A BLOCK VERSION OF GMRES, BICG, BICGSTAB FOR LINEAR SYSTEMS WITH MULTIPLE RIGHT-HAND SIDES

Research aim:

Research a block version of GMRES, BICG, BICGSTAB for linear systems with multiple right-hand side.

The need for computer modeling of increasingly complex structures has led to the need to solve large linear systems.

All methods for solving linear systems can be divided into two classes: direct and iterative. Methods that lead to the solution for a finite number of arithmetic operations. Iterative methods are called, which should be obtained as a result of infinite repetition.

Many iterative methods are based on an iteration loop that accesses the coefficient matrix $\boldsymbol{A}$ once per loop and performs a matrix-vector multiply. To reduce data movement in the algorithm, our approach is to modify the algorithm such that more than one matrix-vector product occurs for a single memory access of $\boldsymbol{A}$. To this end, we investigated alternatives for solving a single right-hand side system based on solving a corresponding block linear system $\boldsymbol{AX} = \boldsymbol{B}$, where $\boldsymbol{X}$ and $\boldsymbol{B}$ are both groups of vectors.

Algorithm B-LGMRES

$r_i = b - Ax_i,\ \beta = \|r_i\|_2$
$R_i = [r_i, z_i, \ldots, z_{i-k+1}]$
$R_i = V_1 \hat{R}$
for $j = 1 : m$
    $U_j = AV_j$
    for $l = 1 : j$
        $H_{l,j} = V_l^T U_j$
        $U_j = U_j - V_l H_{l,j}$
    end
    $U_j = V_{j+1} H_{j+1,j}$
end
$W_m = [V_1, V_2, \ldots, V_m],\ H_m = \{H_{l,j}\}_{1 \le l \le j+1; 1 \le j \le m}$
find y_m s.t. $\|\beta e_1 - H_m y_m\|_2$ is minimized
$z_{i+1} = W_m y_m$
$x_{i+1} = x_i + z_{i+1}$

FIG. 3. *B-LGMRES(m, k) for restart cycle i.*

Algorithm Bl-BIC

ALGORITHM 1: **Block BCG**

X_0 is an $N \times s$ initial guess, $R_0 = B - AX_0$.
$\tilde{R}_0$ is an arbitrary $N \times s$ matrix.
$P_0 = R_0, \tilde{P}_0 = \tilde{R}_0$.
For $k = 0, 1, \ldots$ compute
$\alpha_k = (\tilde{P}_k^T A P_k)^{-1} \tilde{R}_k^T R_k$
$X_{k+1} = X_k + P_k \alpha_k$
$R_{k+1} = R_k - AP_k \alpha_k$
$\tilde{\alpha}_k = (P_k^T A^T \tilde{P}_k)^{-1} R_k^T \tilde{R}_k$
$\tilde{R}_{k+1} = \tilde{R}_k - A^T \tilde{P}_k \tilde{\alpha}_k$
$\beta_k = (\tilde{R}_k^T R_k)^{-1} \tilde{R}_{k+1}^T R_{k+1}$
$\tilde{\beta}_k = (R_k^T \tilde{R}_k)^{-1} R_{k+1}^T \tilde{R}_{k+1}$
$P_{k+1} = R_{k+1} + P_k \beta_k$
$\tilde{P}_{k+1} = \tilde{R}_{k+1} + \tilde{P}_k \tilde{\beta}_k$
end.

Algorithm Bl-BICGSTAB

ALGORITHM 3: **Bl-BiCGSTAB**

X_0 an initial guess; $R_0 = B - AX_0$; $P_0 = R_0$;
$\tilde{R}_0$ an arbitrary $N \times s$ matrix;
For $k = 0, 1, 2, \ldots$
$V_k = AP_k$;
solve $(\tilde{R}_0^T V_k)\alpha_k = \tilde{R}_0^T R_k$;
$S_k = R_k - V_k \alpha_k$;
$T_k = AS_k$;
$\omega_k = \langle T_k, S_k \rangle_F / \langle T_k, T_k \rangle_F$;
$X_{k+1} = X_k + P_k \alpha_k + \omega_k S_k$;
$R_{k+1} = S_k - \omega_k T_k$;
solve $(\tilde{R}_0^T V_k)\beta_k = -\tilde{R}_0^T T_k$;
$P_{k+1} = R_{k+1} + (P_k - \omega_k V_k)\beta_k$;
end.

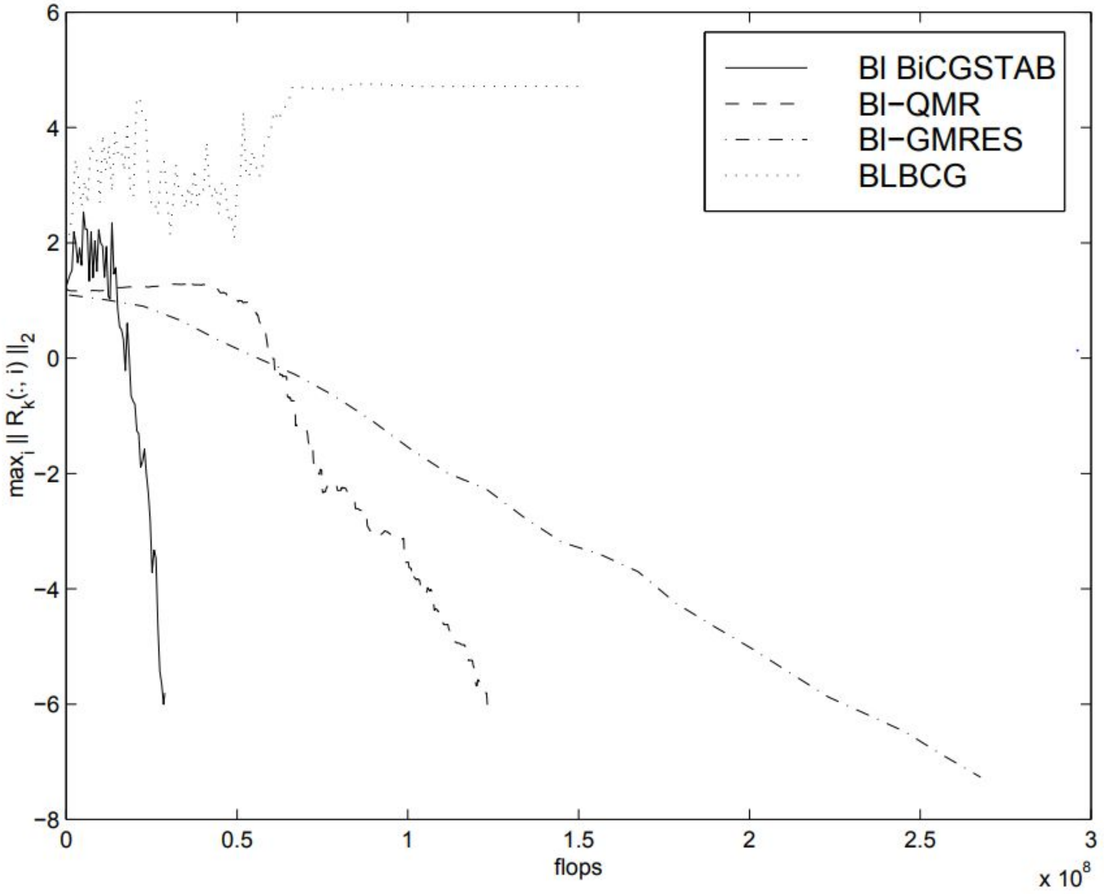
We compared the performance (in term of flops) of the Bl-BiCGSTAB algorithm, the Bl-GMRES algorithm and the BiCGSTAB algorithm applied to each single right-hand side. For all the tests the matrix B was an $N \times s$ random matrix. In Table 2 we list the effectiveness of Bl-BiCGSTAB measured by the ratios $f_1(s)$ and $f_2(s)$ where

$f_1(s)$=flops(Bl-BiCGSTAB)/(flops(BiCGSTAB))

$f_2(s)$=flops(Bl-BiCGSTAB)/(flops(Bl-GMRES))

Matrix	$s = 5$	$s = 10$	$s = 5$	$s = 10$
Utm 1700a ($N = 1700$) ($nnz(A) = 21313$)	$f_1(5) = 0.49$	$f_1(10) = 0.38$	$f_2(5) = 0.62$	$f_2(10) = 0.36$
SAYLR4($N = 3564$) ($nnz(A) = 22316$)	$f_1(5) = 0.77$	$f_1(10) = 0.89$	$f_2(5) = 0.06$	$f_2(10) = 0.12$
SHERMAN5 ($N = 3312$) ($nnz(A) = 20793$)	$f_1(5) = 0.93$	$f_1(10) = 0.94$	$f_2(5) = 0.26$	$f_2(10) = 0.16$
SHERMAN3 ($N = 5005$) ($nnz(A) = 20033$)	$f_1(5) = 0.82$	$f_1(10) = 1.10$	$f_2(5) = 0.27$	$f_2(10) = 0.25$

Comparison of various block methods for solving linear systems



Conclusion

The block methods are of great practical value in applications involving linear systems with multiple right-hand sides. However, they are not as well studied from the theoretical point of view.