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Bachelorarbeit

Implementation and experimental comparison between the COMMUNICATION AVOIDING-GENERALIZED MINIMAL RESIDUAL METHOD and standard GMRES

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Contents

Abstract

1 Introduction

As the CPU-memory performance gap widens the cost for communication increases as well.

Compared to arithmetic costs communication costs are much higher and the widening CPU-memory performance gap promotes the need for communication-avoiding algorithms.

Communication avoiding GMRES is based on s-step GMRES *REF[[J. Erhel, A parallel GMRES version for general sparse matrices, Electron. Trans. Numer. Anal., 3 (1995), pp. 160–176.]]*

2 Notation

For linear algebra, similar notation is considered as in [3] and [2].

- Greek letters denote scalars, lower case Roman letters denote vectors (or - based on the context - dimensions), capital Roman letters denote matrices.
- Capital letters with two subscripts, e.g. '$V_{m,n}$', denote matrices with m rows and n columns.
- Capital *Black letter* letters (e.g. V, Q and R in Black letters are represented by $\mathfrak{V}$, $\mathfrak{Q}$ and $\mathfrak{R}$ resp.) denote matrices that are composed out of other matrices.
- v_k denotes the k^{th} vector in a series of vectors v_0, v_1, ..., , v_k, v_{k+1}, ... of equal length.
- Similarly, V_k denotes the k^{th} matrix in a sequence of matrices V_0, V_1, ... , V_k, V_{k+1}, ... Generally all these matrices have the same number of rows. They may or may not have the same number of columns.
- If V_k is a matrix consisting of s vectors $[v_1, v_2, \ldots, v_s]$, $\underline{V}_k$ comprises vectors $[V_k, v_{s+1}]$. The underline means one more column at the end.
- If again, V_k is a matrix consisting of s vectors $[v_1, v_2, \ldots, v_s]$, $\acute{V}$ consists of vectors $[v_2, v_3, \ldots, v_s]$. The acute denotes one column less at the beginning.
- As a consequence $\underline{\acute{V}}$ denotes one more column at the end and one less column at the beginning, e.g. $\underline{\acute{V}} = [\acute{V}, v_{s+1}]$.
- Depending on the context, both underline or/and acute letters can also refer to row as well.

- Matlab notation is used for addressing elements of matrices and vectors. For example, given a matrix A of size $n \times n$ and two sets of indices α and β, $A(\alpha, :)$ is a submatrix formed by the subset of the rows of A whose indices belong to α. Similarly, $A(\alpha, \beta)$ is a submatrix formed by the subset of the rows of A whose indices belong to α and the subset of the columns of A whose indices belong to β.

3 Related work

s-step methods, CA-ILU(0)

4 Computational kernels

In this thesis *computational kernels* define the parts of an algorithm with the highest costs. These costs include both arithmetic and communication. The term *communication* generally denotes the movement of data either between different processors or between fast and slow memory. Communication optimal algorithms do not eliminate communication completely, but they are constructed with the goal to minimize it. This often results in additional redundant computations.

4.1 Matrix powers kernel (MPK)

[3] p.60
The Matrix Powers Kernel Power iteration, SpMV instead of MV, sparse matrix like a graph $\rightarrow$ spacial, temporal locality not as efficiently used as in dense MV. Avoid communication by sending / receiving all necessary values beforehand (look at reachability of graph(A)) and computing s basis vectors without further communication.

4.2 Tall and skinny QR (TSQR)

Unconditionally stable like Householder QR but less communication

4.3 Block Classical Gram-Schmidt (BCGS)

Dense matrix-matrix multiplications $\rightarrow$ less communication (factor $\Theta(s)$ fewer messages) than unblocked CGS. Also, BCGS requires less communication that BMGS. No reorthogonalization because solving linear system with (std. GMRES uses unblocked MGS-Arnoldi) CA-GMRES uses TSQR which improves orthogonality of the block columns.

5 Arnoldi iteration

first presented in *REF[[W. E. Arnoldi, The principle of minimized iterations in the solution of the matrix eigenvalue problem, Q. Appl. Maths, 9 (1951), pp. 17–29.]]*

s steps of standard Arnoldi produce an $s+1 \times s$ upper Hessenberg Matrix $\underline{H}$ and $m \times s+1$ orthonormal vectors $q_1, q_2, \ldots, q_s, q_{s+1}$ that form a basis for the Krylov subspace $\mathcal{K}_{s+1}(A, r)$ such that $AQ = \underline{Q}\underline{H}$. There are many ways to orthogonalize successive basis vectors. Modified Gram-Schmidt (MGS) is often employed because it provides high numerical stability, however, although not as stable, Classical Gram-Schmidt (CGS) is more suited for parallel implementations because it provides fewer synchronization points.

introduction.. produces $AQ = QH$

5.1 Arnoldi(s)

[238] H. F. Walker, Implementation of the GMRES and Arnoldi methods using Householder transformations, Tech. Rep. UCRL-93589, Lawrence Livermore National Laboratory, Oct. 1985.

5.1.1 The Monomial basis

like powermethod, rapidly growing condition number and vector length $\rightarrow$ scale vector to lengh 1, but: basis vectors are always linearly independent in exact arithmetic. In machine precision they become inevitably dependent at a certain point $\rightarrow$ need a different basis.

5.1.2 The Newton basis

polinomial interpolation at shifts $\theta_1, \theta_2, \ldots, \theta_s$.

Choosing the shifts find estimates of the eigenvalues of A (Ritz values).

The modified Leja ordering

Avoiding complex arithmetic

5.2 Arnoldi(s,t)

5.2.1 Introduction

5.2.2 Scaling the first basis vector

Arnoldi(s,t) produces $\underline{\Omega}$ which differs from MGS-Arnoldi $\hat{\underline{\Omega}}$ by a unitary scaling $\underline{\Theta} = \mathrm{diag}(\theta_1, \theta_2, \ldots, \theta_{st}, \theta_{st+1})$ such that $\hat{\underline{\Omega}} = \underline{\Omega\Theta}$. $\rightarrow$

- QR factorization must not change direction of the first column
- compute $\theta_1 = \langle r_0, q_1 \rangle \ / \ \beta$
- compute q_1 via MGS-Arnoldi (this happens naturally when the first outer iteration is started with MGS-Arnoldi in order to compute Ritz values for the Newton basis)

5.2.3 QR factorization update

overlapping / non overlapping approach.

[3] assumably have some errors in their notation, so the process is outlined slightly differently below.

$[\underline{\mathfrak{Q}}_0, \underline{\acute{V}}_1] = [\underline{\mathfrak{Q}}_0, \underline{\acute{Q}}_1] \cdot \begin{pmatrix} I_{s+1,s+1} & \underline{\acute{\mathfrak{R}}}_{0,1} \\ 0_{s,s+1} & \underline{\acute{R}}_1 \end{pmatrix}$

BGS ...

$AV_k = \underline{V}_k \underline{B}_k$

$A[\mathfrak{Q}_{k-1}, V_k] = [\mathfrak{Q}_{k-1}, \underline{V}_k]\underline{\mathfrak{B}}_k$

where $\underline{\mathfrak{B}}_k$ satisfies: $\underline{\mathfrak{B}}_k = \begin{pmatrix} \mathfrak{H}_{k-1} & 0_{sk,s} \\ h_{k-1} e_1 e_{sk}^T & \underline{B}_k \end{pmatrix}$ with $\mathfrak{H}_0 := H_0$

$A[\underline{\mathfrak{Q}}_{k-1}, \acute{Q}_k] \cdot \begin{pmatrix} I_{sk+1,sk+1} & \acute{\mathfrak{R}}_{k-1,k} \\ 0_{s-1,sk+1} & \acute{R}_k \end{pmatrix} = [\underline{\mathfrak{Q}}_{k-1}, \underline{\acute{Q}}_k] \cdot \begin{pmatrix} I_{sk+1,sk+1} & \underline{\acute{\mathfrak{R}}}_{k-1,k} \\ 0_{s,sk+1} & \underline{\acute{R}}_k \end{pmatrix} \cdot \begin{pmatrix} \mathfrak{H}_{k-1} & 0_{sk,s} \\ h_{k-1} e_1 e_{sk}^T & \underline{B}_k \end{pmatrix}$

We have

$$A[\underline{\mathfrak{Q}}_{k-1}, \acute{Q}_k] = [\underline{\mathfrak{Q}}_{k-1}, \underline{\acute{Q}}_k]\underline{\mathfrak{H}}_k$$

therefore,

$$\underline{\mathfrak{H}}_k = \begin{pmatrix} I_{sk+1,sk+1} & \underline{\acute{\mathfrak{R}}}_{k-1,k} \\ 0_{s,sk+1} & \underline{\acute{R}}_k \end{pmatrix} \cdot \begin{pmatrix} \mathfrak{H}_{k-1} & 0_{sk,s} \\ h_{k-1} e_1 e_{sk}^T & \underline{B}_k \end{pmatrix} \cdot \begin{pmatrix} I_{sk+1,sk+1} & \acute{\mathfrak{R}}_{k-1,k} \\ 0_{s-1,sk+1} & \acute{R}_k \end{pmatrix}^{-1}$$

5.2.4 Reconstructing the upper Hessenberg matrix

flop optimization. how to apply Givens rotations

6 CA-GMRES

The GMRES method starts with an initial approximate solution x_0 and initial residual $r_0 = b - Ax_0$ and finds a correction z_k at iteration k which solves the least-squares problem

$$\min_{z_k} \|b - A(x_0 + z_k)\|_2 \tag{1}$$

where z_k is determined in the Krylov subspace

$$\mathcal{K}_k(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{k-1} r_0\}.$$

The solution at iteration k is then formed by $x_k = x_0 + z_k$. Since $\{r_0, Ar_0, \ldots, A^{k-1} r_0\}$ is usually ill-conditioned the Arnoldi method is incorporated to produce $k+1$ orthonormal

basis vectors $\underline{Q}_k = [q_1, q_2, \ldots, q_k, q_{k+1}]$ with $q_1 = r_0/\|r_0\|_2$ and a $k+1 \times k$ upper Hessenberg coefficient matrix $\underline{H}_k$ where

$$AQ_k = \underline{Q}_k \underline{H}_k.$$

With these conditions z_k can be defined as $z_k = Q_k y$ such that

$$\begin{aligned} \min_{z_k} \|b - A(x_0 + z_k)\|_2 &= \min_y \|r_0 - AQ_k y\|_2 \\ &= \min_y \|r_0 - \underline{Q}_k \underline{H}_k y\|_2. \end{aligned}$$

Since $q_1 = r_0/\|r_0\|_2$ and $\underline{Q}_k$ is orthonormal, one has

$$\begin{aligned} \min_y \|r_0 - \underline{Q}_k \underline{H}_k y\|_2 &= \min_y \|\underline{Q}_k^T r_0 - \underline{H}_k y\|_2 \\ &= \min_y \|\beta e_1 - \underline{H}_k y\|_2 \end{aligned} \tag{2}$$

with $\beta = \|r_0\|_2$. $\underline{H}_k$ is then factored as $\underline{H}_k = \underline{G}_k \underline{R}_k$ with $\underline{G}_k$ being a product of k Givens rotations and $\underline{R}_k$ being upper triangular. The upper triangular system to solve is then given by

$$\min_y \left\|\beta \underline{G}_k^T e_1 - \underline{R}_k y\right\|_2$$

The solution can then be obtained by computing $x_k = x_0 + Q_k y$. Note that the absolute value of the last coordinate of $\beta \underline{G}_k^T e_1$ is $\|b - Ax_k\|_2$, the absolute residual at iteration k.

The CA-GMRES algorithm solves a different least-squares problem than (2).

$$\min_y \left\|\beta e_1 - \underline{RB} R^{-1} y\right\|_2 \tag{3}$$

6.1 Preconditioning

Left, right, split, we consider left preconditioning ($M^{-1}Ax = M^{-1}b$) only. Scaling is a special type of preconditioning. [3] considered two types of scaling in order to prevent rapid basis vector growth:

1. Balancing: replacing A by $A' = DAD^{-1}$ with D diagonal.
2. Equilibration: replacing A by $A' = D_r A D_c$ with D_r and D_c diagonal.

In their experiments solving nonsymmetric linear systems with CA-GMRES [3] found that for practical problems, equilibration established to be quite effective and almost made the basis type irrelevant. We observed something similar after applying the ILU(0) preconditioner to the system.

6.1.1 ILU(0) preconditioner

$M = LU$
in CA-GMRES apply M^{-1} to $r_0 = b - Ax_0$ at initialization and to $q_i = Aq_{i-1}$ int the MPK.

Algorithm 1 Newton CA-GMRES

Require: $n \times n$ linear system $Ax = b$ and initial guess x_0

1: $r_0 := b - Ax_0$, $\beta := \|r_0\|_2$, $q_1 := r_0/\beta$
2: **for** $k = 0$ to $t - 1$ do **do**
3: **if** $k = 0$ **then**
4: Compute $\underline{Q}_0$ and $\underline{H}_0$ using standard Arnoldi
5: Set $\underline{\mathfrak{Q}}_0 := \underline{Q}_0$ and $\underline{\mathfrak{H}}_0 := \underline{H}_0$
6: Compute Ritz values from H_0 and fix basis conversion matrix $\underline{B}_k$
7: Reduce $\underline{H}_0$ from upper Hessenberg to upper triangular form using s Givens rotations G_1, G_2, ..., G_s. Apply the same rotations in the same order to βe_1, resulting in the length $s + 1$ vector ζ_0.
8: **else**
9: Compute $\underline{\acute{V}}_k$ using SpMV and 1-2 AXPY
10: $\underline{\acute{\mathfrak{R}}}_{k-1,k} := \underline{\mathfrak{Q}}_{k-1}^T \underline{\acute{V}}_k$
11: $\underline{\acute{V}}_k' := \underline{\acute{V}}_k - \underline{\mathfrak{Q}}_{k-1} \underline{\acute{\mathfrak{R}}}_{k-1,k}$
12: Compute QR factorization of $\underline{\acute{V}}_k' \to \underline{\acute{Q}}_k \underline{\acute{R}}_k$ using TSQR
13: Compute $\underline{\mathfrak{H}}_{k-1,1} := -\mathfrak{H}_{k-1} \mathfrak{R}_{k-1,k} R_k^{-1} + \underline{\mathfrak{R}}_{k-1,k} \underline{B}_k R_k^{-1}$
14: Compute $H_k := R_k B_k R_k^{-1} + \tilde{\rho}_k^{-1} b_k z_k e_s^T - h_{k-1} e_1 e_{s(k-1)}^T \mathfrak{R}_{k-1,k} R_k^{-1}$
15: Compute $h_k := \tilde{\rho}_k^{-1} \rho_k b_k$
16: $\underline{\mathfrak{H}}_k := \begin{pmatrix} \mathfrak{H}_{k-1} & \underline{\mathfrak{H}}_{k-1,k} \\ h_0 e_1 e_{sk}^T & H_k \\ 0_{1,sk} & h_k e_s^T \end{pmatrix}$
17: Apply Givens rotations G_1, ..., G_{sk} in order to $\begin{pmatrix} \underline{\mathfrak{H}}_{k-1,k} \\ \underline{H}_k \end{pmatrix}$.
18: Reduce $\underline{H}_k$ to upper triangular form using s Givens rotations G_{sk+1}, ..., $G_{s(k+1)}$. Apply the rotations in the same order to $\begin{pmatrix} \zeta_{k-1} \\ 0_s \end{pmatrix}$, resulting in the length $s(k + 1) + 1$ vector ζ_k.
19: **end if**
20: Element $s(k+1)+1$ of ζ_k is the 2-norm (in exact arithmetic) of the current residual $r_{k+1} = b - Ax_{k+1}$ of the current solution x_{k+1}.
21: **if** converged **then**
22: Use the above reduction of $\underline{\mathfrak{H}}_k$ to upper triangular form and ζ_k to solve $y_k := \text{argmin}_y \|\mathfrak{H}_k y - \beta e_1\|_2$
23: Set $x_k := x_0 + \mathfrak{Q}_k y_k$, and exit
24: **end if**
25: **end for**

6.1.2 CA-ILU(0) preconditioner

summarize [2] (can be very long or short, dependent on overall length)

6.2 Convergence metrics

CA-GMRES produces cheap convergence metric, namely the relative residual $\|r_{k+1}\|_2$ / $\|r_0\|_2$. Might not be the best choice, depends too much on initial guess x_0.

If

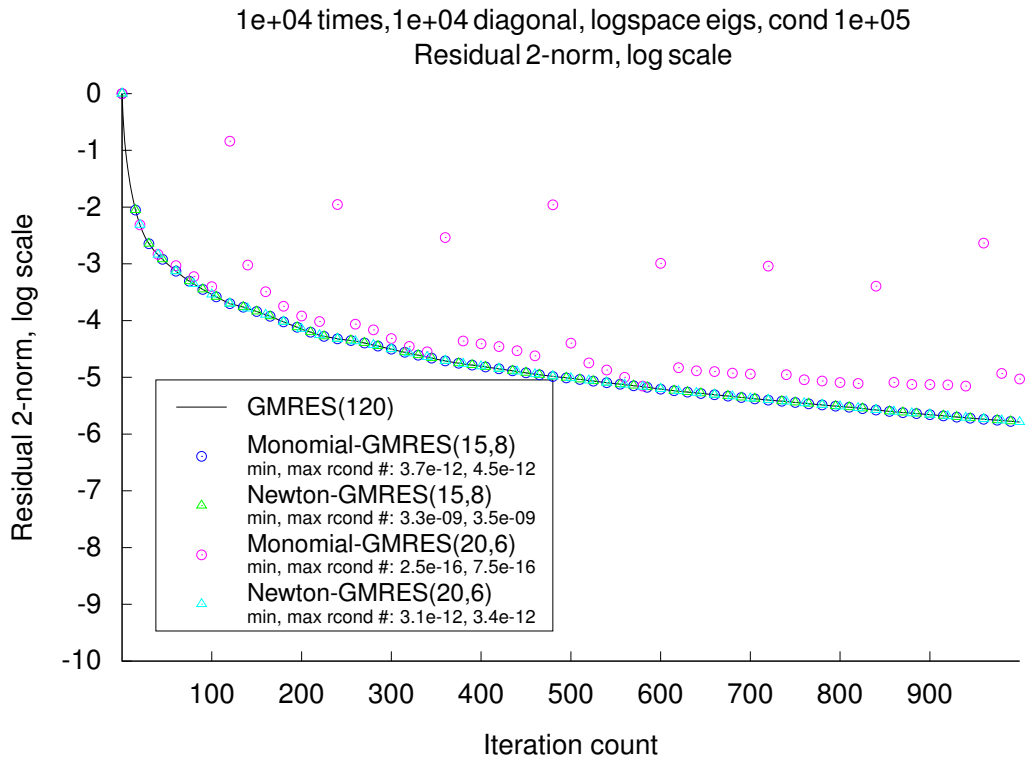
- $\|x_0\|_2$ too large $\rightarrow \|r_0\|$ will be large and iteration will stop too early.
- $x_0 = 0$ harder to make the relative residual small if A is ill-conditioned and x_{k+1} lies nearly in the nullspace of A.

6.3 Implementation details

language: C++, libraries: intel MKL, profiler: ??? (intel VTune Amplifier, TAU, ...) could not implement neither the MPK nor the CA-ILU(0) preconditioner due to time constraints. Also Modified Leja ordering does not deal with under / overflow in the product to maximize like in [3].

6.4 Numerical experiments

How the true solution $\hat{x}$ was generated: $\hat{x}(k) = u(k) + sin(2\pi k/n)$, where the scalar $u(k)$ is chosen from a random uniform [-1, 1] distribution. $\hat{x}$ was chosen in this way because a completely random solution is usually nonphysical, but a highly nonrandom solution (such as a vector of all ones) might be near an eigenvector of the matrix (which would result in artificially rapid convergence of the iterative method).


1e+04 times,1e+04 diagonal, logspace eigs, cond 1e+05
Residual 2-norm, log scale
Residual 2-norm, log scale
Iteration count
0
-1
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100
200
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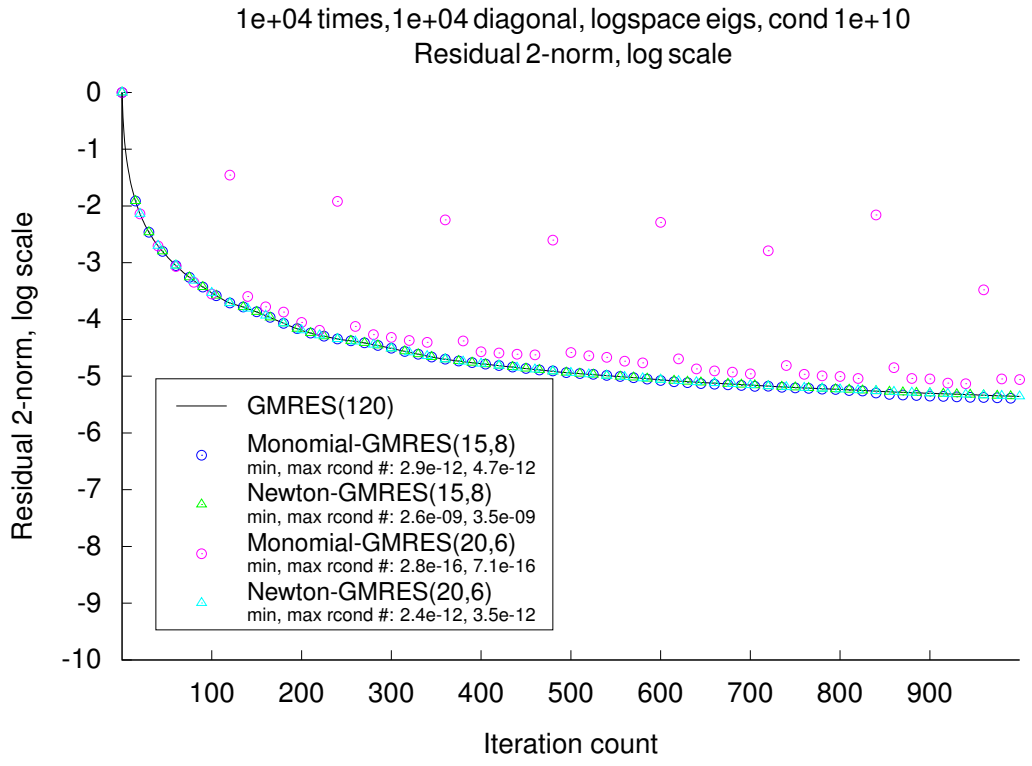
GMRES(120)
Monomial-GMRES(15,8)
min, max rcond #: 3.7e-12, 4.5e-12
Newton-GMRES(15,8)
min, max rcond #: 3.3e-09, 3.5e-09
Monomial-GMRES(20,6)
min, max rcond #: 2.5e-16, 7.5e-16
Newton-GMRES(20,6)
min, max rcond #: 3.1e-12, 3.4e-12


1e+04 times,1e+04 diagonal, logspace eigs, cond 1e+10
Residual 2-norm, log scale
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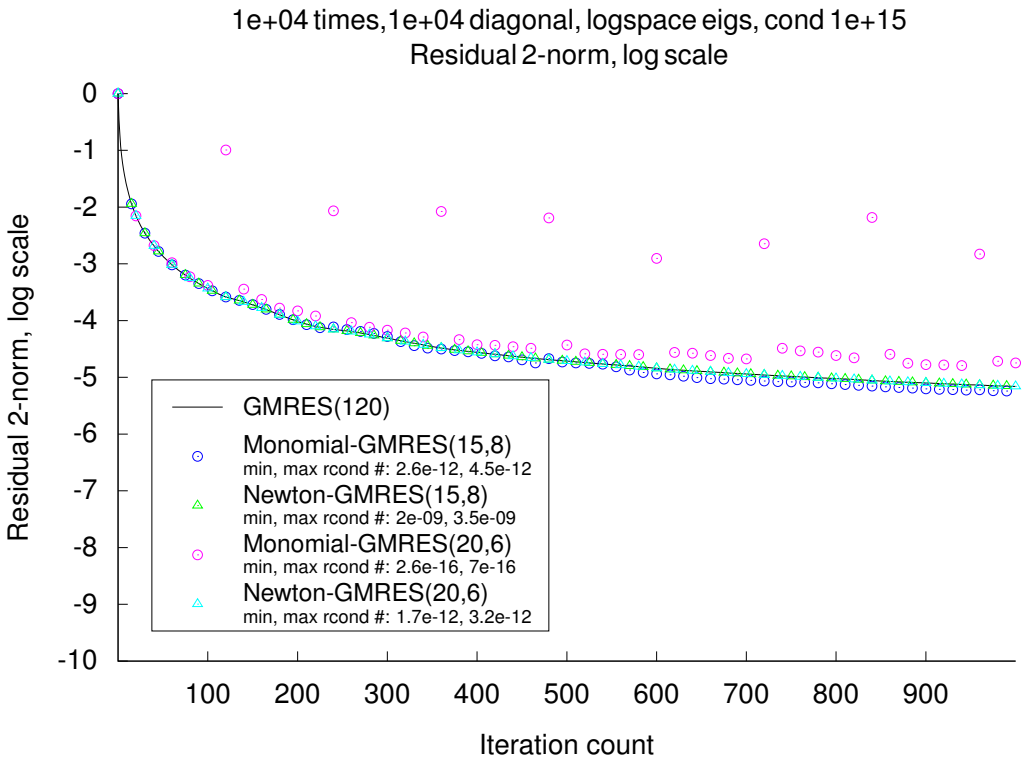
GMRES(120)
Monomial-GMRES(15,8)
min, max rcond #: 2.9e-12, 4.7e-12
Newton-GMRES(15,8)
min, max rcond #: 2.6e-09, 3.5e-09
Monomial-GMRES(20,6)
min, max rcond #: 2.8e-16, 7.1e-16
Newton-GMRES(20,6)
min, max rcond #: 2.4e-12, 3.5e-12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min, max rcond #: 2e-09, 3.5e-09
Monomial-GMRES(20,6)
min, max rcond #: 2.6e-16, 7e-16
Newton-GMRES(20,6)
min, max rcond #: 1.7e-12, 3.2e-12

6.5 Performance experiments

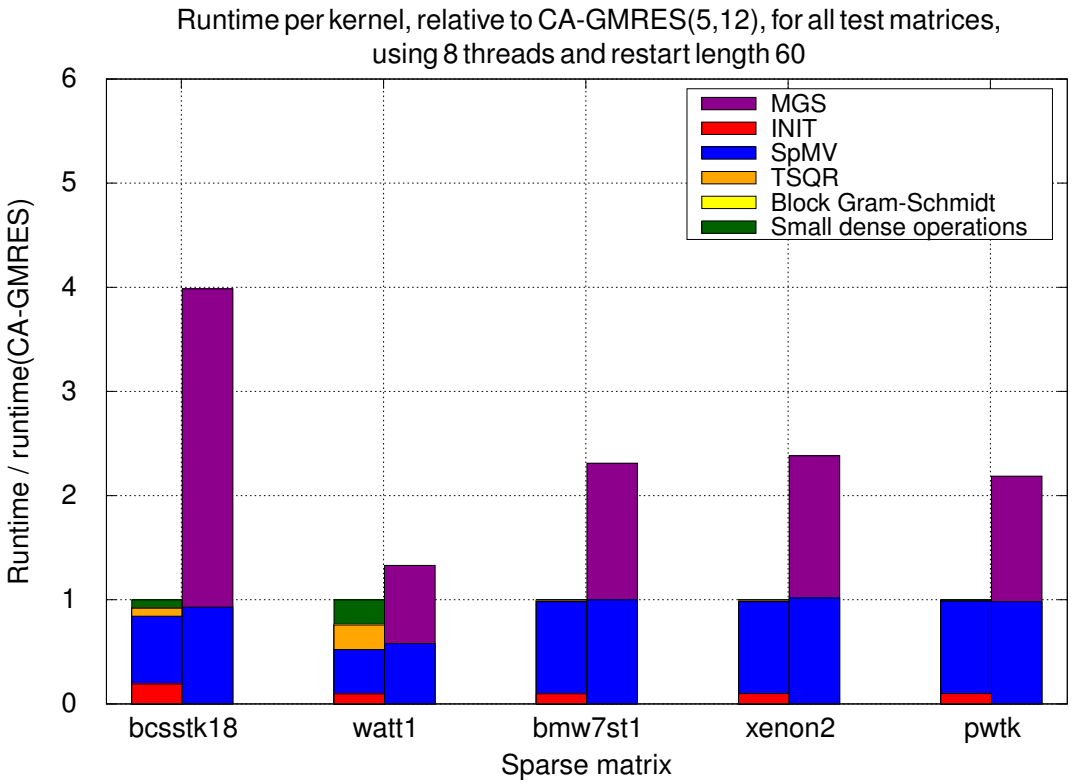

Figure 1: left CA-GMRES, right GMRES

6.5.1 Summary

Conclusion: the MPK is an important kernel and should have been implemented, also restarting with s steps of std. GMRES is not optimal and leaves room for optimization.

7 Conclusion

Krylov subspace methods (summarize this section briefly in introduction)

[1] p.191

- short description:
  Krylov subspace definition: $\mathcal{K}_k(A, r_0) = span\left\{r_0, Ar_0, A^2r_0, \ldots, A^{k-1}r_0\right\}$

All iterative methods build and enhance a KSP with every iteration.

$$\mathbf{r}_k = \mathbf{r}_0 + \sum_{j=1}^{k} c_j A^j \mathbf{r}_0 \quad \rightarrow \quad \mathbf{x}_k = \mathbf{x}_0 + \sum_{j=0}^{k-1} c_{j+1} A^j \mathbf{r}_0$$

what is good for the power method, is bad here, bc. vectors are in theory linearly independent but too close to parallel → in machine arithmetic they become linearly dependent. Need new basis ...

- Arnoldi [1] p.192

$$AQ_k = Q_{k+1} H_{k+1,k}$$

- Summary: ([1] p. 192)
  - 1. construct an orthogonal basis for the Krylov subspace;
  - 2. define an optimality property;
  - 3. use an effective preconditioner.

[1] p.184

- short description: most stable and prominent iterative method, for sym pos def matrices only.
- Algorithm description (just the basics)
  - $\|x - x_k\|_A = min_{y \in \mathcal{K}_k(A,r_0)} \|x - y\|_A$
    After k-steps, x_k minimizes in the KSP the A-norm x - y (only if A is SPD, or else it's not a norm)
  - follows basic concept: $\mathbf{x}_{new} = x_{old} + constant \cdot searchdirection$ (better version *steepest descent*)
  - $\mathbf{r}_k$ is multiple of q_{k+1} (q from Arnoldi; q is not directly used in CG)
    → (1) orthogonal residuals $\mathbf{r}_i^T \mathbf{r}_k = 0, \quad i < k$
    → (2) $(x_i - x_{i-1})^T A (x_k - x_{k-1}) = 0 \quad \rightarrow \quad \Delta\mathbf{x}_i^T A \Delta\mathbf{x}_k = 0, \quad i < k$
    in other words: the corrections in $\mathbf{x}$ are orthogonal in the A-inner product, hence the term 'conjugate' in CG. The term 'gradients' comes from minimizing the energy equation/quadratic form:

    $$E(x) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} - b^T\mathbf{x} \rightarrow min$$

    Set the derivative (gradient) to zero, i.e. $E'(x) = 0$:

    $$A\mathbf{x} - b = 0$$

    and we're back to the original problem. So minimizing energies and solving the linear equation $A\mathbf{x} = b$ are basically the same.

  - H is symmetric, and therefore tridiagonal. Arnoldi simplifies to Lanczos → short 'three-term' recurrences (only have to look at a few previous orthogonal vectors, not all of them).

- p.191 what about general matrices? Any non-singular matrix A can be transformed into SPD matrix via $A^TA \rightarrow$ bad condition number $\kappa(A)$.

  {The condition number of the matrix A^TA is the square of the condition number of A [...] A large condition number both increases the number of iterations required and limits the accuracy to which a solution can be obtained. [4] p. 89 (2.7.40)} consider Krylov subspace methods that are directly based on general matrix $A \rightarrow$ GMRES

GMRES (summarize this section briefly in introduction)

- short description: general form of MINRES (=like CG it is only for symmetric matrices, but must not be PD) MINRES minimizes $\|\mathbf{r}_k\|_2$ and CG minimizes energy norm of the residual $\|\mathbf{r}_k\|_{A^{-1}}$ or the energy norm of the error $\|\mathbf{x}^* - \mathbf{x}_k\|_A$ respectively. [1] (p. 198)

- algorithm description:

- $\|b - A\mathbf{x}_k\|_2 = min_{y \in \mathcal{K}_k(A,r_0)} \|b - Ay\|_2$
  After k-steps, $\mathbf{x}_k$ minimizes in the KSP the ℓ^2-norm $b - Ay$

- GMRES vs. CG:
  - CG forces the residual $\mathbf{r}_k$ to be orthogonal to the Krylov subspace $\mathcal{K}_k(A, r_0)$;
  - GMRES seeks the residual with minimum ℓ_2-norm within the Krylov subspace.

- Summary:
  The main components of a single iteration of GMRES are
  1. perform a step of the Arnoldi process;
  2. update the QR factorization of the updated upper Hessenberg matrix;
  3. solve the resulting least squares problem.

References

[1] Uri M. Ascher and Chen Greif. *A First Course in Numerical Methods*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2011.

[2] Laura Grigori and Sophie Moufawad. Communication avoiding ilu0 preconditioner. *SIAM Journal on Scientific Computing*, 37:C217–C246, 04 2015.

[3] Mark Hoemmen. *Communication-avoiding Krylov Subspace Methods.* PhD thesis, Berkeley, CA, USA, 2010. AAI3413388.

[4] William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. *Numerical Recipes in C.* Cambridge University Press, 1992.

Appendices

Appendix A

discussion of test matrices