Inexact Newton Dogleg Methods

Homer Walker
Mathematical Sciences Department
Worcester Polytechnic Institute
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Joint work with Roger Pawlowski (SNL), J. N. Shadid (SNL), J. P. Simonis (WPI).

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**Nonlinear problem:**  \[ F(u) = 0, \quad F : \mathbb{R}^n \to \mathbb{R}^n. \]

Start with classical ... 

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**Newton’s Method:**

Given an initial \( u \).

Iterate:

- Solve \( F'(u)s = -F(u) \).
- Update \( u \leftarrow u + s \).
Globalizations.

Idea: Repeat as necessary . . .

- *Test* a step for acceptable progress.
- If unacceptable, *modify* it and test again.

Major approaches:

- *Backtracking* (linesearch, damping).
- *Trust region*. 
**Trust region globalization.**

- \( s = \arg \min_{\|w\| \leq \delta} \| F(u) + F'(u) w \|. \)

- Can’t be computed exactly.
**The dogleg step.** \[ f(u) \equiv \frac{1}{2} \| F(u) \|^2. \]

- \[ s^{\text{CP}} \equiv \arg \min_{0 \leq \lambda < \infty} \| F(u) - F'(u) \lambda \nabla f(u) \|. \]
- \[ \Gamma^{\text{DL}}: 0 \to s^{\text{CP}} \to s^{\text{N}}. \]
- \[ s = \arg \min_{\| w \| \leq \delta, w \in \Gamma^{\text{DL}}} \| F(u) + F'(u) w \|. \]
Work toward a general *inexact Newton* adaptation.

**Inexact Newton Method** (Dembo–Eisenstat–Steihaug 1982):
Given an initial $u$.
Iterate:

Find *some* $\eta \in [0, 1)$ and $s$ that satisfy

$$\|F(u) + F'(u) s\| \leq \eta \|F(u)\|.$$ 

Update $u \leftarrow u + s$. 
Possible **big** issue: *Evaluating $s^{CP}$ requires $F'T$-products.*

**Proposed general framework.**

- Find $s^{IN}$ such that $\|F(u) + F'(u) s^{IN}\| \leq \eta \|F(u)\|$.
- Choose $\hat{g} \approx \nabla f(u)$ and compute $\hat{s}^{CP} = \arg \min_{0 \leq \lambda < \infty} \|F(u) - F'(u) \lambda \hat{g}\|$.
- Define $\hat{\Gamma}^{DL} : 0 \to \hat{s}^{CP} \to s^{IN}$.
- Choose $s \in \hat{\Gamma}^{DL}$, test, etc.
More issues . . .

Minor consideration: For any $\eta \in (0, 1)$, $\|F(u) + F'(u) s\|$ may not decrease monotonically along $\hat{T}_{DL}$. 
More issues (cont.) . . .

More serious consideration: Unless $\eta \in [0, 1)$ is small (how small?), we may have
\[
\langle s^{\text{IN}}, s^{\text{CP}} \rangle < \| s^{\text{CP}} \|^2 \quad \text{or} \quad \| s^{\text{IN}} \| < \| s^{\text{CP}} \|.
\]
Inexact Newton Dogleg Method:

Given $\eta_{\text{max}} \in [0, 1)$, $\delta_{\text{min}} > 0$, $t \in (0, 1)$, $0 < \theta_{\text{min}} < \theta_{\text{max}} < 1$, and initial $u$ and $\delta \geq \delta_{\text{min}}$.

Iterate:

Choose $\eta \in [0, \eta_{\text{max}}]$ and $s^{\text{IN}}$ such that

$$\|F(u) + F'(u) s^{\text{IN}}\| \leq \eta \|F(u)\|.$$

Determine $\hat{g}$ and admissible $s \in \hat{\Gamma}^{\text{DL}}$.

While $\text{ared} < t \cdot \text{pred}$ do:

Choose $\theta \in [\theta_{\text{min}}, \theta_{\text{max}}]$.

Update $\delta \leftarrow \max\{\theta \delta, \delta_{\text{min}}\}$.

Redetermine admissible $s \in \hat{\Gamma}^{\text{DL}}$.

Update $u \leftarrow u + s$ and update $\delta$.

- $s \in \hat{\Gamma}^{\text{DL}}$ is admissible $\iff \min\{\|s^{\text{IN}}\|, \delta_{\text{min}}\} \leq \|s\| \leq \delta$.

- $\text{ared} \equiv \|F(u)\| - \|F(u + s)\|$, $\text{pred} \equiv \|F(u)\| - \|F(u) + F'(u) s\|$.

- Choose $\theta$, update $\delta$ a la Dennis–Schnabel (1983).
Recall: $u$ is a **stationary point** of $\|F\| \iff \|F(u)\| \leq \|F(u) + F'(u) s\| \forall s$.

**Theorem:** Assume $F$ is continuously differentiable. Suppose $\{u_k\}$ is produced by the INDL Method and, for some $\epsilon > 0$,

$$\frac{\langle \hat{g}_k, \nabla f(u_k) \rangle_2}{\|\hat{g}_k\|_2 \|\nabla f(u_k)\|_2} \geq \epsilon$$

for every $k$. If $u_*$ is a limit point of $\{u_k\}$, then $u_*$ is a stationary point of $\|F\|$. If additionally $F'(u_*)$ is nonsingular, then $F(u_*) = 0$ and $u_k \to u_*$. Moreover, for all sufficiently large $k$, the initial $s_k$ is accepted without modification in the while-loop, and $s_k = s_k^{IN}$ is an admissible step.

Note: If $s_k = s_k^{IN}$ for all large $k$, then **convergence is ultimately controlled by the “forcing terms”** $\eta_k$. 
Choosing an admissible \( s \in \hat{\Gamma}^{DL} \).

The Standard Strategy.

If \( \|s^{\text{IN}}\| \leq \delta \),
\[ s = s^{\text{IN}} \]
Else if \( \|\hat{s}^{\text{CP}}\| \geq \delta \),
\[ s = (\delta/\|\hat{s}^{\text{CP}}\|)\hat{s}^{\text{CP}} \]
Else
\[ s = (1 - \gamma)\hat{s}^{\text{CP}} + \gamma s^{\text{IN}} \]
for \( \gamma \in (0, 1) \) such that \( \|s\| = \delta \)

- An admissible \( s \in \hat{\Gamma}^{DL} \) is uniquely determined.
- \( s^{\text{IN}} \) is always computed; \( \hat{s}^{\text{CP}} \) may not be.
- If \( \eta \) isn’t small, we may have \( s = s^{\text{IN}} \) when \( s = \lambda\hat{s}^{\text{CP}} \) would be preferred.
An Alternative Strategy.

If \( \| \hat{s}_{\text{CP}} \| \geq \delta \),
\[
s = \left( \frac{\delta}{\| \hat{s}_{\text{CP}} \|} \right) \hat{s}_{\text{CP}}
\]
Else if \( \| F(u) + F'(u) \hat{s}_{\text{CP}} \| \leq \eta \| F(u) \| \),
\[
s = \hat{s}_{\text{CP}}
\]
Else if \( \| s_{\text{IN}} \| \leq \delta \),
\[
s = s_{\text{IN}}
\]
Else
\[
s = (1 - \gamma) s_{\text{CP}} + \gamma s_{\text{IN}}
\]
for \( \gamma \in (0, 1) \) such that \( \| s \| = \delta \)

- An admissible \( s \in \hat{\Gamma}_{\text{DL}} \) is uniquely determined.
- \( \hat{s}_{\text{CP}} \) is always computed; \( s_{\text{IN}} \) may not be.
- \( s \) is appropriately biased toward \( \hat{s}_{\text{CP}} \).
Further refinements.

- If needed, $s^{\text{IN}}$ can be computed as $s^{\text{IN}} = \hat{s}^{\text{CP}} + z$, where $\|\hat{r}^{\text{CP}} + F'(u) z\| \leq \eta \|F(u)\|$ and $\hat{r}^{\text{CP}} \equiv F(u) + F'(u) \hat{s}^{\text{CP}}$.

- Having both $\hat{s}^{\text{CP}}$ and $s^{\text{IN}}$, we can choose $s = (1 - \gamma) \hat{s}^{\text{CP}} + \gamma s^{\text{IN}}$ so that $\|s\| \leq \delta$ and $\|F(u) + F'(u) s\|$ is minimal (easy).
Numerical experiments.

- **Test problems**: Three benchmark flow problems in 2D; two in 3D.

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

- **Discretization**: Pressure stabilized streamline upwind Petrov–Galerkin FEM.

- **Algorithms and software**: Newton–GMRES implementations in the Sandia NOX nonlinear solver suite, with GMRES and domain-based (overlapping Schwarz) ILU preconditioners from the Sandia Aztec package. The simulation driver was the Sandia MPSalsa parallel reacting flow code.

- **Problem sizes**: 25,263 to 179,685 unknowns.

- **Machine**: 4-15 nodes (8-30 CPUs) on a 16-node, 32-CPU IBM Linux cluster.
**2D test problems.**

Thermal Convection Problem

Lid Driven Cavity Problem

Backward-Facing Step Problem

**3D test problems.** Thermal convection and lid driven cavity problems in the unit cube.
The forcing terms.

- **Small constant:** \( \eta_k = 10^{-4} \).

- **Adaptive:** \( \eta_k = \min \{ \eta_{\text{max}}, \tilde{\eta}_k \} \), where

\[
\tilde{\eta}_k = \frac{\|F(u_k)\| - \|F(u_{k-1}) + F'(u_{k-1}) s_{k-1}\|}{\|F(u_{k-1})\|}
\]
Robustness study.

2D and 3D Thermal Convection $Ra = 10^3, 10^4, 10^5, 10^6$

2D Lid Driven Cavity $Re = 1000, 2000, \ldots, 10,000$

3D Lid Driven Cavity $Re = 100, 200, \ldots, 1000$

2D Backward Facing Step $Re = 100, 200, \ldots, 700, 750, 800$
**Robustness study.** The table shows *total numbers of failures.*

<table>
<thead>
<tr>
<th>Method</th>
<th>Forcing Term</th>
<th>2D Problems</th>
<th>3D Problems</th>
<th>All Problems</th>
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</thead>
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<tr>
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<td>0</td>
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<td>Stand. Strat.</td>
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<td>10</td>
<td>0</td>
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<tr>
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<tr>
<td>“Full Step”</td>
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<td></td>
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<td>18</td>
<td>5</td>
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</table>

*GMRES solves starting from zero.

**GMRES solves starting from the Cauchy point.*
**Efficiency study.**

- 2D Thermal Convection  \( Ra = 10^3, 10^4, 10^5 \)
- 3D Thermal Convection  \( Ra = 10^3, 10^4, 10^5, 10^6 \)
- 2D Lid Driven Cavity  \( Re = 100, 200, \ldots, 1000 \)
- 3D Lid Driven Cavity  \( Re = 100, 200, \ldots, 900 \)
- 2D Backward Facing Step  \( Re = 100, 200, \ldots, 700, 750, 800 \)
### Efficiency study.

<table>
<thead>
<tr>
<th>Method</th>
<th>Forcing Term</th>
<th>Inexact Newton Steps</th>
<th>Function Evals.</th>
<th>GMRES Iterations</th>
<th>GMRES Iterations per INS</th>
<th>Normal'd Time</th>
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<tbody>
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<td>147</td>
<td>1.23</td>
</tr>
</tbody>
</table>

*GMRES solves starting from zero.

**GMRES solves starting from the Cauchy point.*
**Concluding observations.**

- These globalizations have good theoretical support.

- They are effective on these test problems, *especially with adaptive forcing terms*.

- Methods, strategies, and refinements bear further study ...
  - more experimentation,
  - comparisons with other globalizations (*see Simonis’s talk*).