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Bergische Universität GH Wuppertal

Fachbereich Mathematik

Andreas Frommer and Uwe Glässner

# Solving Shifted Linear Systems with GMRES and Applications to Lattice Gauge Theory

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Frommer, A., Glässner, U.

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## 1. Introduction

The Krylov subspaces $K_m(M,r) = \text{span}\{r, Mr, \ldots, M^{m-1}r\}$ and $K_m(M+\alpha I, r)$ of a matrix $M \in \mathbf{C}^{n\times n}$ and a vector $r \in \mathbf{C}^n$ are identical for all $\alpha \in \mathbf{C}$. This fact can be used in Krylov subspace iterative methods (where the $m$-th residual $r^m = b - Mx^m$ of the $m$-th iterate $x^m$ lies in $K_m(M, r^0)$) to simultaneously solve the two systems

$$Mx = b\ , \quad (M+\alpha I)\widehat{x} = b$$

with very low additional cost for the second system for which no further matrix multiplications are needed. See [1] for the QMR and TFQMR method and [3] for BiCG. In case that $M$ is hermitian positive definite, similar considerations for the CG method can be found in [5,6]. Here we show how the restarted GMRES method can be modified to again allow for a cheap computation of iterates for the shifted system $(M+\alpha I)\widehat{x} = b$.

## 2. Restarted GMRES

GMRES is based on the Arnoldi process for computing an orthonormal basis $v^1, v^2, \ldots v^m$ of $K_m(M,r)$. More precisely, denoting $V_m = [v^1|v^2|\ldots|v^m] \in \mathbf{C}^{n\times m}$, the Arnoldi process yields an "upper Hessenberg" matrix $H_m^* \in \mathbf{C}^{(m+1)\times m}$ such that

$$MV_m = V_{m+1}H_m^*\ .$$

The restarted GMRES algorithm is given in Fig. 1 for a fixed restart value $m$. There, $e_1$ denotes the vector $e_1 = (1, 0, \ldots, 0)^T \in \mathbf{C}^{m+1}$. The iterate $x^{j+1}$ satisfies the optimality property

$$||b - Mx^{j+1}|| = \min_{x \in x^j + K_m(M,r^j)} ||b - Mx||\ .$$

To fix notations, quantities related to the shifted system $(\alpha I + M)\widehat{x} = b$ will be afflicted with a hat. If we run the restarted GMRES method for the shifted system, $\widehat{r}^m$ will be different from $r^m$ and not colinear to $r^m$, even if $\widehat{r}^0 = r^0$. Hence, after the first restart (i.e. for $j=1$ in Fig. 1), the respective Krylov subspaces become different and no savings for the shifted system are possible any more. We therefore propose to modify the iteration for the shifted system such that $\widehat{r}^m = \gamma_m r^m$ for all $m$. The right part of Fig. 1 shows how this can be obtained by merely solving small linear systems involving the matrix

$$\widehat{H}_m^* = H_m^* + \alpha \cdot \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \\ 0 & \ldots & 0 \end{bmatrix} \in \mathbf{C}^{(m+1)\times m}.$$

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choose $x^0$, set $r^0 = b - Mx^0, \beta_0 = ||r^0||$
for $j = 0, 1, \ldots$ until convergence do
    compute $V_{m+1}$ and $H_m^*$ for $K_m(M, r^j)$
        via the Arnoldi process
    compute $y^j \in \mathbf{C}^m$, the minimizer
        of $||\beta_j e_1 - H_m^* y||_2$
    set $x^{j+1} = x^j + V_m y^j$
        $r^{j+1} = V_{m+1} z^j$ where $z^j = \beta_j e_1 - H_m^* y^j$
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take $x^0 = \widehat{x}^0 = 0$, set $r^0 = \widehat{r}^0 = b, \beta_0 = ||r^0||, \gamma_0 = 1$
for $j = 0, 1, \ldots$ until convergence do
    compute $V_{m+1}$, $H_m^*$ for $K_m(M, r^j)$ and
        $y^j, x^{j+1}, r^{j+1}$ and $z^j$ from GMRES($m$)
    solve $\left[\widehat{H}_m^* | z^j\right] \begin{bmatrix} \widehat{y}^j \\ \gamma_{j+1} \end{bmatrix} = \gamma_j \beta_0 e_1$
    set $\widehat{x}^{j+1} = \widehat{x}^j + V_m \widehat{y}^j$, $\widehat{r}^{j+1} = \gamma_{j+1} r^{j+1}$
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Figure 1: GMRES($m$) (left) and shifted GMRES($m$) (right)

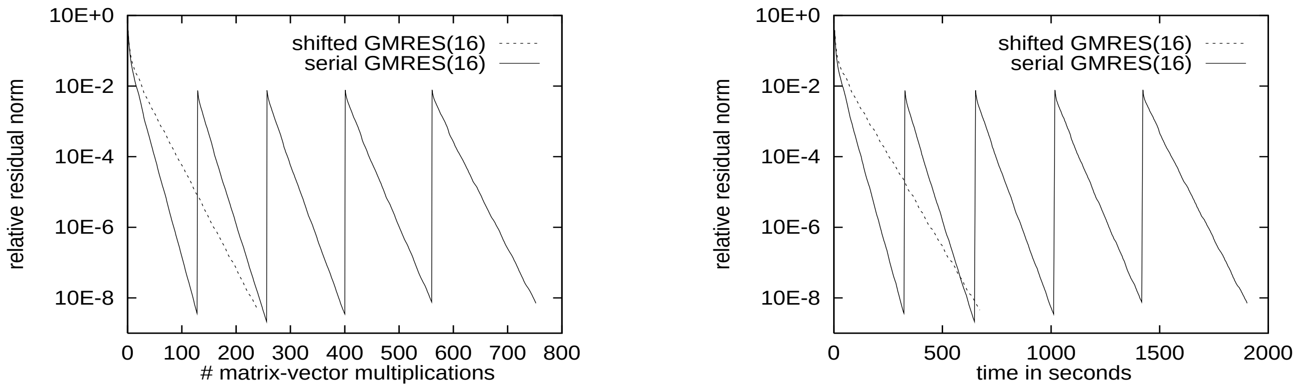


Figure 2: iteration numbers and run times for shifted GMRES(16) vs. serial GMRES(16)

The following result on the convergence of the shifted GMRES($m$) method was proven in [2] (see also [4] for $m = 1$).

Theorem: Assume that $M$ is positive real, i.e. $Re(x^H Mx) > 0$ for all $x \neq 0$ and let $\alpha > 0$. Then

(i) $\lim_{j\to\infty} x^j = M^{-1}b$

(ii) $\lim_{j\to\infty} \widehat{x}^j = (M + \alpha I)^{-1}b$, and, in addition, $|\gamma_j| < 1$ for all $j$.

Note that the last relation may be interpreted as the shifted system converging more rapidly than the original one.

## 3. Application in Lattice Gauge Theory

The odd-even preconditioned *Wilson fermion matrix* has the form

$$M_{ee}(\kappa) = \frac{1}{\kappa^2} I - D_{oe}\ D_{eo}\ .$$

It represents a nearest neighbor coupling on a four-dimensional space-time lattice, each point of which carries 12 complex variables. Typically, in lattice gauge theory one seeks solutions of several systems $M_{ee}(\kappa) = \varphi$ with a 'point source' $\varphi$ for several values of $\kappa$ ranging in $[0, \kappa_c)$, and $M_{ee}(\kappa)$ is positive real for all $\kappa \in [0, \kappa_c)$. We are therefore precisely in the situation of Theorem 1 if we take the original system to be the one with the largest value of $\kappa$. Figure 2 shows the results of the shifted GMRES(16) algorithm on a $8^4$ lattice for five values of $\kappa$ in comparison to a 'serial' solution process where GMRES(16) is used for each $\kappa$ value separately, taking the final approximation of the previous $\kappa$ as an initial guess for the next. We see that the shifted GMRES(16) is 3 times faster than the 'serial' method. The measurements were done on a Sun Sparcstation 20.

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*Address:* Frommer, Andreas, Bergische Universität Wuppertal, Fachbereich Mathematik, D-42097 Wuppertal
Glässner, Uwe, Bergische Universität Wuppertal, Fachbereich Physik, D-42097 Wuppertal