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Newton-Krylov Methods
and Krylov Subspace Methods
Think: n very large, A and \( I_n \) sparse. 

Nonlinear problem: 

\[ \begin{array}{l}
\mathbb{R}^n \leftarrow \mathbb{R}^n \\
I : 0 = f(x) \end{array} \]

... and Newton-Krylov methods for the

Linear problem: 

\[ \begin{array}{l}
A \in \mathbb{R}^{n \times n} \\
q = Ax \end{array} \]

... and Krylov subspace methods for the

We'll consider ...
There are by now many Krylov subspace methods, e.g.,

**Krylov Subspace Method:**

\[
\{0 \in \mathbb{R}^n \mid x_0, x_{1+}, \ldots, x_{n-1} \} \quad \text{span} \equiv \mathcal{K} \quad x \in \mathcal{K},
\]

\[
\exists z \quad x + 0 \cdot z = x
\]

Given \( x_0 \), determine …
steps.

So a "smart" Krylov subspace method will find the solution in at most $n$ steps.

Lemma: If $A$ is nonsingular, then $\dim \mathcal{K}^{r+1} \geq \dim \mathcal{K}^{r}$ and $\dim \mathcal{K}^{r+1} \geq \dim \mathcal{K}^{r}$. Some $z \in \mathcal{K}^{r}$.

\[ z + 0 x = q_{r-1} A^{-1} \iff \forall \mathcal{K}^{r+1} \geq \dim \mathcal{K}^{r} \]

They require only products of $A$ (and sometimes $A^T$) with vectors.

certain features.
\[ T_r \preceq \mathcal{K}_r \quad \forall r \in \mathcal{K}_r \]

Orthogonal Residual (OR): Choose \( z \in \mathcal{K}_r \) so that

\[ \min_{\mathcal{K}_r} \| z + c \|^2 = \min_{\mathcal{K}_r} \| z - q \|^2 \]

Minimal Residual (MR): Choose \( z \in \mathcal{K}_r \) to solve

... for specificing \( z \) ...
\[
\begin{align*}
\text{MINRES (Paige-Saunders 1975)} & \iff \text{MR} \\
\text{SYMMLQ (Paige-Saunders 1975)} & \iff \text{OR}
\end{align*}
\]

Indefinite: \( \mathbf{A} = \mathbf{A}^T \bullet \)

\[
\begin{align*}
\text{Conjugate Residual (Hestenes-Stiefel 1952)} & \iff \text{MR} \\
\text{Conjugate Gradient (Hestenes-Stiefel 1952)} & \iff \text{OR}
\end{align*}
\]

\( \mathbf{A} > 0 \iff \mathbf{A} = \mathbf{A}^T \bullet \)

MR/OR with Short Recurrence

\( \text{MR/OR} \iff \mathbf{A} = \mathbf{A}^T \)
Given $A', q, x', tol, \text{itmax}$.

Conjugate Gradient Method:

\[ z + x \rightarrow x \] 
\[ \frac{z}{\|z\|} \rightarrow d' \text{ and } \frac{d'/z}{z} \rightarrow g' \]
\[ dp \rightarrow p \]
\[ dp + z \rightarrow z \]
\[ \frac{d'}{z} \rightarrow d \text{ and } dp \rightarrow dp \]
\[ dp + u \rightarrow dp' \]

Compute $d$.

\[ \frac{d'}{z} \rightarrow d' \text{ and } dp \rightarrow dp' \]
\[ dp' + u \rightarrow dp' \]

If $d < tol$, go to End.

Iterate: For $i = 0, \ldots, \text{itmax}$, do:

\[ 0 = g', 0 = z, \frac{z}{\|z\|} = x' - q = \frac{d'}{z}, \text{Ax} = A, y, \text{tol}, \text{itmax} \]
\[ \mathbf{a}_0 \text{ on } 0 = n \quad [1, 0] \times [1, 0] = \mathbf{a} \quad \text{in } f = n \nabla \]

CG performance — accuracy:
\[ m = 16, 32, 64, 128. \quad m \times m \text{ grid}. \]

\[ \text{CG, no preconditioning.} \quad \text{CG, 1 machine epsilon 10^{-16}.} \]

\[ \begin{align*}
\phi &\quad \phi \\
0 &\quad n \\
[1, 1] \times [1, 1] &\quad = \mathcal{A} \quad \text{in} \quad f = n \nabla
\end{align*} \]

CG performance — scalability.
Preconditioning is key to scalability.

\[
\hat{y}_{I-1}^W = x, \quad q = \hat{y}_{I-1}^W \quad \triangleleft \quad \text{Right:}
\]

\[
q_{I-1}^W = x \hat{V}_{I-1}^W \quad \triangleleft \quad \text{Left:}
\]

In practice, all Krylov subspace methods usually require preconditioning.
PCG performance — scalability

\[ \mathbf{A} \mathbf{e} = 0 \ \text{on} \ \Gamma \quad \mathbf{f} = n \nabla \]
So we must give up either MR/0R or short recurrences.

Faber and Mantel (1984): For General A, the MR and 0R criteria cannot be implemented with short recurrences.

What about methods for General A?
MR leads to the Generalized Minimal Residual Method (Saad-Schultz 1986).

OR leads to the Arnoldi method or FOM (Full Orthogonalization Method).

First possibility: Stick with MR/OR and give up short recurrences.
\( m \) can be important.

\( \text{GMRES}^m \) may not converge. It usually works well, but the choice of

which restarts are necessary with \( x^m \rightarrow x^0 \) after \( m \) steps.

For most large-scale problems, the method implemented is \( \text{GMRES}^m \),

storage, plus \( k \) products of \( A \) with vectors,

\( \mathcal{O}(hn) \) arithmetic and requires \( \mathcal{O}(hn) \) iterations costs \( \mathcal{O}(hn) \) arithmetic

Carrying out \( k \) iterations costs \( \mathcal{O}(hn) \) arithmetic and requires \( \mathcal{O}(hn) \) iterations.

Converges in \( \leq n \) iterations (in exact arithmetic) but may stagnate.

Monotone decreasing residual norms.

\textbf{Basic GMRES properties.}
Given $A$, $q$, $x$, tol, $\text{itmax}$:

**GMRES($m$)** (standard Gram-Schmidt Implementation):

- **Initialize**: $r = q - Ax$, $x_0 = 0$, $\text{itno} = 0$.
- **Iterate**: For $k = 1$, \ldots, $m$, do:
  - $r_k = r - x_0 A r / \beta = r - Ax$, $\beta = ||r||$.
  - $x_k = r_k / \beta$.
  - $r_k = q - Ax_k$.
  - $x_0 = x_0 + x_k$.
- **Solve**: Let $k$ be the final iteration number from Iterate.
- Else update $\text{itno} = \text{itno} + 1$.

Determine $\gamma_k$ such that

- If $k < 1$, apply $\gamma_{k-1} = 1$.
- If $k = 1$, form $H_1 = I$; else form $H_k = I + \gamma_k H_{k-1}$.
- For $i = 1$, \ldots, $k$, do:
  - Set $H_k y + 1, \gamma_k H y$. 
  - Set $y = I y + 1, \gamma_k y$.
  - Update $y + 1, \gamma_k y$.

Set $y + 1, \gamma_k y$. 

Update $y + 1, \gamma_k y$.

For $i = 1$, \ldots, $k$, do:

- Initialize: $r = q - Ax$, $x_0 = 0$.
- Update $\text{itno} = \text{itno} + 1$.
- Iterate:
  - Solve $r = Ax$, $x_0 = 0$.
  - Update $\text{itno} = \text{itno} + 1$.
- Else iterate:
  - Reset $y = 0$.
  - Update $\text{itno} = \text{itno} + 1$.

If $\gamma_k ||r|| / \beta < \text{tol}$, accept $x$; otherwise, return to Initialize.

Update $x = x + r / \beta$.

Solve $H_k y = r$, where $y_0 = 0$.

Final: Let $k$ be the final iteration number from Iterate.

Else update $\text{itno} = \text{itno} + 1$.
\[ f = \frac{x \theta}{n \vartheta} \varphi + n c + n \nabla \]
• BICGSTAB — Biconjugate Gradient Stabilized (van der Vorst 1992).

• GMRES — Generalized Minimal Residual (Fletcher-Reeves 1991).

• CGS — Conjugate Gradient Squared (Sonnefeld 1989).

• BCG — Biconjugate Gradient (Lanczos 1952, Fletcher 1976).

Second possibility: Give up MR/OR and pursue short recurrences.
Newton's Method:

Update \( x \rightarrow x + s \).

Solve \( \frac{d}{dx} f(x) = 0 \).

Iterate:

Given an initial \( x \).

The model method is...
Which linear solver to use?

How to "globallize" the method?

When to stop the linear iterations?

| Issue: | Result: a Newton iterative method (truncated Newton method). |

\[
(x)_{k+1} = s(x)_k A
\]

Idea: Use an iterative linear solver to solve approximately
Given an initial $x$.

Inexact Newton Method:

$$ (s + x)\mathcal{H} \approx s(x)\mathcal{H} + (x)\mathcal{H} $$

Find some $\mu \in [0,1]$ and $s$ that satisfy

$$(x)\mathcal{H} || y \geq || s(x)\mathcal{H} + (x)\mathcal{H} ||$$

update $x \rightarrow x + s$. Interate:

An inexact Newton method (Dembo-Eisenstat-Steihaug 1982) is any method each step of which reduces the norm of the local linear model.
The "forcing term" is a critical issue in choosing the stopping criterion for iterative linear solvers. Typically, the stopping criterion is based on the norm of the residual.

\[ \| (x)_{n+1} \|_u \geq \| s(x)_n H + (x)_n H \| \]

Apply the iterative linear solver to the system until

\[ (x)_n H = s(x)_n H \]

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

Regard Newton iterative methods as a special case.
\[ *x \leftarrow \mathcal{N} x \iff (\| (\mathcal{N} x) J \|) O = \mathcal{N} \hat{u} \]  

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

\[ *x \leftarrow \mathcal{N} x \iff 0 \leftarrow \mathcal{N} \hat{u} \]  

\[ \| m (\mathcal{N} x) J \| \equiv (\mathcal{N} x) J \| m \| \text{ linear in norm } \]  

\[ *x \leftarrow \mathcal{N} x \iff 1 < \lambda_{\max} \leq \mathcal{N} \hat{u} \]  

\textbf{Theorem:} Suppose \( \mathcal{N} \) is invertible. If \( \{ \mathcal{N} x \} \) is inexact Newton sequence with \( x_0 \) sufficiently near \( x^* \), then

forcing terms.
Update $s + x \rightarrow x$.

$$(u - 1)\theta - 1 \rightarrow u \text{ and } s \theta \rightarrow s \text{ with } \theta \in [\theta_{\min}, \theta_{\max}]$$

Choose $\theta \in [\theta_{\min}, \theta_{\max}]$, do:

While $\|(x)_H\| \leq \|(s + x)_H\| < \|(s + x)_H\|$

Choose initial $u \in [0, u_{\max}]$ and $s$ such that

Iterate:

Given an initial $x$ and $t \in (0, 1)$, $u_{\max} \in (0, 1)$, $\theta_{\min}$ and $\theta_{\max}$.

Inexact Newton Backtracking (INB) Method:

A Globally convergent method (Eisenstat-Walker 1994) is...
asymptotic convergence is determined by the initial \( y \).

- \( \mathcal{F}(x) = 0 \), \( \mathcal{F}(x)^{T} \) is nonsingular, and

  - \( \mathcal{F}(x) \) converges to \( x \) such that \( \mathcal{F}(x)^{T} \) is singular at each one.

- \( \mathcal{F}(x) \) has limit points, and \( \mathcal{F}(x)^{T} \) is singular at each one.

\[ \infty \leftarrow \| y^{\ast} \| \]

Possibilities:

\( s \) and \( n \) are accepted for all sufficiently large \( \lambda \).

Furthermore, the initial \( \mathcal{F}(x)^{T} \) is nonsingular, then \( \mathcal{F}(x)^{T} \) is nonsingular, and \( \mathcal{F}(x)^{T} \) is singular at each point \( x \) such that

**Theorem:** If produced by the INB method has a limit point \( \{ y^{\ast} \} \)
exact evaluation of $v(x)_I$ and $v(x)_J$ by automatic differentiation.

$$\left[ (x)_I - (\alpha h + x)_I \right] \frac{h}{I} \approx v(x)_I$$

approximation of $v(x)_J$ by finite differences, e.g.,

They allow matrix-free implementations through

Krylov subspace methods have special appeal for solving

work toward a Newton-Krylov implementation.
The first CG step is the steepest descent step.

\[ s(x) f(x) \Delta \Delta \left[ \mathcal{L} - \frac{\mathcal{L}^2}{\mathcal{L}} \right] + s(x) f \mathbf{\Delta} + (x) f = \}

The \( k \)th CG step minimizes over \( \mathcal{K} \).

Symmetric positive-definite, then \( \ldots \)

\[ s(x) f(x) \Delta \mathbf{\Delta} \rightleftharpoons \mathbf{\Delta} \\
\]

For optimization, say \( \min_x \mathbf{\Delta} \), \( \mathbf{\Delta} \leftarrow \mathbf{\Delta} \) \( \forall x \in \mathcal{K} \).

Linear residual norm \( \| s(x) f + (x) f \| = \) linear model norm

GMRES and other MR methods minimize over \( \mathcal{K} \).

They have desirable optimality properties.
Choose \( \theta \in \theta \text{ max} \) to minimize a quadratic or cubic that interpolates

\[ \| (x - \theta \text{ max})^T \| \]

•

Take \( \| \cdot \| = \| \cdot \| = 2 \) •

Choose \( \theta \text{ max} = 1 \) \( \text{‘. ‘} \theta \text{ min} = 5 \) •

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

Choose \( n \text{ max} \) near 1, e.g., \( n \text{ max} = 9 \) •

Minor details:

A practical Newton–Krylov implementation of Algorithm 1N3B
the danger of over-solving!

These give desirable convergence rates, but there remains...

\[
\text{local quadratic convergence:} \quad \iff \quad \left(\| (x^k + I)x^k \| O = \nu \right) \quad \bullet
\]

\[
\text{local superlinear convergence:} \quad \iff \quad 0 \iff \nu \quad \bullet
\]

\[
\text{local linear convergence:} \quad \iff \quad 1 > \text{constant} \geq \nu \quad \bullet
\]

From Dembo–Eisenstat–Steinhaus (1982), we know...

---

Choosing the forcing terms.
Streamlines for $Re = 10,000$.

\[ 0 \begin{bmatrix} I \end{bmatrix} = \frac{u \phi}{\phi \theta} \quad \text{and} \quad 0 = \phi \quad \text{on} \quad \theta^1 \text{ on top.} \quad \text{on the sides and bottom.} \]

\[
\left[ \begin{bmatrix} I \end{bmatrix} \times \begin{bmatrix} I \end{bmatrix} \right] = \mathcal{A} \quad \text{in} \quad 0 = \phi \nabla \frac{\mathcal{E}}{\phi \theta} - \phi \nabla \frac{\phi \mathcal{E}}{\phi \theta} + \phi \nabla (\omega R / I)
\]

Example: The driven cavity problem.

\[ \text{Linear Residual Norm} \quad \text{Nonlinear Function Norm} \quad \text{New Nonlinear Iterations} \]

\[ \text{Total GMRES(20) Iterations} \]

\[ \text{Log Residual Norm} \]

\[
\left\{ \frac{\gamma + \frac{\gamma}{\Gamma}||y||}{\Gamma} \right\}_{1}^{D_{\text{empir--Stevens}} 1983}, \quad \text{FOR } \mu_{\text{min}} = \mu \]
Some practical safeguards are also necessary...

\[ \exists \gamma > 1 \quad \text{with order or if} \quad \gamma \to I. \]

\[ z \geq x > 1 \quad \exists \gamma \geq 0 \quad \left( \frac{\| (1 - \gamma x) A \|}{\| \gamma x A \|} \right) \gamma = \gamma \mu \]

Choice 2: \[ \{ \gamma_{\max}, \gamma \} \text{ min } \mu = \gamma \mu \]

\[ \| x - (1 - \gamma x) \| \| x - \gamma x \| \| \gamma \mathcal{A} \| \geq \| x - (1 + \gamma x) \| \] with \[ x \to I \cdot \gamma \cdot \mathcal{A} \]

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

Choice 1: \[ \{ \gamma_{\max}, \gamma \} \text{ min } \mu = \gamma \mu \]

Two forcing term choices that reduce overestimating (Eisenstat-Walker 1996)
The inverted triangle indicates the safeguard value was used.

Performance on the driven cavity problem, $Re = 500$. 

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**For safeguarded Choice 1**
Software: INB implementation in the Sandia MPsaLa parallel reactive flow code, with

Discretization: Pressure stabilized streamline upwinding Petrov-Galerkin FEM.

Equations as appropriate:

PDEs: Low Mach number Navier-Stokes equations with heat and mass transport

Problems: Three 2D CFD benchmark problems and two large scale 3D flow simulations.

Numerical experiments on CFD problems.

Goal: to test the effectiveness of backtracking alone and in combination with various forciing

Term choices.

Joint work with J. N. Shadiad and R. S. Tuminaro, Sandia National Labs (JCP 1997).

Machines: Intel Paragons at Sandia National Labs.

Sandia Aztec package.

GMRES routine and domain-based (overlapping Schwarz) ILU preconditioners from the
Backward facing step. Streamlines for $Re = 850$.

\[ 0 = \mathbf{n} \cdot \Delta \quad \text{and} \quad n_2 \Delta \frac{H}{l} + d\Delta - = n\Delta \cdot n \]

The driven cavity and backward facing step.
Thermal convection. Flow and temperature contours at $Ra = 1',000,000$.

\[ L_z \Delta = L \Delta \cdot n \quad '0 = n \cdot \Delta \quad 'Ra + n_z \Delta + d \Delta - = n \Delta \cdot \frac{dp}{L} \]

Here, $L = 1$. Thermal convection.
### Numbers of Failures with Backtracking (top rows) and without (bottom rows)

<table>
<thead>
<tr>
<th>Backward Focusing Step</th>
<th>Driven Cavity</th>
<th>Thermal Convection</th>
<th>10-4</th>
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<tr>
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<td>1</td>
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### Benchmark Problem Experiments

A robustness study...
<table>
<thead>
<tr>
<th>Time (Seconds)</th>
<th>Iterations</th>
<th>GMRES Steps</th>
<th>Back-Tracks</th>
<th>Inexact Newton Steps</th>
<th>Forcing Term ( \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>44.5</td>
<td>1531</td>
<td>0</td>
<td>5</td>
<td>10.4</td>
<td>Choice 1</td>
</tr>
<tr>
<td>511.5</td>
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</table>

**Without Backtracking**

<table>
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<tr>
<th>Time (Seconds)</th>
<th>Iterations</th>
<th>GMRES Steps</th>
<th>Back-Tracks</th>
<th>Inexact Newton Steps</th>
<th>Forcing Term ( \theta )</th>
</tr>
</thead>
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<td>0</td>
<td>5</td>
<td>10.4</td>
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</tbody>
</table>

**With Backtracking**
Performance with backtracking:

<table>
<thead>
<tr>
<th>Time (Seconds)</th>
<th>Iterations Gmres</th>
<th>Back-Steps Newton</th>
<th>Inexact Newton Term</th>
</tr>
</thead>
<tbody>
<tr>
<td>3915.1</td>
<td>15,360</td>
<td>6</td>
<td>24</td>
</tr>
<tr>
<td>3953.9</td>
<td>15,477</td>
<td>7</td>
<td>25</td>
</tr>
<tr>
<td>3554.5</td>
<td>13,450</td>
<td>6</td>
<td>28</td>
</tr>
<tr>
<td>Choice 1</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

- No failures with backtracking.
- Divergence without backtracking for all forcing terms.
- 3D non-uniform mesh: 477,855 unknowns; 256 processors.
- Navier-Stokes equations plus mass transport.
No strategy always works best.

Very accurate Jacobians may be necessary.

Many inexact Newton steps may be necessary.

Globalization (backtracking) is necessary (but not sufficient).

A good long-term choice is necessary (but not sufficient).

Newton-Krylov methods can be very effective on these problems, but...

Summary observations.