Restarted Krylov Subspace Methods for the Matrix Sign Function

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5. Summary and Future Work
Simulation of lattice QCD with the overlap Dirac operator requires the (repeated) solution of linear systems of equations

\[
(I + \Gamma_5 \text{sgn}(A)) x = y
\]  

(1)

with

\[
\Gamma_5 = I_n \otimes (\gamma_5 \otimes I_3),
\]

\[
\gamma_5 = \gamma_1 \gamma_2 \gamma_3 \gamma_4,
\]

with Dirac gamma matrices \( \gamma_j \)

\[
A = \Gamma_5 D_w(\mu), \ D_w(\mu) \text{ Wilson Dirac operator at chemical potential } \mu,
\]

\[
A \in \mathbb{C}^{N \times N}, \ N = 12n, \ n: \text{ number of lattice sites},
\]

\[
\text{sgn} : \mathbb{C} \setminus i\mathbb{R} \rightarrow \{-1, 1\} \text{ sign function}.
\]

For \( \mu \equiv 0 \) the matrix \( A \) is (essentially) Hermitian, otherwise non-Hermitian.
\( A \) is large, sparse and highly structured:

- \( N = 12n, \ n = n_1^4, \ n_1 \in \mathbb{N}. \)

<table>
<thead>
<tr>
<th>( n_1 )</th>
<th>4</th>
<th>8</th>
<th>16</th>
<th>32</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 12N )</td>
<td>3,072</td>
<td>49,152</td>
<td>786,432</td>
<td>12,582,912</td>
</tr>
</tbody>
</table>

- Discretization of Wilson Dirac operator involves only nearest neighbor coupling, i.e., typically \( 1 + 4 \cdot 12 = 49 \) nonzeros per row.

Solution method of choice for (1): **Krylov subspace methods.**

**Advantages:**

- storage, LU-factorization of matrix not required; instead only its action on given vector.
- Can stop short of full machine precision accuracy.
- Theory, software, preconditioning techniques well established.

**Crucial subproblem:** every iteration step requires action of \( \text{sgn}(A) \) on given vector.
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Matrix Functions

Fundamental computational task

Given \( A \in \mathbb{C}^{N \times N}, f : D \rightarrow \mathbb{C} \) analytic, \( \Lambda(A) \subset D \), \( b \in \mathbb{C}^{N}, \| b \| = 1 \).

Compute \( f(A)b \).

Applications

\[
\begin{align*}
  f(z) &= 1/z & \text{linear systems of equations} \\
  f(z) &= e^{tz}, t \in \mathbb{R} & \text{initial value problems} \\
  f(z) &= \log(z) & \text{continuous-time Markov chains} \\
  f(z) &= \text{sgn}(z) & \text{lattice QCD, eigenvalues, control} \\
  f(z) &= 1/\sqrt{z} & \text{lattice QCD} \\
  f(z) &= \sqrt{z} & \text{stochastic ODEs, domain decomposition}
\end{align*}
\]
Compute $f(A)b$ without computing $f(A)$

I. If $A$ is small: **techniques specific** to every $f$ (and $A$)
   - $f(z) = 1/z$: Gaussian elimination.
   - $f(z) = e^z$: Padé approximation (+ ‘scaling and squaring’).

[Higham, 2008]

II. If $A$ is large and sparse (or structured): **projection methods** (model reduction)
   - Project $A$ (and $b$) onto a space $\mathcal{K}$ of low dimension.
   - Evaluate $f(A_{\mathcal{K}})b_{\mathcal{K}}$ using methods of type I and ‘lift’ the result to the original dimension.

Here: methods of type II, where $\mathcal{K}$ is a Krylov-space!
Compute $f(A)b$ without computing $f(A)$

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     [Higham, 2008]

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Here: methods of type II, where $\mathcal{K}$ is a Krylov-space!
Matrix Functions
Definition via Jordan canonical form

\[ f(A) = X f(J) X^{-1} \]  \hspace{1cm} \text{[Giorgi (1928)]}  

\[ J = \text{diag}(J(\lambda_1), \ldots, J(\lambda_K)) = X^{-1} A X \]  
\( \lambda_1, \ldots, \lambda_K \in \Lambda(A) \)  

Jordan canonical form of \( A \), (geometric multiplicity),

\[ f(J) := \text{diag}\left( f(J(\lambda_1)), \ldots, f(J(\lambda_K)) \right), \]

\[ f(J(\lambda)) := \begin{bmatrix}  f(\lambda) & f'(\lambda) & \cdots & \frac{f(n-2)(\lambda)}{(n-2)!} & \frac{f(n-1)(\lambda)}{(n-1)!} \\ f(\lambda) & \cdots & \frac{f(n-3)(\lambda)}{(n-3)!} & \frac{f(n-2)(\lambda)}{(n-2)!} \\ \vdots & \vdots & \vdots & \vdots \\ f(\lambda) & f'(\lambda) \\ f(\lambda) \end{bmatrix} \]
Matrix Functions

Definition via Cauchy integral

$$f(A) = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda)(\lambda I - A)^{-1} d\lambda$$  \[\text{Frobenius (1896)}\]

with a contour $\Gamma \subset \mathbb{C}$ such that $\Lambda(A) \subset \text{int} \, \Gamma$. 
Every function applied to a (fixed) matrix is a polynomial. More precisely,

\[ f(A) = q(A) \]

where \( q \in \mathcal{P}_{K-1} \) satisfies Hermite interpolation conditions

\[ q^{(\ell)}(\lambda_j) = f^{(\ell)}(\lambda_j), \quad \ell = 0, \ldots, n_j - 1; \quad j = 1, \ldots, k \quad (2) \]

and the minimal polynomial of \( A \) is given by

\[ m_A(z) = \prod_{j=1}^{k} (z - \lambda_j)^{n_j} \in \mathcal{P}_K, \quad n_1 + \cdots + n_k = K. \quad (3) \]

Shorthand for (2), (3):

\[ q = l_{m_A} f. \]
Analogously, for any vector $b \in \mathbb{C}^N$, 

$$f(A)b = q(A)b$$

where 

$$q = I_{m_{A,b}}f \in \mathcal{P}_{L-1}$$

and 

$$m_{A,b}(z) = \prod_{j=1}^{\kappa} (z - \lambda_j)^{\nu_j} \in \mathcal{P}_L, \quad \nu_1 + \cdots + \nu_\kappa = L,$$

denotes the minimal polynomial of $b$ with respect to $A$. 
The vector $f(A)b$ we seek lies in some Krylov space

$$K_m(A, b) := \text{span}\{b, Ab, \ldots, A^{m-1}b\} = \{p(A)b : p \in \mathbb{P}_{m-1}\}, \quad m \leq L,$$

$L$ being the smallest index such that $A^L K_L = K_{L+1}$.

The polynomial $q$ such that $f(A)b = q(A)b$ is determined by (Hermite) interpolation conditions at the eigenvalues of $A$ (those relevant for $b$).

This motivates constructing approximations

$$f(A)b \approx q_{m-1}(A)b \in K_m(A, b)$$

with $q_{m-1}$ determined by interpolation conditions.
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Krylov Subspace Approximation
Arnoldi-like decomposition

Numerically stable generation of Krylov spaces (Arnoldi-, Lanczos process, Chebyshev recurrence etc.) yield Arnoldi-like decompositions

\[ AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^\top \]

\[ \text{range}(V_m) = \mathcal{K}_m(A, b), \quad V_m^H V_m = I \]

\[ b = V_m e_1, \]

\[ H_m \text{ unreduced upper Hessenberg}, \]

\[ e_m = [0, \ldots, 0, 1]^\top \in \mathbb{C}^m. \]

- Simplification: \( H_m \) Hermitian tridiagonal for \( A \) Hermitian (Hermitian Lanczos process).
- Algorithm: multiply most recent basis vector \( v_m \) with \( A \), orthogonalize against \( v_1, \ldots, v_m \).
Krylov Subspace Approximation

A Key Relation

For Arnoldi(-like) decomposition of $\mathcal{K}_m(A, b)$

\[ AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T, \]

denote $\gamma_m := \prod_{j=1}^m h_{j+1,j}$. 

For any polynomial $p \in \mathcal{P}_{m-1}$ there holds

\[ p(A)b = V_m p(H_m)e_1 \]

and, for $p \in \mathcal{P}_m$ with leading coefficient $\alpha_m$,

\[ p(A)b = V_m p(H_m)e_1 + \alpha_m \gamma_m v_{m+1}. \]

Krylov Subspace Approximation of $f(A)b$

Given Arnoldi-like decomposition of $\mathcal{K}_m$ set

$$f(A)b \approx f_m := V_m f(H_m)e_1$$

[Druskin & Knizhnerman (1989)],
[Gallopoulos & Saad (1992)],
[Hochbruck & Lubich (1995)]

**Interpretation:** Let $w_m := m_{H_m} \in \mathcal{P}_m$ denote the minimal polynomial of $H_m$ (≡ characteristic polynomial since $H_m$ nonderogatory). Then

$$f(H_m) = [l_{w_m}f](H_m)$$  
by interpolation property

$$V_m[l_{w_m}f](H_m)e_1 = [l_{w_m}f](A)b$$  
by key relation since $[l_{w_m}f] \in \mathcal{P}_{m-1}$

**Advantage:** avoids $A$, avoids explicit interpolation, requires only evaluation of (first column of) $f(H_m)$ for (small) matrix $H_m$.

**Drawback:** requires basis $V_m$ (extensive storage), even in Hermitian case.
Three Interpretations

- **Subspace approximation.** $H_m = V_m^H A V_m$ represents $A$ on $\mathcal{K}_m(A, b)$ w.r.t. $V_m$. Approximate $f(A)$ with $f(H_m)$ there.

- **Cauchy integral.** For a contour $\Gamma$ with $W(A) \subset \text{int} \Gamma$,

$$f(A)b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda)(\lambda I - A)^{-1} b \, d\lambda$$

$$\approx \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) V_m(\lambda I - H_m)^{-1} V_m^H b \, d\lambda = V_m f(H_m) e_1.$$  

$x_m(\lambda)$: Galerkin approx. of $x(\lambda) := (\lambda I - A)^{-1} b$ w.r.t. $\mathcal{K}_m(A, b)$.

- **Interpolation.** If $p \in P_{m-1}$ Hermite-interpolates $f$ at nodes $\Lambda(H_m)$, then

$$f(A)b \approx p(A)b = V_m p(H_m) e_1 = V_m f(H_m) e_1.$$
Three Interpretations

- **Subspace approximation.** \( H_m = V_m^H A V_m \) represents \( A \) on \( \mathcal{H}_m(A, b) \) w.r.t. \( V_m \). Approximate \( f(A) \) with \( f(H_m) \) there.

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Three Interpretations

- **Subspace approximation.** \( H_m = V_m^H A V_m \) represents \( A \) on \( \mathcal{K}_m(A, b) \) w.r.t. \( V_m \). Approximate \( f(A) \) with \( f(H_m) \) there.

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- **Interpolation.** If \( p \in \mathcal{P}_{m-1} \) Hermite-interpolates \( f \) at nodes \( \Lambda(H_m) \), then

\[
f(A)b \approx p(A)b = V_mp(H_m)e_1 = V_m f(H_m)e_1.
\]
The Arnoldi Approximation \((V_m^H V_m = I)\)

**Special case:**
- \(f(z) = 1/z\), then \(f_m = m\)-th FOM-iterate for \(Ax = b\) \((f_0 = 0)\).
- If, in addition, \(A\) is Hpd, then \(f_m\) is the \(m\)-th CG-iterate.

**Alternatives:**
- Interpolation at harmonic Ritz values [Van den Eshof & al. (2002)], equivalent to CR/MINRES/GMRES for \(f(z) = 1/z\).
- Two-sided (or nonsymmetric) Lanczos process, equivalent to BiCG \(f(z) = 1/z\).
- Block orthonormal basis (see restarts), equivalent to FOM\((m)\) \(f(z) = 1/z\).
The Arnoldi Approximation ($V_m^H V_m = I$)

Special case:
- $f(z) = 1/z$, then $f_m = m$-th FOM-iterate for $Ax = b$ ($f_0 = 0$).
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Alternatives:
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Restarting
Motivation

For large matrices basic approximation scheme too expensive

- **A non-Hermitian:** at step $m$ need to store $m$ vectors of size $N$, orthogonalization costs $O(m^2 N)$ flops.

- **A Hermitian:** Can exploit short recurrence for basis generation, but still need complete basis to form approximation $V_m f(H_m) e_1$.
  Alternative: generate basis twice (two-pass variant).

Restarting well-known from Krylov subspace methods for linear systems/eigenvalues.

**Basic scheme:**

- Generate Krylov subspace of affordable dimension $m$.
- Compute approximation w.r.t. this space.
- Generate new Krylov space to compute correction to this approximation.
- repeat until sufficiently accurate.
Solution of $Ax = b$ given by $f(A)b$ with $f(z) = 1/z$.

Popular solution procedure: (restarted GMRES, restarted FOM)

- Given initial approximation $x_0 = 0$ generate Krylov space $\mathcal{K}_m(A, b)$ of dimension $m$ and approximate solution (FOM) $x_m = V_mH_m^{-1}e_1$ to $A^{-1}b$.
- Correction $c$ to $x_m$ obtained by solving residual equation:

$$A^{-1}b = x_m + c, \quad Ac = b - Ax_m =: r_m.$$ 

- (approximate) solution of residual equation in new Krylov space $\mathcal{K}_m(A, r_m)$, hence storage requirements fixed.

Generalization to other functions $f$ not obvious: no residual available.
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For function $f$, nodes $\vartheta_1, \ldots, \vartheta_m \in \mathbb{C}$, denote by

$$w_m(z) := \prod_{j=1}^{m}(z - \vartheta_j)$$

nodal polynomial,

$$l_{w_m}f \in \mathcal{P}_{m-1}$$

Hermite interpolant to $f$ at $\{\vartheta_j\}_{j=1}^{m}$,

$$\Delta_{w_m}f := \frac{f - l_{w_m}f}{w_m}$$

$m$-th order divided difference of $f$ w.r.t. $w_m$.

Then

$$f = l_{w_m}f + \Delta_{w_m}f \cdot w_m,$$

$$f(A)b = [l_{w_m}f](A)b + [\Delta_{w_m}f](A) w_m(A)b$$

$$= V_m[l_{w_m}f](H_m)e_1 + [\Delta_{w_m}f](A)(V_m w_m(H_m)e_1 + \gamma_m v_{m+1})$$

$$= f_m + \gamma_m[\Delta_{w_m}f](A)v_{m+1}.$$
Theorem [Eiermann & E., 2006]

Given a function $f$, matrix $A \in \mathbb{C}^{n \times n}$, vector $b \in \mathbb{C}^n$, and the Arnoldi decomposition $AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^\top$, then the error of the Krylov subspace approximation $f_m$ of $f(A)b$ is given by

$$f(A)b - f_m = g(A)v_{m+1},$$

(4)

where $g(z) = \gamma_m[\Delta w_m f](z)$ and $w_m \in P_m$ denotes the (monic) nodal polynomial associated with $\Lambda(H_m)$.

Naive approach: update $f_m$ by explicit evaluation of divided differences (block Newton interpolation).

This is (severely) unstable.
$k$ standard Arnoldi decompositions of $A$

$$AV_j = V_jH_j + h_{j+1}v_{jm+1}e_m^T, \quad j = 1, 2, \ldots, k,$$

of the $m$-dim. Krylov spaces $\mathcal{K}_m(A, v_{(j-1)m+1})$, glued together,

$$A\hat{V}_k = \hat{V}_k\hat{H}_k + h_{k+1}v_{km+1}e_{km}^T,$$

where $\hat{V}_k := [V_1 \ V_2 \ \cdots \ V_k] \in \mathbb{C}^{n \times km},$

$$\hat{H}_k := \begin{bmatrix} H_1 \\ E_2 & H_2 \\ \vdots & \vdots & \ddots \ E_k & H_k \end{bmatrix} \in \mathbb{C}^{km \times km}, \quad E_j := h_j e_1 e_m^T \in \mathbb{R}^{m \times m}.$$

(5) is an Arnoldi-like decomposition of $\mathcal{K}_m(A, b)$. Compute

$$\hat{f}_k := \hat{V}_k f(\hat{H}_k)e_1 = \hat{f}_{k-1} + V_k[f(\hat{H}_k)e_1](k-1)m+1:km.$$
An Example


Heat equation on \((0, 1)^3\), i.e., \(f = f_0 e^{tA_h}\), \(A_h \approx \Delta\), \(\dim(A_h) = 125\,000\)

\[
\begin{array}{c|c|c}
m & k & \text{time [s]} \\
\hline
\infty & 1 & 1948 \\
20 & 20 & 206 \\
10 & 45 & 146 \\
6 & 87 & 153 \\
\end{array}
\]

(Power Mac G5 1.6 GHz, 1.5 GB RAM, MATLAB 7)
Instead of $f(A)b$, evaluate $r(A)b$ where $f(z) \approx r(z) = \sum_{\ell=1}^{n_p} \frac{\alpha_{\ell}}{\omega_{\ell} - z}$ is a suitably accurate rational approximation of $f$. Now

$$r(\hat{H}_k)e_1 = \sum_{\ell=1}^{n_p} \alpha_{\ell}(\omega_{\ell} I - \hat{H}_k)^{-1}e_1 =: \sum_{\ell=1}^{n_p} \alpha_{\ell}\hat{r}_\ell.$$ 

Due to block bidiagonal structure of $\hat{H}_k$, each of the $n_p$ systems $(\omega_{\ell} I - \hat{H}_k)\hat{r}_\ell = e_1$ can be solved recursively:

$$(\omega_{\ell} I - H_1)r_{\ell,1} = e_1, \quad (\omega_{\ell} I - H_j)r_{\ell,j} = E_j r_{\ell,j-1}, \quad j = 2, \ldots, k,$$

where $\hat{r}_\ell = [r_{\ell,1}^T, r_{\ell,2}^T, \ldots, r_{\ell,k}^T]^T$. Last block of $r(\hat{H}_k)e_1$ now obtained as

$$[O, \ldots, O, I] r(\hat{H}_k)e_1 = \sum_{\ell=1}^{n_p} \alpha_{\ell}r_{\ell,k}.$$
Example: $f(z) = e^z$, best uniform rational approximation of $f$ on $D = (-\infty, 0]$ of type $(16, 16)$ [Cody, Meinardus & Varga (1969)].
Example: \( f(z) = \text{sgn} \, z \),
best uniform rational approximation of \( f \) on \( D = [-10, -1] \cup [1, 10] \) of type \((19, 20)\) [Zolotarev (1877)],

\[
\text{Poles and weights explicitly known in terms of Jacobi elliptic functions.}
\]
An Example
[Afanasjew, Eiermann, E. & Güttel (2006)]

Quasi-static Maxwell’s equation on a cube

\[ f = f_0 e^{tA_h} \]
\[ A_h \approx \sigma^{-1} \nabla \times (\mu^{-1} \nabla \times \cdot) \]
\[ \dim(A_h) = 565326 \]
\[ \Lambda(A_h) \subset [-10^8, 0] \]
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Compensate for deterioration of convergence due to restarting by augmenting the Krylov subspace with nearly invariant subspaces.

Identify a subspace which slows convergence, approximate this space and eliminate its influence from the iteration process.

In practice: Approximate eigenspaces associated with eigenvalues close to singularities of $f$ (for $f = \exp$, approximate eigenspaces which belong to "large" eigenvalues).

Deflated restarting: Technique

1st restart cycle:

\[ AV_1 = V_1 H_1 + h_2 \mathbf{v}_{m+1} e_m^\top. \]

2nd restart cycle: Extract \( \ell \) wanted eigenvalues of \( H_1 \)

\[ H_1 [X_2 \ast] = [X_2 \ast] \begin{bmatrix} T_2 & \ast \\ O & \ast \end{bmatrix} \]

\((T_2 \in \mathbb{C}^{\ell \times \ell} \text{ is upper triangular and } X_2 \in \mathbb{C}^{m \times \ell} \text{ has orthonormal columns}). Set \( Y_2 := V_1 X_2 \).

\[ AY_2 = Y_2 T_2 + h_2 \mathbf{v}_{m+1} u_2^\top, \text{ where } u_2 = X_2^\top e_1 \text{ (dense!)}. \]

Extend this decomposition by \( m \) Arnoldi steps

\[ A [Y_2 \ V_2] = [Y_2 \ V_2] \begin{bmatrix} T_2 & G_2 \\ h_2 e_1 u_2^\top & H_2 \end{bmatrix} + h_3 \mathbf{v}_{2m+1} e_{2m+\ell}^\top, \]

where \([Y_2 \ V_2] \text{ has orthonormal columns, } V_2 e_1 = \mathbf{v}_{m+1}, \ H_2 \in \mathbb{C}^{m \times m} \text{ is upper Hessenberg}. \]
deflated restarting: technique

3rd restart cycle: extract $\ell$ wanted eigenvalues:

\[
\begin{bmatrix}
T_2 & G_2 \\
h_2 e_1 u_1^T & H_2
\end{bmatrix}
\begin{bmatrix}
x_2 \\
h_2 e_1 u_1^T
\end{bmatrix} =
\begin{bmatrix}
x_2 \\
h_2 e_1 u_1^T
\end{bmatrix}
\begin{bmatrix}
T_3 & 0 \\
0 & * 
\end{bmatrix}
\ldots
\]

after $k$ restart cycles:

\[
A \tilde{V}_k = \tilde{V}_k \tilde{H}_k + h_{k+1} v_{km+1} e_k^T,
\]

\[
\tilde{V}_k = \begin{bmatrix} V_1 | Y_2 | V_2 | \ldots | Y_k | V_k \end{bmatrix} \in \mathbb{C}^{n \times \tilde{k}}, \quad \tilde{k} = km + (k - 1)\ell,
\]

\[
\tilde{H}_k = \begin{bmatrix}
H_1 & & & & \\
& T_2 & G_2 & & \\
& E_2 & F_2 & H_2 & \\
& & & \ddots & \ddots \\
& & & & E_k & T_k & G_k \\
& & & & & E_k & F_k & H_k
\end{bmatrix} \in \mathbb{C}^{\tilde{k} \times \tilde{k}}.
\]
Structure of $\tilde{H}_k$

$k = 5, \ell = 2, m = 6$

non-Hermitian $A$

Hermitian $A$
Deflated restarting
Different interpretations

Theorem [Eiermann, E., Güttel, 2008]
Given the thick-restart decomposition after \( k \) restart cycles
\[
A\tilde{V}_k = \tilde{V}_k \tilde{H}_k + h_{k+1} v_{km+1} e_k^T
\]
\( (\ell \text{ Ritz vectors per restart, } m \text{ mvm per cycle}) \), there holds
\[
\tilde{f}_k = \tilde{V}_k f(\tilde{H}_k)e_1 = p_{km-1}(A)b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda)\tilde{z}_{k,(m,\ell)}(\lambda) \, d\lambda,
\]
where \( p_{km-1} \in \mathcal{P}_{km-1} \) interpolates \( f \) in
\[
\Lambda(\tilde{H}_k) \setminus \left( \bigcup_{j=2}^{k-1} \Lambda(T_j) \right),
\]
and where \( \tilde{z}_{k,(m,\ell)} \) is the approximate solution of \((\lambda I - A)x = b\) generated by \( k \) cycles of \( \text{FOM}(m, \ell) \) [Morgan (2002)].
**Numerical Example**

Maxwell’s equation revisited

Maxwell’s equation, \( n = 565326, m = 70 \) and \( m = \infty \)

Matrix-vector products

error

\( \ell = 0 \)

\( \ell = 2 \)

\( \ell = 10 \)

\( \ell = 20 \)

full Arnoldi

\[
f = \exp(tA_h)b
\]

\[
A_h \approx \nabla \times (\mu^{-1} \nabla \times \cdot)
\]

\( \dim A_h = 565326 \)

\( \Lambda(A_h) \subset [-10^8, 0] \)

\( m = 70 \)

target = 0
Outline

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   - Matrix Functions
   - Krylov Subspace Approximation

3. Restarting
   - Motivation
   - Basic Procedure
   - Deflated Restarting

4. Application to the Matrix Sign Function
   - Other Approaches
   - Numerical Experiments

5. Summary and Future Work
Other Approaches

Hermitian Case

Much work in last 10 years on $\text{sgn } A, A = A^H$, for QCD.

- polynomial approximation
- rational approximation (partial fraction expansion), multishift CG
- Hermitian Lanczos process
- relaxed accuracy within inner/outer iteration

For references see
[Cundy, van den Eshof, Frommer, Krieg, Lippert & Schäfer (2005)]
as well as previous QCD-NA Workshop proceedings.
Given a partial Schur decomposition of $A$

$$AU_k = U_k T_k, \quad T_k \in \mathbb{C}^{k \times k} \text{ upper triangular}, \quad U_k^H U_k = I_k,$$

$m$ steps of (modified) Arnoldi process yield orthonormal basis of range $U_k \oplus \mathcal{K}_m(A, b)$ and the Arnoldi-like decomposition

$$A[U_k \ V_m] = [U_k \ V_m] \begin{bmatrix} T_k & U_k^H AV_m \\ O & H_m \end{bmatrix} + h_{m+1,m} v_{m+1} e_k^T.$$

Associated Krylov subspace approximation

$$f(A)b \approx [U_k \ V_m] \begin{bmatrix} f(T_k) & F \\ O & f(H_m) \end{bmatrix} [U_k \ V_m]^H b$$

$$= U_k f(T_k) U_k^H b + U_k F V_m^H b + V_m f(H_m) V_m^H b.$$
The coupling matrix $F$ is the solution of the Sylvester equation

$$T_k F - FH_m = f(T_k) U_k^H A V_m - U_k^H A V_m f(H_m)$$

(inexpensive, elimination-type solution scheme)

- Requires reasonably accurate eigenvalue approximations as an initial preprocessing phase.
- Similar approach using spectral projection in place of orthogonal projection on eigenspace. No coupling block, but need left eigenvectors in addition to (right) eigenvectors.
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Numerical Experiments
Wilson Dirac operator at nonzero chemical potential

Matrix taken from [Bloch et al. (2007)] (4 × 4 lattice, $N = 3072$).

sparsity structure

spectrum
Numerical Experiments
Wilson Dirac operator at nonzero chemical potential

Explicit deflation

Deflated restarting DR$(m, \ell)$

<table>
<thead>
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<th>Method</th>
<th>init.</th>
<th>total</th>
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</thead>
<tbody>
<tr>
<td>full</td>
<td>460 s</td>
<td>460 s</td>
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<tr>
<td>Schur 30</td>
<td>5 s</td>
<td>33 s</td>
</tr>
<tr>
<td>Schur 60</td>
<td>8 s</td>
<td>36 s</td>
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<td>spectral 30</td>
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<td>spectral 60</td>
<td>16 s</td>
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<table>
<thead>
<tr>
<th>Method</th>
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</thead>
<tbody>
<tr>
<td>full</td>
<td>460 s</td>
</tr>
<tr>
<td>TR(100,30)</td>
<td>1100 s</td>
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<tr>
<td>TR(100,60)</td>
<td>2496 s</td>
</tr>
<tr>
<td>TR(120,30)</td>
<td>2059 s</td>
</tr>
</tbody>
</table>
Execution times of deflated restarting (DR) not yet competitive.
DR does, however, have fixed memory costs.
DR spends 98% of execution time in full matrix function routine. Rational function approximation to sgn will eliminate this by allowing an update formula. (under investigation, CF-approximation in the complex plane)

Acceleration of convergence due to deflation does not set in immediately, likely to be improved by using harmonic Ritz values in the deflation.
Krylov subspace approximations are an effective tool for approximating $f(A)b$.

- Initial (preliminary) experiments with DR promising, many improvements still possible and under investigation.
- Matrix sign evaluation in QCD challenging, appears more difficult than matrix exponential.
- Not mentioned: a posteriori error estimators are available.
- Also not mentioned: asymptotic convergence theory available.
- Availability of AMG methods in combination with rational approximation would completely change the picture.
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