Variants of the Block-QMR Method and Applications in Quantum Chromodynamics [1]

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Keywords: quantum chromodynamics, block-QMR iterations, linear system, shifted systems

ABSTRACT

Numerical computations in lattice quantum chromodynamics (QCD) require the solution of large sparse systems of linear equations. These systems are so large that they can only be tackled by iterative solution techniques. In certain QCD simulations, a sequence of closely related linear systems has to be solved. In a quenched simulation, all systems have the same coefficient matrix, but differ in their right-hand sides. In the multiboson framework, systems with coefficient matrices that differ only by an additive shift have to be solved. In this paper, we describe variants of the block-QMR method that are tailored to these two classes of multiple linear systems. Numerical results with linear systems from QCD simulations are reported.

INTRODUCTION

Quantum chromodynamics (QCD) is generally believed to be the fundamental physical theory of the strong interaction between matter. To evaluate the theory without recourse to perturbation theory, *lattice QCD* works with discretizations on a four-dimensional space-time lattice [2]. Lattice QCD requires enormous computing power and efficient numerical algorithms in order to solve huge sparse systems of linear equations arising from a discretized Dirac operator, the fermionic matrix. The coefficients of the matrix are related to the fluctuating gluonic background field. In this paper, we only consider the Wilson fermion framework

[1]Numerical Analysis Manuscript No. 97–3–01, Bell Laboratories, Murray Hill, New Jersey, May 1997. Available on WWW at {`http://cm.bell-labs.com/cs/doc/97`}.

[2]The work of these authors was partially sponsored by Deutsche Forschungsgemeinschaft under grant Fr 755/10-1

[11], where the underlying system

$$\mathbf{M}_\kappa\,\boldsymbol{\psi} = \left(\frac{1}{\kappa}\mathbf{I} - \mathbf{D}\right)\,\boldsymbol{\psi} = \boldsymbol{\varphi} \tag{1}$$

represents a nearest-neighbor coupling of the form

$$\frac{1}{\kappa}\boldsymbol{\psi}_x - \left(\sum_{j=1}^{4}\mathbf{m}_{x,x-\mathrm{e}_j}\boldsymbol{\psi}_{x-\mathrm{e}_j} + \sum_{j=1}^{4}\mathbf{m}_{x,x+\mathrm{e}_j}\boldsymbol{\psi}_{x+\mathrm{e}_j}\right) = \boldsymbol{\varphi}_x.$$

Here, x represents the 4-dimensional grid coordinates and the $\mathbf{e}_j$ are unit vectors. Each "component" $\boldsymbol{\psi}_x$ is from $\mathbb{C}^{12}$, and the coupling terms $\mathbf{m}_{x,y}$ are complex 12×12 matrices. The quantity κ is a scalar parameter.

In this paper, we discuss efficient iterative algorithms for the solution of the following two different families of closely related systems of the form (1).

(i) In a *quenched* simulation, one needs to solve (1) repeatedly, where $\mathbf{M}_\kappa$ is a fixed matrix, but with 12 different right-hand sides $\boldsymbol{\varphi}$, corresponding to the 12 unit vectors at a given lattice point.

(ii) In the *multiboson* framework [9], one would like to perform a heat bath on auxiliary fields for reasons of efficiency [3]. This amounts to solving several systems of the form (1) with the same matrix $\mathbf{D}$, but different complex parameters κ, and a different, Gaussian randomly distributed right-hand side $\boldsymbol{\varphi} = \boldsymbol{\varphi}_\kappa$ for each value of κ.

Multiple systems of the type (i) can be solved efficiently by means of the block-QMR method [6]. Exploiting the special structure of the family (ii) is more intricate. Note that the coefficient matrices of the systems in (ii) differ from the fixed matrix $\mathbf{D}$ only by an additive shift, namely $1/\kappa$, while the right-hand sides are different and in general unrelated.

In the next two sections, we briefly review the block-QMR method for the iterative solution of systems (i), and we discuss an adaptation of block-QMR to shifted systems (ii). We then present results from numerical experiments with physically realistic configurations on a relatively small 4^4 lattice, and finally, we make some concluding remarks.

THE BLOCK-QMR METHOD

Recall that the family (i) consists of multiple linear systems of the type

$$\mathbf{A}\,\mathbf{x}^{(j)} = \mathbf{b}^{(j)}, \quad j = 1, 2, \ldots, m_0. \tag{2}$$

Here, $\mathbf{A}$ is a fixed, nonsingular, in general complex non-Hermitian, $N \times N$ matrix, and $\mathbf{b}^{(j)} \in \mathbb{C}^N$. Assuming that all right-hand sides $\mathbf{b}^{(j)}$, $j = 1, 2, \ldots, m_0$, are available simultaneously—as it is the case in quenched QCD simulations—solving the m_0 systems (2) is equivalent to solving the block system of linear equations

$$\mathbf{A}\,\mathbf{X} = \mathbf{B}, \tag{3}$$

where $\mathbf{B} = \begin{bmatrix} \mathbf{b}^{(1)} & \mathbf{b}^{(2)} & \cdots & \mathbf{b}^{(m_0)} \end{bmatrix}$ and $\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)} & \mathbf{x}^{(2)} & \cdots & \mathbf{x}^{(m_0)} \end{bmatrix}$.

Instead of applying an iterative method, such as the quasi-minimal residual (QMR) algorithm [7], to each of the m_0 systems (2) individually, it is potentially more efficient to apply a suitable block version of the iterative method to the block system (3). For Krylov-subspace methods, such as QMR, the advantage of block iterations over individual runs can be formulated precisely; see, e.g., [6]. Essentially, the argument is that a block Krylov-subspace method selects its iterates from a sequence of subspaces that are higher dimensional than the subspaces from which the iterates of the individual runs are chosen, even though generating the "block" subspaces and all m_0 sequences of "individual" subspaces requires roughly the same computational work.

The block-QMR method [6] is an extension of the QMR algorithm [7] for systems with single right-hand sides to block systems (3). Let $\mathbf{X}_0 \in \mathbb{C}^{N\times m_0}$ be an arbitrary initial guess for the exact solution $\mathbf{A}^{-1}\mathbf{B}$ of (3), and set $\mathbf{R}_0 := \mathbf{B} - \mathbf{A}\,\mathbf{X}_0$. The block-QMR method constructs approximate solutions of (3) that are of the form

$$\mathbf{X}_\mu = \begin{bmatrix} \mathbf{x}_\mu^{(1)} & \mathbf{x}_\mu^{(2)} & \cdots & \mathbf{x}_\mu^{(m_0)} \end{bmatrix} \in \mathbb{C}^{N\times m_0}, \quad \mu = 1, 2, \dots, \tag{4}$$

where $\mathbf{x}_\mu^{(j)} \in \mathbf{x}_0^{(j)} + \mathcal{K}_\mu(\mathbf{A}, \mathbf{R}_0)$ for each $j = 1, 2, \dots, m_0$. Here, for each $\mu = 1, 2, \dots$,

$$\mathcal{K}_\mu(\mathbf{A}, \mathbf{R}_0) := \operatorname{colspan}_\mu \begin{bmatrix} \mathbf{R}_0 & \mathbf{A}\mathbf{R}_0 & \cdots & \mathbf{A}^{N-1}\mathbf{R}_0 \end{bmatrix} \tag{5}$$

is the *μ-th block Krylov subspace* (generated by $\mathbf{A}$ and $\mathbf{R}_0$). In (5), the following notation is used. For any matrix $\mathbf{M}$ and any integer $0 < \mu \leq \operatorname{rank}\mathbf{M}$, we denote by $\operatorname{colspan}_\mu \begin{bmatrix}\mathbf{M}\end{bmatrix}$ the μ-dimensional subspace spanned by the first μ linearly independent columns of $\mathbf{M}$ that one encounters when scanning the columns from left to right for linear independence.

The block-QMR method uses a recently developed Lanczos-type process [1] that produces two sequences of *biorthogonal* basis vectors for $\mathcal{K}_\mu(\mathbf{A}, \mathbf{R}_0)$ and the μ-th block Krylov subspace (generated by $\mathbf{A}^{\mathrm{T}}$ and $\mathbf{L}$) $\mathcal{K}_\mu(\mathbf{A}^{\mathrm{T}}, \mathbf{L})$; here, $\mathbf{L} \in \mathbb{C}^{N\times m_0}$ is an arbitrarily chosen matrix, different from the zero matrix. More precisely, after μ steps, the Lanczos-type process has produced *right* and *left Lanczos vectors*

$$\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_\mu \quad \text{and} \quad \mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_\mu, \tag{6}$$

respectively, such that

$$\begin{aligned} \operatorname{span}\{\, \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_\mu \,\} &= \mathcal{K}_\mu(\mathbf{A}, \mathbf{R}_0), \\ \operatorname{span}\{\, \mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_\mu \,\} &= \mathcal{K}_\mu(\mathbf{A}^T, \mathbf{L}), \\ \mathbf{w}_i^{\mathrm{T}}\mathbf{v}_k &= 0 \quad \text{for all} \quad i \neq k = 1, 2, \dots, \mu. \end{aligned}$$

An important feature of the Lanczos-type process is that the Lanczos vectors (6) are generated by means of recurrences of limited length, namely $(2m_0+1)$-term recurrences. For the right Lanczos vectors, these recurrences can be summarized in compact form as follows:

$$\mathbf{A}\,\mathbf{V}_\mu = \mathbf{V}_n\,\mathbf{T}_\mu + \widehat{\mathbf{V}}_\mu^{\mathrm{dl}}, \quad \mu \geq 1. \tag{7}$$

Here, $\mathbf{V}_\mu := \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_\mu \end{bmatrix}$, $\mathbf{T}_\mu$ is an $n \times \mu$ banded matrix with upper and lower bandwidth m_0 containing the recurrence coefficients, and $\widehat{\mathbf{V}}_\mu^{\mathrm{dl}}$ is a matrix with mostly zero or very small entries that accounts for "deflation" of linearly or almost linearly dependent columns in the block Krylov sequence $\mathbf{R}_0, \mathbf{A}\mathbf{R}_0, \ldots, \mathbf{A}^{N-1}\mathbf{R}_0$ in (5). The recurrences (7) are complemented by "initial" recurrences

$$\mathbf{V}_{m_1} \boldsymbol{\rho} + \widehat{\mathbf{V}}_0^{\mathrm{dl}} = \mathbf{R}_0 \tag{8}$$

that are used to biorthogonalize the columns of the "right" initial block $\mathbf{R}_0$ against the columns of the "left" initial block $\mathbf{L}$. In (8), $m_1 \leq \operatorname{rank} \mathbf{R}_0 \leq m_0$, and $\boldsymbol{\rho}$ is an upper triangular $m_1 \times m_0$ matrix. The left Lanczos vectors in (6) are generated by means of recurrences similar to (7) and (8).
In the block-QMR method, the right Lanczos vectors are used to parametrize any possible iterate (4) as follows:

$$\mathbf{X}_\mu = \mathbf{X}_0 + \mathbf{V}_\mu \mathbf{Z}, \quad \text{where} \quad \mathbf{Z} \in \mathbb{C}^{\mu \times m_0}. \tag{9}$$

By (7) and (8), the block residual associated with (9) is given by

$$\mathbf{R}_\mu = \mathbf{R}_0 - \mathbf{V}_n \mathbf{T}_\mu \mathbf{Z} - \widehat{\mathbf{V}}_\mu^{\mathrm{dl}} \mathbf{Z} = \mathbf{V}_n \left(\begin{bmatrix} \boldsymbol{\rho} \\ \mathbf{0} \end{bmatrix} - \mathbf{T}_\mu \mathbf{Z} \right) - \widehat{\mathbf{V}}_\mu^{\mathrm{dl}} \mathbf{Z}. \tag{10}$$

Following the QMR philosophy introduced in [7] and assuming that the columns $\mathbf{v}_j$ of the matrix $\mathbf{V}_n$ are all normalized to have Euclidean length 1, in the block-QMR method, the free parameter matrix $\mathbf{Z}$ in (9) is determined so that the Euclidean norm of the bracketed term in (10) is minimized. More precisely, in (9), one chooses $\mathbf{Z} = \mathbf{Z}_\mu$ as the solution of the matrix least-squares problem

$$\left\| \begin{bmatrix} \boldsymbol{\rho} \\ \mathbf{0} \end{bmatrix} - \mathbf{T}_\mu \mathbf{Z}_\mu \right\|_2 = \min_{\mathbf{Z} \in \mathbb{C}^{\mu \times m_0}} \left\| \begin{bmatrix} \boldsymbol{\rho} \\ \mathbf{0} \end{bmatrix} - \mathbf{T}_\mu \mathbf{Z} \right\|_2 . \tag{11}$$

This choice amounts to a *quasi-minimization* of the norm of the residual (10). In the block-QMR method, the matrix least-squares problem (11) is solved by means of standard techniques based on a QR decomposition of $\mathbf{T}_\mu$. In particular, this allows to obtain the solution $\mathbf{Z}_\mu$ by updating the solution $\mathbf{Z}_{\mu-1}$ from the previous step. Moreover, the associate update $\mathbf{X}_{\mu-1} \longrightarrow \mathbf{X}_\mu$ for the actual iterates (9) turns out to be a simple rank-one update. For a description of this update procedure and for further implementation details, we refer the reader to [6].

EXPLOITING THE SHIFTED STRUCTURE

Recall that QCD simulations in a multiboson framework require the solution of multiple linear systems of the type

$$(\mathbf{A} - \sigma_j \mathbf{I})\, \mathbf{x}^{(j)} = \mathbf{b}^{(j)}, \quad j = 1, 2, \ldots, m_0. \tag{12}$$

Here, $\mathbf{A}$ is again a fixed $N \times N$ matrix, and $\sigma_j \in \mathbb{C}$, $j = 1, 2, \ldots, m_0$, are shifts.
For the special case that all right-hand sides in (12) are identical, i.e.,

$$\mathbf{b}^{(j)} = \mathbf{b} \quad \text{for all} \quad j = 1, 2, \ldots, m_0, \tag{13}$$

and if one is willing to use the initial guess $\mathbf{x}_0^{(j)} = \mathbf{0}$ for all j, it is straightforward to exploit the shift structure when solving the m_0 systems by Krylov-subspace methods; see, e.g., [4] and the references given therein. In fact, in this special case, the Krylov subspaces for all m_0 systems are identical:

$$\mathcal{K}_\mu(\mathbf{A} - \sigma_j \mathbf{I}, \mathbf{b}) = \mathcal{K}_\mu(\mathbf{A}, \mathbf{b}) \quad \text{for all} \quad j = 1, 2, \ldots, m_0 \quad \text{and} \quad \mu \geq 1. \tag{14}$$

This means that the expensive part of the Krylov-subspace method, namely the computation of suitable basis vectors for the underlying Krylov subspaces has to be performed only once, independently of the number m_0 of linear systems to be solved.
The general case (12) (or even (13) if nonzero initial guesses $\mathbf{x}_0^{(j)} \neq \mathbf{0}$ are chosen) is less straightforward, as the Krylov subspaces of the individual solves now depend on j. One possibility to still exploit the shift structure of (12) is to employ the Lanczos-type process sketched in the previous section. Applying this algorithm to the matrix $\mathbf{A}$, the right initial block

$$\mathbf{R}_0 := \begin{bmatrix} \mathbf{r}^{(1)} & \mathbf{r}^{(2)} & \cdots & \mathbf{r}^{(m_0)} \end{bmatrix}, \quad \mathbf{r}^{(j)} := \mathbf{b}^{(j)} - (\mathbf{A} - \sigma_j \mathbf{I})\, \mathbf{x}_0^{(j)}, \tag{15}$$

and an arbitrary nonzero left initial block $\mathbf{L} \in \mathbb{C}^{N \times m_0}$, we generate basis vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_\mu$ for the μ-th block Krylov subspace $\mathcal{K}_\mu(\mathbf{A}, \mathbf{R}_0)$ defined in (5). Using these basis vectors, for each $j = 1, 2, \ldots, m_0$, we define a μ-th iterate $\mathbf{x}_\mu^{(j)}$ for the j-th system in (12) as follows:

$$\mathbf{x}_\mu^{(j)} = \mathbf{x}_0^{(j)} + \mathbf{V}_\mu\, \mathbf{z}_\mu^{(j)}, \tag{16}$$

where $\mathbf{z}_\mu^{(j)} \in \mathbb{C}^\mu$ is the solution of the (vector) least-squares problem

$$\left\| \begin{bmatrix} \boldsymbol{\rho}_j \\ \mathbf{0} \end{bmatrix} - \left(\mathbf{T}_\mu - \sigma_j \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \end{bmatrix} \right) \mathbf{z}_\mu^{(j)} \right\|_2 = \min_{\mathbf{z} \in \mathbb{C}^\mu} \left\| \begin{bmatrix} \boldsymbol{\rho}_j \\ \mathbf{0} \end{bmatrix} - \left(\mathbf{T}_\mu - \sigma_j \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \end{bmatrix} \right) \mathbf{z} \right\|_2. \tag{17}$$

In (16), as before, we set $\mathbf{V}_\mu := \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_\mu \end{bmatrix}$. Furthermore, in (17), $\mathbf{T}_\mu$ and $\boldsymbol{\rho}$ are the matrices of Lanczos recurrence coefficients given by (7) and (8), and the vector $\boldsymbol{\rho}_j$ is defined as the j-th column of $\boldsymbol{\rho}$. Note that the shift σ_j now explicitly enters the j-th least-squares problem (17). Using (7) and (8), it is easy to verify that the choice (17) of $\mathbf{z}_\mu^{(j)}$ guarantees that the associated iterate $\mathbf{x}_\mu^{(j)}$ just quasi-minimizes (over $\mathbf{x}_0^{(j)} + \mathcal{K}_\mu(\mathbf{A}, \mathbf{R}_0)$) the residual norm $\|\mathbf{b}^{(j)} - (\mathbf{A} - \sigma_j \mathbf{I})\, \mathbf{x}\|_2$ of the j-th system in (12).

NUMERICAL RESULTS

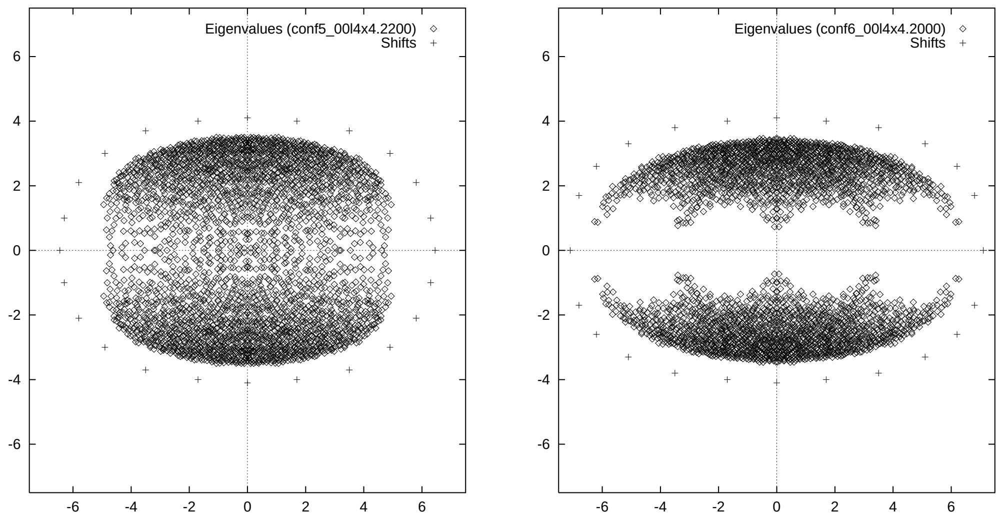

Figure 1: Eigenvalues of $\mathbf{D}$ and shifts for $\beta = 5.0$ (left) and $\beta = 6.0$ (right)

	QMR			block-QMR		
	# Mult. $\mathbf{D}$	# Mult. $\mathbf{D}^{\mathrm{T}}$	total	# Mult. $\mathbf{D}$	# Mult. $\mathbf{D}^{\mathrm{T}}$	total
$\beta = 5.0$	696	631	1327	589	565	1154 (87 %)
$\beta = 6.0$	1203	1171	2374	712	688	1400 (59 %)

Table 1: Quenched simulation: number of matrix-vector multiplications, $\kappa = 0.15$

	QMR			shifted block-QMR		
	# Mult. $\mathbf{D}$	# Mult. $\mathbf{D}^{\mathrm{T}}$	total	# Mult. $\mathbf{D}$	# Mult. $\mathbf{D}^{\mathrm{T}}$	total
$\beta = 5.0$	2455	2376	4831	1779	1730	3509 (73 %)
$\beta = 6.0$	2700	2635	5335	1817	1765	3582 (67 %)

Table 2: Heat-bath computation: number of matrix-vector multiplications

In this section, we report results from numerical experiments on a (relatively small) 4^4 lattice. We used 2 different (confined) sample configurations $\mathbf{D}$ (where $\mathbf{M}_\kappa = (1/\kappa)\mathbf{I} - \mathbf{D}$) corresponding to the values $\beta = 5.0$ and $\beta = 6.0$ of the "temperature" parameter β. These two "extremal" values represent bounds for the physically interesting range of β, also on larger lattices. Figure 1 shows the eigenvalue distribution of $\mathbf{D}$ for either configuration.
In Table 1, we report results from a quenched simulation, giving the total number of matrix-vector multiplications necessary to solve (1) for 12 different right-hand sides $\boldsymbol{\varphi}$ corresponding to the 12 unit vectors at the lattice point (2,2,2,1) and $\kappa = 0.15$. We compare the block-QMR method (with $m_0 = 12$) against the standard QMR algorithm [7] applied to each of the 12 systems individually. All initial guesses, as well as left Lanczos starting vectors, were chosen randomly. Our stopping criterion was to check for the relative residual norm being less than 10^{-7}. All computations were run in double precision. Table 1 clearly shows that the block-QMR approach reduces the computational requirements substantially, in particular for larger values of β.
In Table 2, we show results for a heat-bath computation in the multiboson situation. We now solved $m_0 = 24$ shifted systems, $\mathbf{M}_{\kappa_j}\boldsymbol{\psi}^{(j)} = ((1/\kappa_j)\mathbf{I} - \mathbf{D})\boldsymbol{\psi}^{(j)} = \boldsymbol{\varphi}^{(j)}$ with complex shift parameters κ_j lying outside the convex hull of the spectrum of $\mathbf{D}$ as indicated by the crosses in Figure 1. The vectors $\boldsymbol{\varphi}^{(j)}$ are Gaussian randomly distributed. We compare a shifted block-QMR approach (the one described in the previous section) with the results of 24 individual runs where all systems are solved independently with the standard QMR method. The initial guesses $\mathbf{x}_0^{(j)}$ were chosen as random vectors, and the stopping criterion was identical to our previous experiment. For the shifted block-QMR approach, we chose the left starting block $\mathbf{L}$ so that $\mathbf{L}^{\mathrm{T}}\mathbf{R}_0$ is diagonal. As before, we see that the block approach yields savings over the non-block version.

CONCLUSION

We presented variants of the block-QMR method for solving families of related linear systems. We have demonstrated that these block-QMR variants can successfully be applied in two typical QCD computations, resulting in savings of up to 50%. Our implementations did not yet make use of the γ_5-symmetry property of the underlying QCD systems. The γ_5-symmetry can be used to completely avoid multiplications with $\mathbf{D}^{\mathrm{T}}$ in the block-QMR method [5, 8, 10].

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