Joint work with R. Pawlowski and J. N. Shadid (Sanda National Labs) and J. P. Simons (WPI).

October 22, 2003
Worcester Polytechnic Institute
Mathematical Sciences Department
Homer Walker

Globally Convergent Newton-Krylov Methods
Newton's Method:

\[ s + x \rightarrow x \]

Update \( x \)

\[
(x)_{n+1} = s(x)_n
\]

Solve \( F \)

Iterate:

Given an initial \( x \).

The model method is:

\[
\Pi_n \leftarrow \Pi_n : F \equiv 0 = (x)_n
\]

Nonlinear problem:
Solving $H(x) - s(x)^H$ may be problematic.

But it's only local... need to globalization.

Convergence is usually mesh-independent for PDE problems.

$$\|x^n - x^{n+1}\| \leq \|x^n - x^{n+1}\|^2$$

Quadratic local convergence.

Properties of Newton's method.
Krylov subspace methods $\Leftrightarrow$ Newton–Krylov methods $\Delta$

Iterative linear algebra methods $\Leftrightarrow$ Newton iterative methods $\Delta$

Focus on the large-scale case.
There are by now many Krylov subspace methods, e.g.,

Terminology: $x_k$ is the $k$th Krylov subspace.

Given $x_0$, determine $x = \hat{q}$

Krylov Subspace Method: For $A x = q$
differentiation

by automatic

exact evaluation of \( \alpha_{x}^{H} \) and \( \alpha (x)^{H} \)

\[
\left[ (x)^{H} - (\alpha y + x)^{H} \right] \frac{y}{1} \approx \alpha (x)^{H}
\]

by finite differences, e.g.

approximation of \( \alpha_{x}^{H} \)

\[
\cdots \text{matrix-free implementations through} \quad \left( (x)^{H} \right) \quad \text{with vectors}
\]

They require only products of \( (x)^{H} \) (and sometimes \( (x)^{H} \))

\[
(x)^{H} - s (x)^{H}
\]

Krylov subspace methods have special appeal for solving
The first CG step is the steepest descent step.

\[ s(x)f \Delta_L s \frac{\Delta}{I} + s_L(x)f \Delta + (x)f = \]

local quadratic model

The kth CG step minimizes over \( k \).

\[ \cdots \]

positive-definite, then \( \cdots \)

\( \text{For optimization, say minimizing } \| \frac{\partial}{\partial} \|, \text{ say minimizing } \}

\[ \| \frac{\partial}{\partial} \|, \text{ say minimizing } \}

\[ \text{linear residual norm } \]

\[ = \| s(x)f \Delta + (x)f \| = \]

linear residual norm

GMRES and other "residual minimizing" methods minimize over \( k \).

They have desirable optimality properties.
Update: $s + x \rightarrow x$

\[ \| (x)_H \| \geq \| s(x)_H + (x)_H \| \]

Find some $u \in (0, 1)$ and $s$ that satisfy

Iterate:

Given an initial $x$.

Exact Newton Method:

\[ (s + x)_H \approx s(x)_H + (x)_H \]

An inexact Newton method (Dembo Eisenstat Steihaug 1982) is any method each step of which reduces the norm of the local linear model. An inexact Newton method.

When to stop the Krylov iterations?
The "forcing term" \( \eta \).

Iterations becomes the issue of choosing the issue of when to stop the linear

\[
\| (x) H \| \eta \geq \| s (x) H + (x) H \|
\]

Apply the iterative linear solver to \( (x) H - s (x) H \) until \( (x) H - s (x) H \) gets small.

Choose \( \eta \in [0, 1) \).

Regardless, Newton-Krylov methods are a special case.
\[ \mathbf{v}^* x \triangleq \mathbf{y} x \iff \left\| (\nabla \mathbf{y} x)^T \right\| O = \mathbf{y} u \]

If also \( F \) is Lipschitz continuous at \( x^* \), then

\[ \mathbf{v}^* x \triangleq \mathbf{y} x \iff 0 \iff \mathbf{y} u \]

\[ \left\| m (\mathbf{y} x)_{x} \right\| \equiv (\mathbf{y} x)_{x} \quad \text{linear in norm} \]

\[ \mathbf{v}^* x \triangleq \mathbf{y} x \iff 1 > x_{\max} \geq \mathbf{y} u \]

Newton sequence with \( x_0 \) sufficiently near \( x^* \), then

\[ \text{Theorem: Suppose } F \text{ and } \mathbf{y} \text{ are invertible.} \]

\( \{x^k\} \) is an inexact forcing terms.

Debo-Eisenbud-Stehnaue (1982): Local convergence is controlled by the
Streamlines for $Re = 10,000$.

On the sides and bottom, \begin{equation}
0 = \frac{\partial \phi}{\partial \theta} \quad \text{and} \quad 0 = \phi \bigg|_{\text{top}}.
\end{equation}

On \( \theta \), \begin{equation}
0 = \phi \nabla \left( \frac{1}{\theta} \frac{\partial \phi}{\partial \theta} - \phi \nabla \left( \frac{\partial \phi}{\partial \theta} \right) \right) + \phi \nabla (\omega R/1).
\end{equation}

In \([0,1] \times [0,1] = \Omega\), \begin{equation}
\text{Example: The driven cavity problem.}
\end{equation}

\begin{equation}
(x)_{\Omega} - s(x)_{\Omega} \overset{\text{overrelaxing}}{=} \text{These give desirable local convergence rates, but there remains the danger of}
\end{equation}
Performance on the driven cavity problem, Re = 500. "Gaps" indicate over-solving.

\[
\begin{align*}
\min \quad & \frac{1}{2} \int_0^T \left( ||x(t) + \frac{1}{2}x_f(t)||^2 \right) dt \\
\text{subject to} \quad & x(t) = \begin{cases} 0, & t \leq 0 \\ \frac{1}{2} \frac{x_f(t)}{T}, & t > 0 \end{cases}
\end{align*}
\]
Some practical safeguards are also necessary.

\[ \| x^* - \gamma x \| \geq \| x^* - x \| \gamma \] with \( x^* \leftarrow \gamma x \)

\[ \frac{\| (1 - \gamma x) A \|}{\| 1 - \gamma x \| (1 - \gamma x) A + (1 - \gamma x) A - \| (\gamma x) A \|} = \gamma L \]

\[ \{ \gamma_{\text{max}}, \gamma_{\text{min}} \} = \gamma L \]

"Choice I":

A forcing term choice that reduces oversolving (Eisenstat-Walker 1996).
Performance on the driven cavity problem, Re = 500.

The inverted triangle indicates the safeguard value was used.
If unacceptable, modify it and test again.

Test a step for acceptable progress.

Idea: Repeat as necessary...

... but we can make it more likely...

We can't guarantee convergence to a solution...

Globalizations of Newton-like methods.

Another major issue: How to globalization the method?
Update $x \rightarrow x + s$.

\[(u - I) \theta - I \rightarrow u \text{ and } s \theta \rightarrow s \theta \rightarrow \max_{\theta} \min_{\theta} \theta \]

Choose $\theta \in \theta$ and $s \theta \rightarrow \max_{\theta} \min_{\theta} \theta$.

While $\| (x)_{\theta} \| ([u - I]t - I] < \| (s + x)_{\theta} \|$

Choose $\theta \in \min_{\theta} \max_{\theta} \theta$ and such that

\[\| (x)_{\theta} \| u \geq \| (s)_{\theta} \lambda + (x)_{\theta} \| \]

Iterate:

Given an initial $x$ and $t \in (0, 1)$,

\[\theta \in (0, 1) \}

Inexact Newton Backtracking (INB) Method:

A backtracking method (Eisenstadt-Walker 1994) is . . .

\[\text{Backtracking (line search, damping)} \]

Classical approach #1: Backtracking (line search, damping)
asymptotic convergence is determined by the initial \( n \)'s.

\[
(**x)_{t} \not\in F, \text{ is nonsingular, and converges to } x^{\ast} \text{ such that } F^{\ast}(x^{\ast}) = 0, \text{ and } F^{\ast}(x^{\ast}) \text{ is nonsingular, then}
\]

\[
\text{Possibilities:}
\]

all sufficiently large \( k \). Furthermore, the initial \( s \) and \( n \) are accepted for the INB method has a limit point \( x^{\ast} \) such that \( F^{\ast}(x^{\ast}) = 0 \) and \( x^{\ast} \not\in F \) and produced by \( \{ x \} \).

**Theorem:** Assume that \( F \) is continuously differentiable. If
Choose \( \theta \in \theta_{\text{max}, \text{min}} \) to minimize a quadratic or cubic that interpolates

\[
\left\| (X^\intercal X + \gamma I)^{-1} X^\intercal y \right\|
\]

- Take \( \| \cdot \| \) to be an inner-product norm, e.g.,

Choose \( \text{min} \theta = 0.5 \)

Choose \( \text{max} \theta = 1 \), e.g.,

Choose \( \gamma \) small, e.g., \( \gamma = 10^{-4} \)

Choose \( u_{\text{max}} \) near 1, e.g., \( u_{\text{max}} = 0.9 \)

Practical recommendations...
Update $x \rightarrow x + s$.

determine a final $s$.

Apply the More-Thuente line search to

$$ ||(x)^A - u || \geq || s(x)^A + (x)^A || $$

Choose $n_k \in [0, n_{\text{max}}]$ and initial $s$ such that

Iterate:

Given an initial $x$ and $n_{\text{max}} \in [0, 1)$.

Inexact Newton More-Thuente line search (INML) Method:

A line search method (More-Thuente, 1984) is ...
Finally, update $s \rightarrow \chi_s$.

\[ (*) \text{ and } (**), \chi \in \chi_{\text{min}}, \chi_{\text{max}} \]

Also, holds if \( \chi \leq \chi' \). \( \chi \in \chi_{\text{min}}, \chi_{\text{max}} \)

\( (*) \text{ may or may not hold.} \chi = \chi_{\text{min}}, \chi_{\text{max}} \)

\( (*) \text{ may not hold.} \chi_{\text{min}}, \chi_{\text{max}} \)

Possible outcomes for the final \( \chi \):

The algorithm generates iterates within a given \( \chi_{\text{min}}, \chi_{\text{max}} \) range.

\[ |(0), \phi | g \geq |(\chi), \phi | \text{ (**)} \quad \text{and} \quad (0), \phi \sigma + (0) \phi \geq (\chi) \phi \text{ (*)} \]

To find \( \chi \) such that

\[ \| s \chi + x \| \frac{2}{1} \equiv (\chi) \phi \text{ (**) for } \]

More-Thuente linear search:
Choose $\gamma_{\text{min}} = 10^{-12}$, $\gamma_{\text{max}} = 10^6$.

Choose $\gamma = 10^{-4}$, $\beta = 0.9999$.

Practical recommendations . . .

\[ x^* \leftarrow x^* \text{ and } 0 = (x^*)^T F_1(x^*) \text{, such that } F_1(x^*) \text{ is nonsingular} \]

\[ 0 \leftarrow (x^*)^T F_1(x^*) \text{, bounded, then } F_1 \text{ is nonsingular for each } x \text{ and } F_1 \text{ has a subsequence such that } \{ F_1^r(x^*) \} \text{ is nonexpansive} \]

\[ \text{The More-Traub interior line search satisfies (**) and } \{ F_1^r(x^*) \} \text{ is determined by the INNL method such that, for each } x, \text{ the } x \text{ determined by} \]

\[ \text{differentially on } \mathcal{I} \text{ is given and } F \text{ is Lipschitz continuously} \]

Theorem: Suppose that $x^0$ is given and $F$ is Lipschitz continuously
Can't be computed exactly.

\[ \cdot \left\| n \left( n \right) \mathcal{I} + (n) \mathcal{I} \right\| ^{\tilde{q}} \| m \| ^{\tilde{q}} = s \]
\[ s = \arg \min_{\|w\| \leq \delta} F(w) \Rightarrow F'(w)w \Rightarrow F'(w) \Rightarrow s_N. \]

The dogleg step: 

\[ \text{FPL}: 0 \rightarrow s_{CP} \rightarrow s_N. \]
\[
\|s(n)_{\mathcal{F}} + (n)_{\mathcal{F}}\| - \|(n)_{\mathcal{F}}\| \equiv \text{pred} \quad \|s + n)_{\mathcal{F}}\| - \|(n)_{\mathcal{F}}\| \equiv \text{pred} \quad \]

Update \( s + n \rightarrow n \) and update \( \theta \).

Redetermine \( s \in \mathcal{I} \).

\{ \text{max} \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \theta \th...
... but this is not entirely satisfactory.

\[ \text{else if } s \leq \| s \|_{N_{CD}} \]

\[ \| s \|_{CD} = \frac{s}{s} \cdot \text{if } s \geq \| s \|_{N_{CD}} \]

\[ \text{else if } s \leq \| s \|_{N_{CD}} \]

\[ \| s \|_{CD} = \frac{s}{s} \cdot \text{if } s \geq \| s \|_{N_{CD}} \]

The Standard Strategy.

- Choosing \( s \in \mathcal{D} \).
- For now we're using \( s \).
- Computing \( s_{CD} \) requires \( p \)-products.

Some Issues.
Furthermore, \( s^N \rightarrow s^N \) for all sufficiently large \( N \).

If additionally \( \mathcal{F} \) is nonsingular, then \( \mathcal{I} = (x) \mathcal{F} \) and \( 0 = (x) \mathcal{F} \).

\( \mathcal{I} \) is a stationary point of \( \mathcal{F} \).

\[ \| s(x) \mathcal{I} + (x) \mathcal{I} \| \geq \| (x) \mathcal{I} \| \mathcal{I} \| \mathcal{I} \| \text{ of } \mathcal{I} \]

**Theorem:** Assume that \( \mathcal{F} \) is continuously differentiable. If \( x^* \) is a limit point of \( \{ x^N \} \) produced by the INDL method, then \( x^* \) is a stationary point of \( \mathcal{F} \).

Def.: For every \( s \in \mathbb{R}^n \), if \( x \in \mathbb{R}^n \) is a stationary point of \( \mathcal{F} \), then..
Machine: 8-node (16-CPU) IBM cluster.

- Chaco load-balancing code.
- From the Aztec package,
- GMRES routine and domain-based (overlapping Schwarz) ILU preconditioners
- Globally-robust NK methods implemented in NOX solver package.
- MPSElae parallel reactive flow code.

Software: Sandia National Labs codes, as follows...

Discretization: Pressure stabilized streamline upwinding Petrov-Galerkin FEM.

PDEs: Low Mach number Navier–Stokes equations with heat transport as appropriate.

Problems: Very large-scale 2D and 3D benchmark steady-state CFD problems.

Goal: To compare robustness and efficiency of these Globally-robust NK solvers.

Numerical experiments:
The driven cavity and backward facing step problems.

\[ \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0 \]

Driven Cavity: \( Re = \begin{cases} 1000, 2000, \ldots, 10000 & \text{in 2D} \\ 100, 200, \ldots, 1000 & \text{in 3D} \end{cases} \)

Backward facing step: \( Re = 100, 200, \ldots, 700, 750, 800 \).

2D backward facing step. Streamlines for \( Re = 850 \).
The thermal convection problem.

\[ \frac{1}{Pr} \cdot \nabla \cdot \mathbf{u} = -\nabla p + \nabla^2 \mathbf{u} + Ra T \mathbf{g}, \]

\[ \nabla \cdot \mathbf{u} = 0, \]

\[ \mathbf{u} = \mathbf{n} \cdot \nabla T = \nabla^2 T \]

2D thermal convection. Flow and temperature contours at \( Ra = 10^3, 10^4, 10^5, 10^6 \).

\( Pr = 1 \) and \( Ra = 10^3, 10^4, 10^5, 10^6 \).
<table>
<thead>
<tr>
<th></th>
<th>4</th>
<th>3</th>
<th>5</th>
<th>5</th>
<th>1</th>
<th>0</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Full Step</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>5</td>
<td>1</td>
<td>0</td>
<td>Double</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>5</td>
<td>4</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>More Thermal</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>Quadratic Only</td>
<td>Backtracking</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>5</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Quadratic/Cubic</td>
<td>Backtracking</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Easy</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>5</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Easy</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Method</td>
<td></td>
</tr>
</tbody>
</table>

2D Results:

A robustness study...
and constant 10–4 Forcing terms (bottom rows).

Numbers of failures with Choice 1 Forcing terms (top rows).

<table>
<thead>
<tr>
<th>Method</th>
<th>3D Backward</th>
<th>3D Lid Driven</th>
<th>Thermal Conv</th>
<th>Thermal Conv</th>
</tr>
</thead>
<tbody>
<tr>
<td>Backward Facing Step</td>
<td>100 &gt; Re &gt; 500</td>
<td>100 &gt; Re &gt; 500</td>
<td>Easier</td>
<td>Easier</td>
</tr>
<tr>
<td>Driven Cavity</td>
<td>600 &gt; Re &gt; 1000</td>
<td>100 &gt; Re &gt; 1000</td>
<td>Thermal Conv</td>
<td>Thermal Conv</td>
</tr>
<tr>
<td>Easier</td>
<td>Ra = 10^6</td>
<td>Ra &gt; 10^6</td>
<td>3D Backward</td>
<td>3D Lid Driven</td>
</tr>
</tbody>
</table>

3D Results: A robustness study (cont.) …
<table>
<thead>
<tr>
<th>Trust Region</th>
<th>More-Thuente</th>
<th>(Quadratic Only)</th>
<th>(Quadratic/Cubic)</th>
<th>Backtracking</th>
<th>Backtracking</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.1</td>
<td>138.77</td>
<td>NA</td>
<td>10.71</td>
<td>0.97</td>
<td>147.16</td>
</tr>
<tr>
<td></td>
<td>9.25</td>
<td>57.91</td>
<td>15.99</td>
<td>0.15</td>
<td>148.65</td>
</tr>
<tr>
<td></td>
<td>9.54</td>
<td>52.65</td>
<td>17.22</td>
<td>0.13</td>
<td>148.61</td>
</tr>
<tr>
<td></td>
<td>9.49</td>
<td>48.79</td>
<td>17.24</td>
<td>0.14</td>
<td>48.79</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>48.79</td>
</tr>
</tbody>
</table>

**Choice I** Forcing terms (top rows) and constant $10^{-4}$ forcing terms (bottom rows).

An **efficiency study** over cases in which all globalized methods succeeded.
To be continued...

No combination is a panacea. Many ingredients contribute to success.

Efficiency:
Adaptive forcing terms significantly improve both robustness and

The globalizations alone improve robustness.

Difficult large-scale test problems:
These globalized Newton-Krylov methods are very effective on these

Summary observations.