
  - Successive substitution: 21-35 iterations $\Longrightarrow$ 350-584 CPU

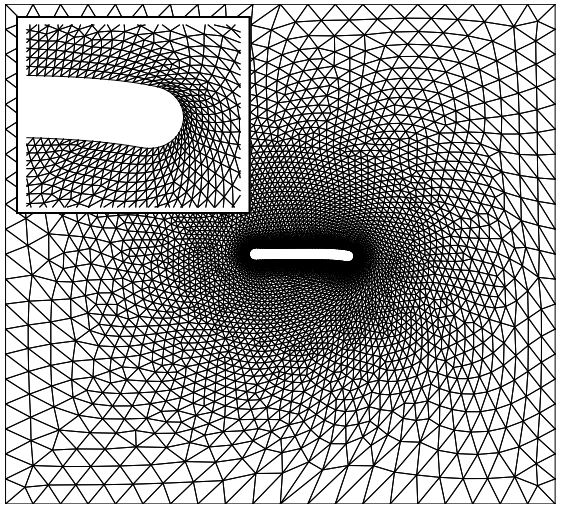
w/ N. Aluru and J.Y. Kim



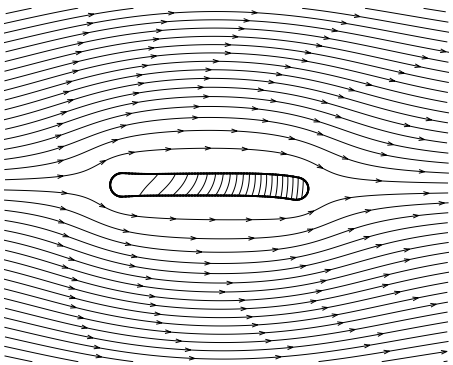
Domain and boundary conditions



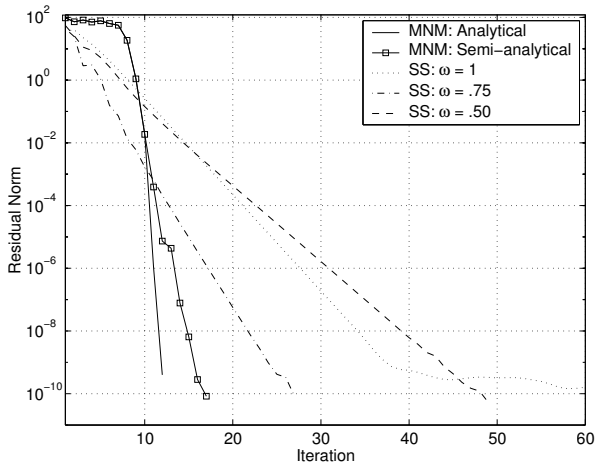
Initial mesh



Deformed mesh



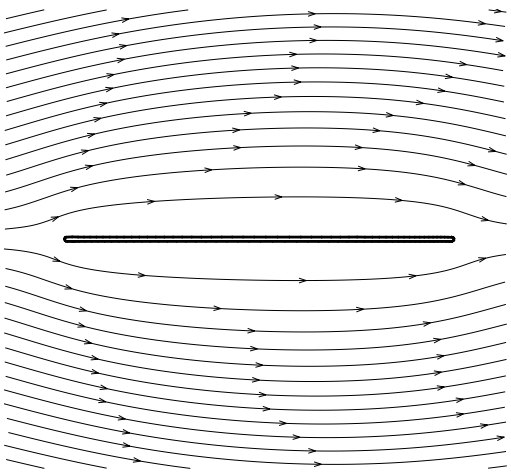
Flow field

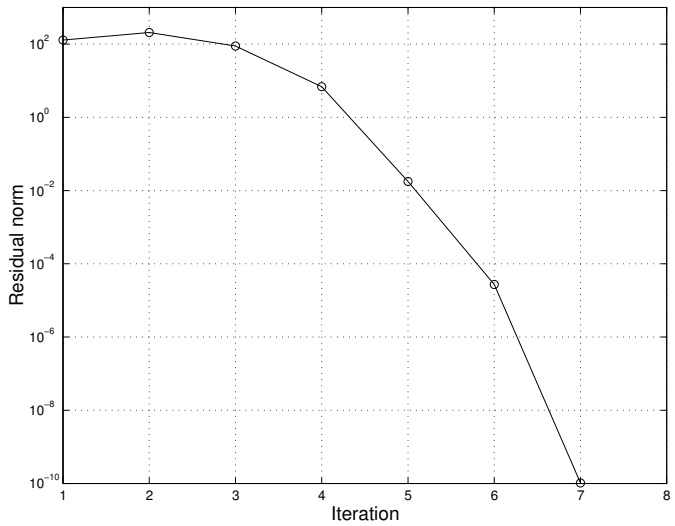


Convergence

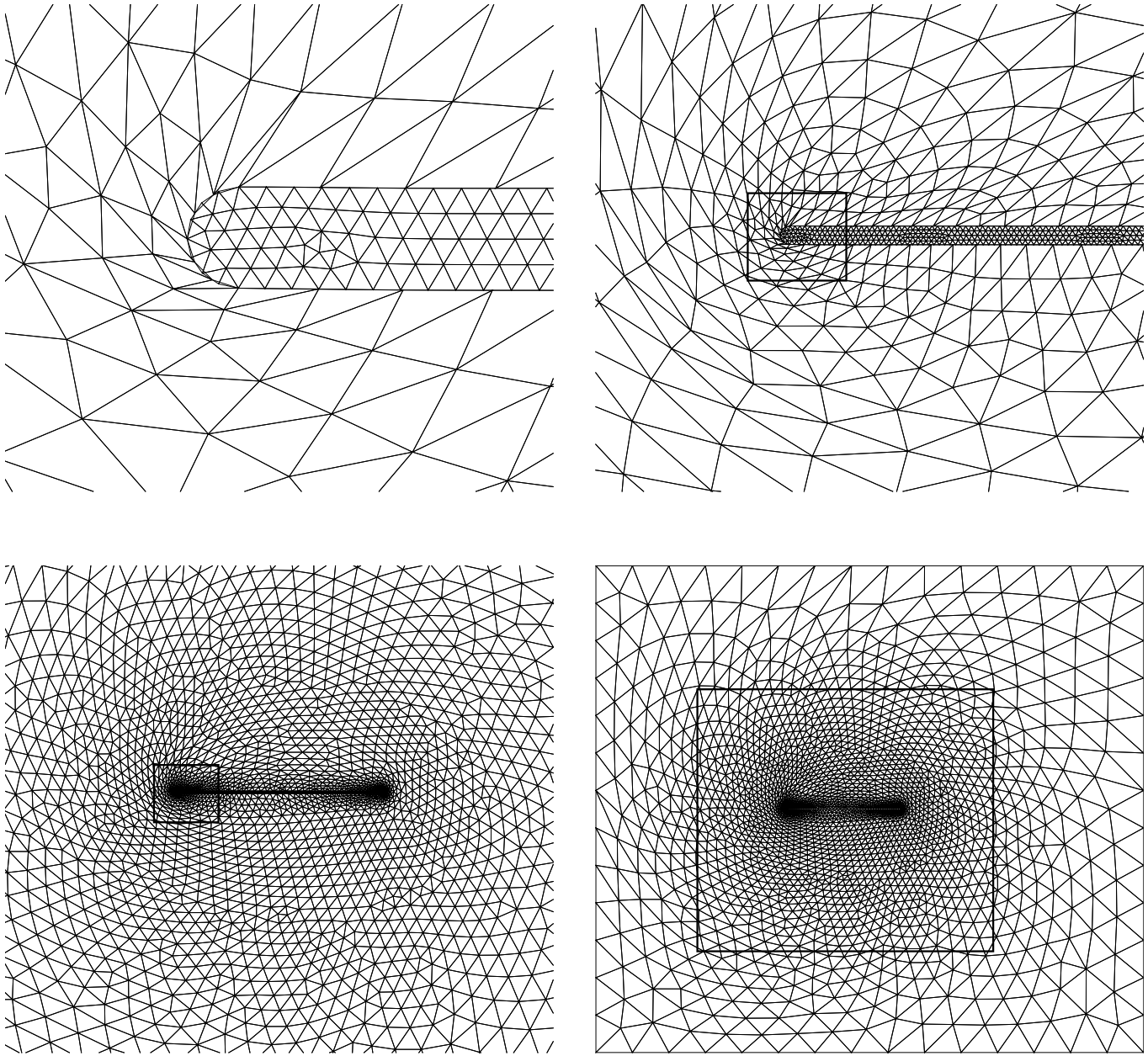
Nonconforming mesh

- Common refinement
- Enforce interfacial momentum mass balance w/ Galerkin method
- Fluid and solid meshes contain 5,662 and 2,178 elements





w/ J.Y. Kim



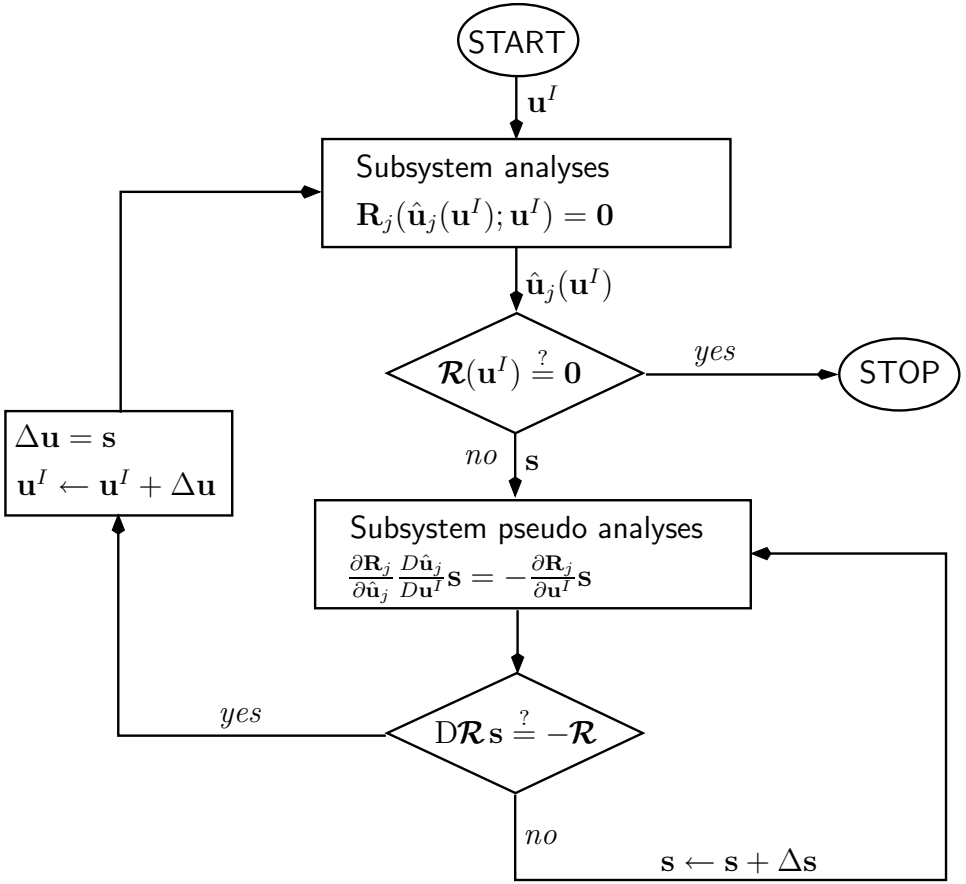
Multi-level Newton method: Domain decomposition

- n subdomain analyses:
  - Usual balance equations:
- Interface analysis
  - Usual interface equations: $\boldsymbol{\mathcal{R}}(\mathbf{u}^I; \hat{\mathbf{u}}_1(\mathbf{u}^I), \hat{\mathbf{u}}_2(\mathbf{u}^I), \cdots, \hat{\mathbf{u}}_n(\mathbf{u}^I)) = \mathbf{0}$
  - Iteratively solve Newton update

$$
\begin{aligned}
\mathrm{D}\boldsymbol{\mathcal{R}}\,\mathbf{s} &= \left[\frac{\partial \boldsymbol{\mathcal{R}}}{\partial \mathbf{u}^I} + \sum_{j=1}^{n}\left(\frac{\partial \boldsymbol{\mathcal{R}}}{\partial \mathbf{u}_j}\frac{D\hat{\mathbf{u}}_j}{D\mathbf{u}^I}\right)\right]\mathbf{s} \\
&= \left[\frac{\partial \boldsymbol{\mathcal{R}}}{\partial \mathbf{u}^I}\mathbf{s} - \sum_{j=1}^{n}\left(\frac{\partial \boldsymbol{\mathcal{R}}}{\partial \mathbf{u}_j}\left[\frac{\partial \mathbf{R}_j}{\partial \mathbf{u}_j}\right]^{-1}\frac{\partial \mathbf{R}_j}{\partial \mathbf{u}^I}\mathbf{s}\right)\right]
\end{aligned}
$$

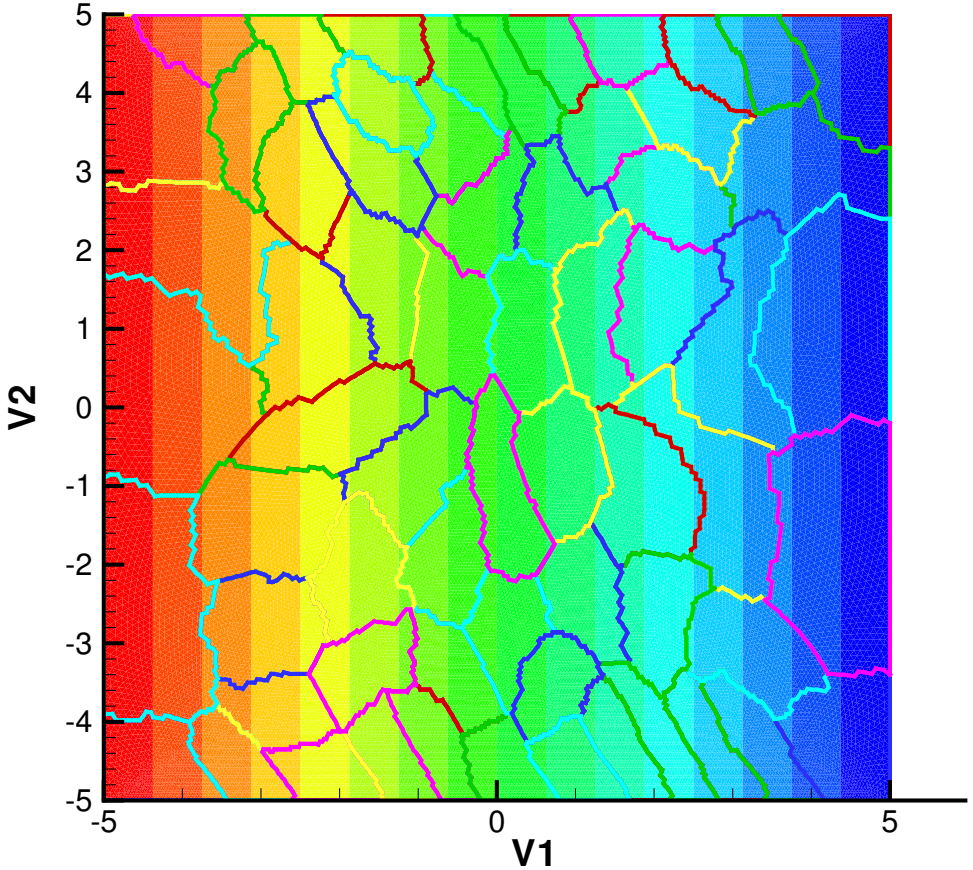
- Matrix free parallelization
- Local nonlinearities

Multi-level Newton method



Heat conduction example

- Steady heat conduction: $\mathbf{R}$
- Interfacial temperature: $\mathbf{u}^I$
- Interfacial energy balance: $\boldsymbol{\mathcal{R}}$
- Partitioning w/ METIS (Chaco)
- Parallelization w/ MPI
- Load balancing w/ Charm++ (PGSLib)
- $\approx 100,000$ elements & $\approx 60,000$ DOF
- Unstructured mesh
- Linear: one outer Newton iteration



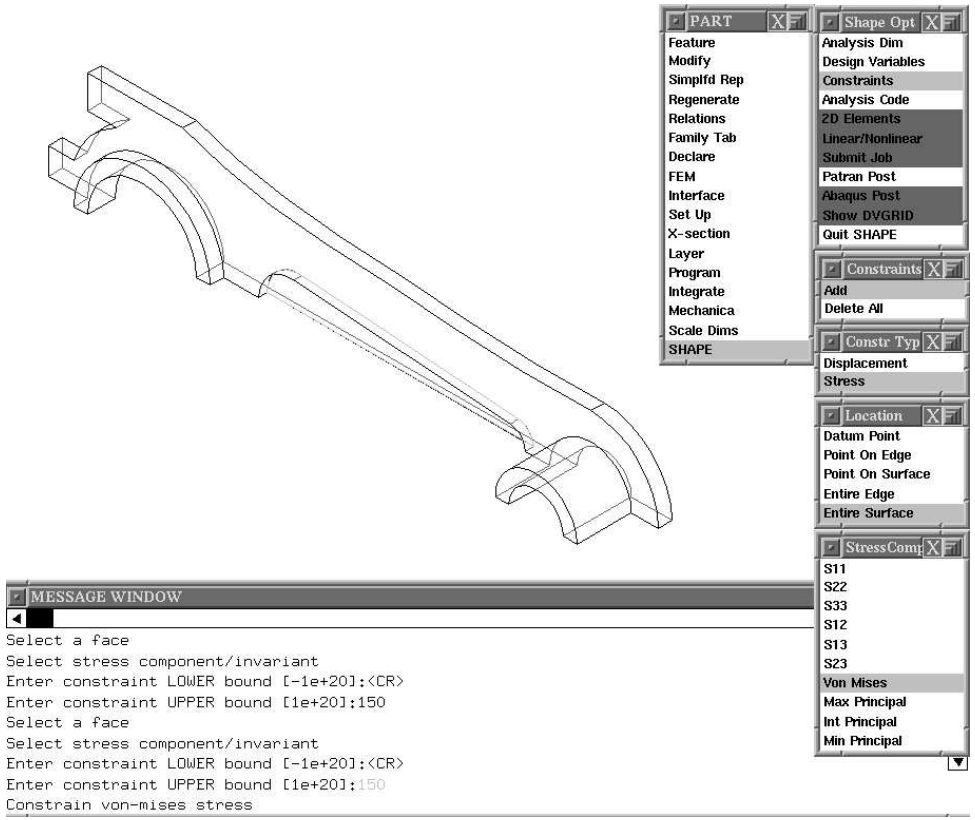
w/ D. Kulkarni

Optimization environment

- Pro/Engineer solid modeler
  - Feature-based modeling
  - OCTREE
  - Pro/Develop API

- MSC/Nastran DSA

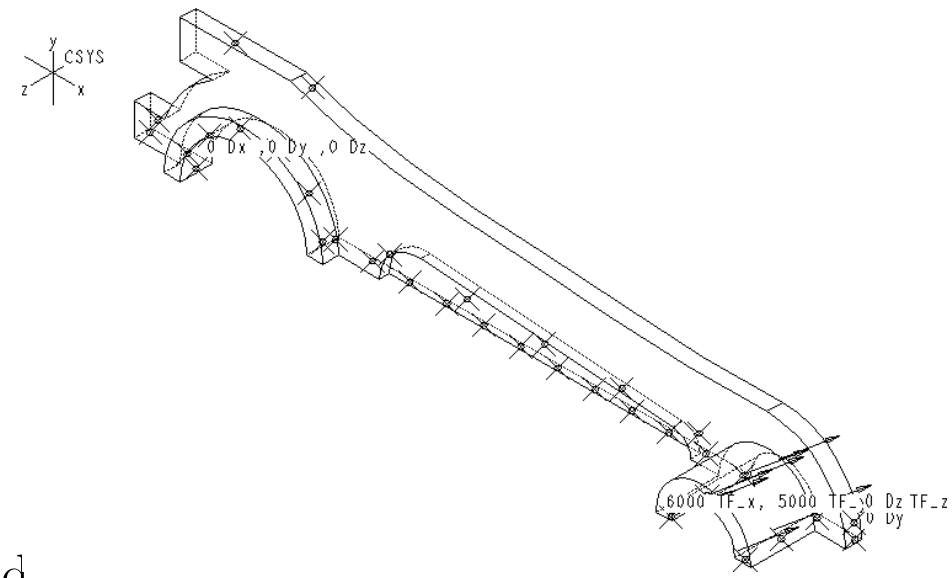
- DOT SLP



w/ S. Chen

Analysis model

- Quarter symmetry employed
- Initial finite element mesh:
  - 2215 parabolic tetrahedrons
  - 4642 nodes
- Linear static analysis
- Steel material properties
- Boundary conditions
  - Encastre condition at crankshaft end
  - Distributed force at pin end
- Maximum von Mises stress of 79.1 MPa

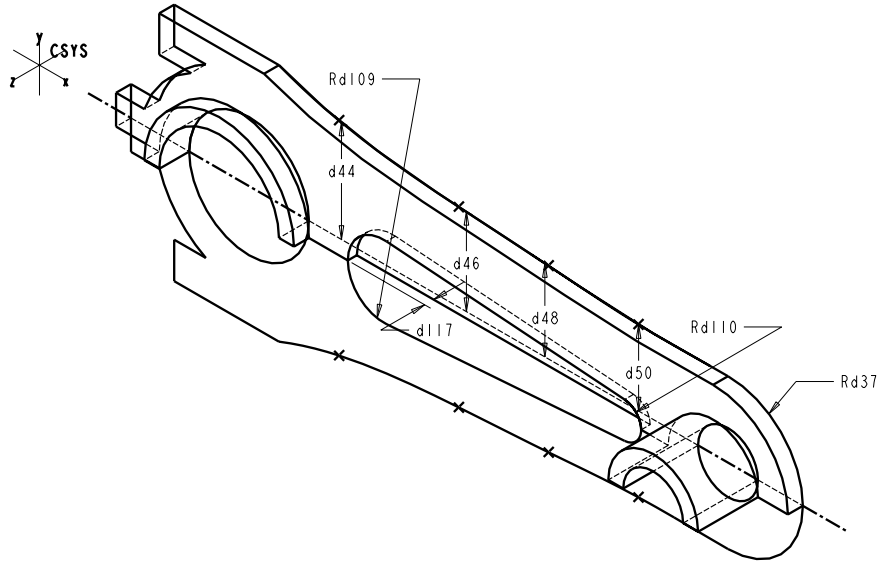


Design model

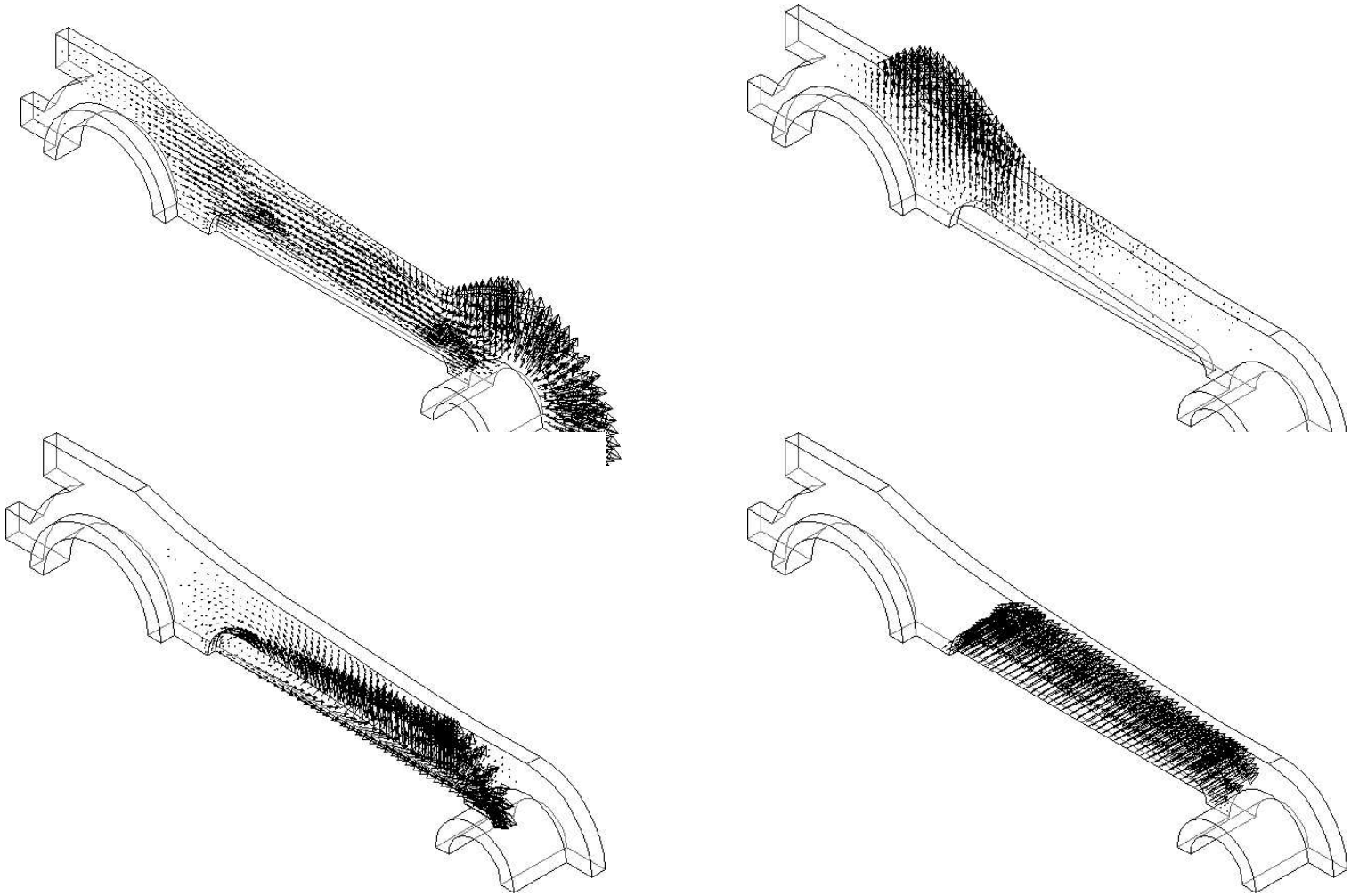
- Minimize volume/mass

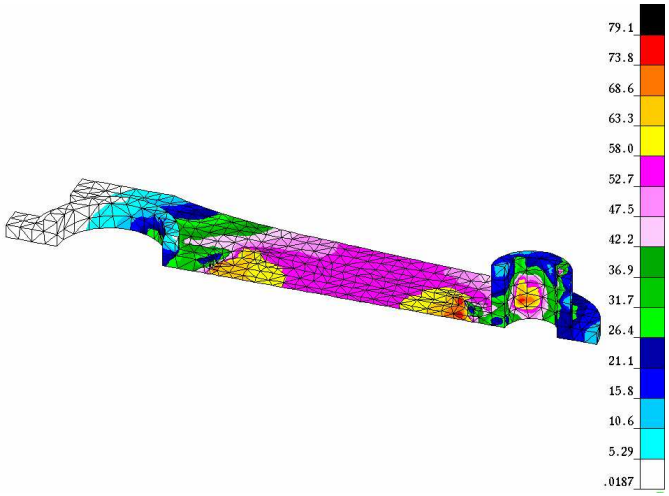
- 8 Design variables
  - Neck contour
  - Web radii
  - Outer pin end radius
  - Web depth

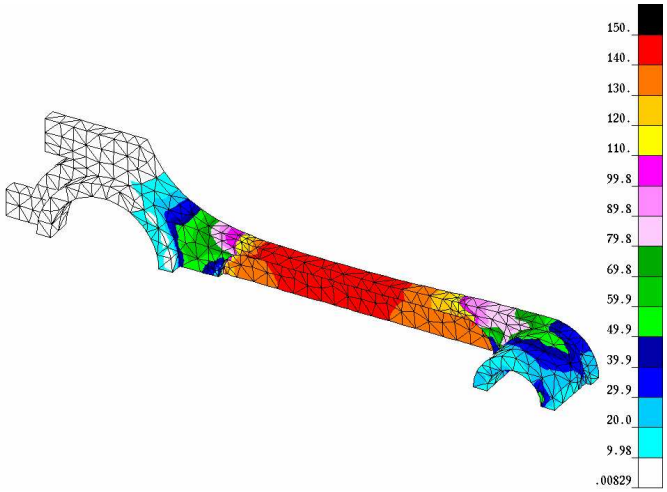
- Constrain von Mises $\leq$ 150 MPa



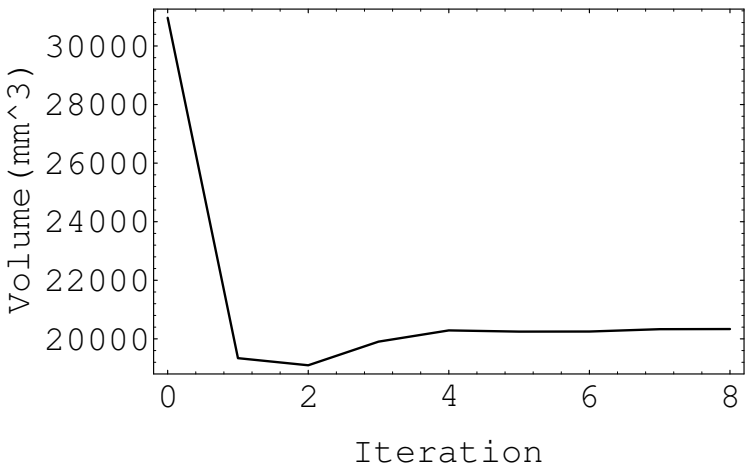
Velocity field

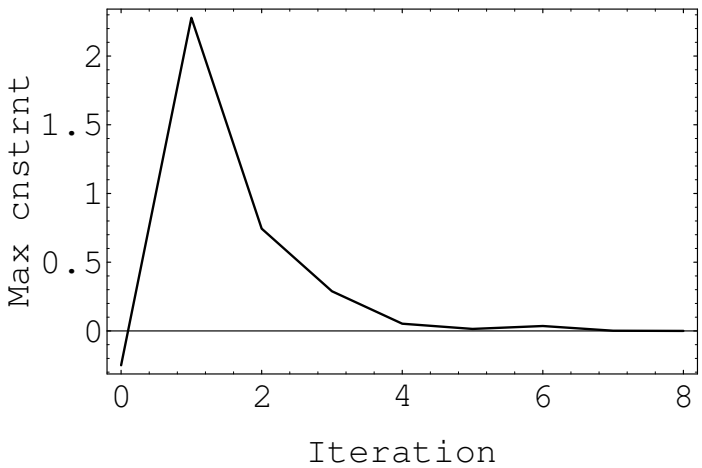



79.1
73.8
68.6
63.3
58.0
52.7
47.5
42.2
36.9
31.7
26.4
21.1
15.8
10.6
5.29
.0187


150.
140.
130.
120.
110.
99.8
89.8
79.8
69.8
59.9
49.9
39.9
29.9
20.0
9.98
.00829

Optimization history





- Convergence in 8 iterations
- 34.3% volume reduction
- Optimal design satisfies performance/geometric constraints

Discussion

- Only initial user interaction
- Update solid model dimensions each iteration
- Update finite element mesh each iteration
  - Remeshing
  - Laplacian smoothing
- Velocity field calculations each iteration
- Applicable to other analyses

Conclusion

- Many applications
  - Reliability & uncertainty
  - Design of experiments
  - Response surface optimization

- Numerous examples
  - Precipitation nucleation & growth
  - Polymer processing
  - Metal forming
  - Controller design
  - Crystal growth
  - Mechanisms