Sparse linear solvers: iterative methods

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Plan

Sparse linear solvers

- Sparse matrices and graphs
- Classes of linear solvers

Krylov subspace methods

- Conjugate gradient method

Iterative solvers that reduce communication

- CA solvers based on s-step methods
- Enlarged Krylov methods

Plan

Sparse matrices and graphs

- Most matrices arising from real applications are sparse.
- A 1M-by-1M submatrix of the web connectivity graph, constructed from an archive at the Stanford WebBase.

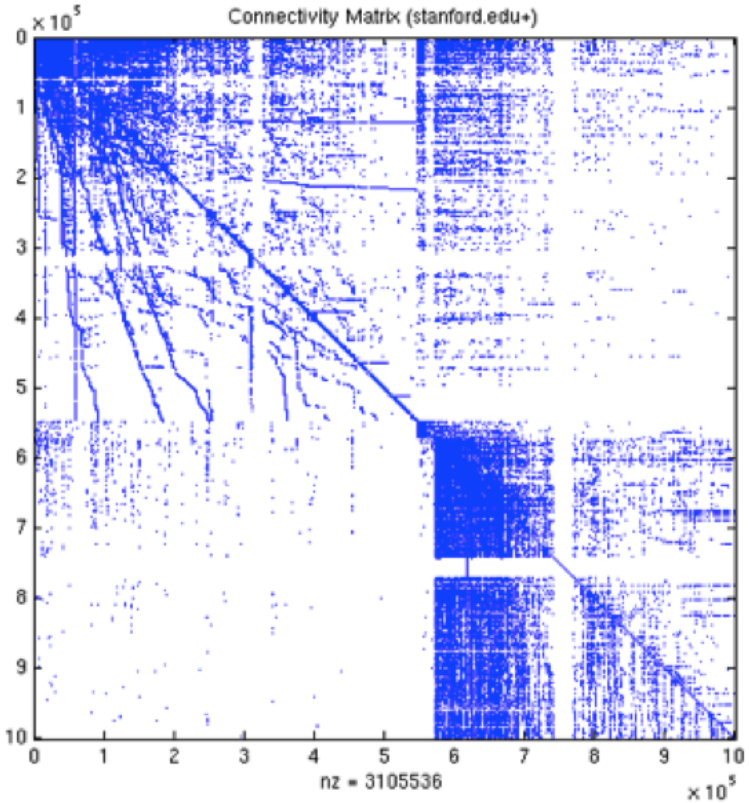


Figure : Nonzero structure of the matrix

Sparse matrices and graphs

- Most matrices arising from real applications are sparse.
- GHS class: Car surface mesh, $n = 100196, nnz(A) = 544688$

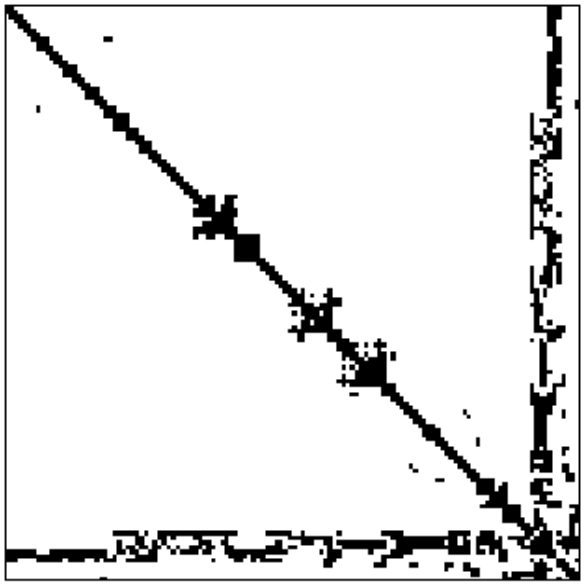


Figure : Nonzero structure of the matrix

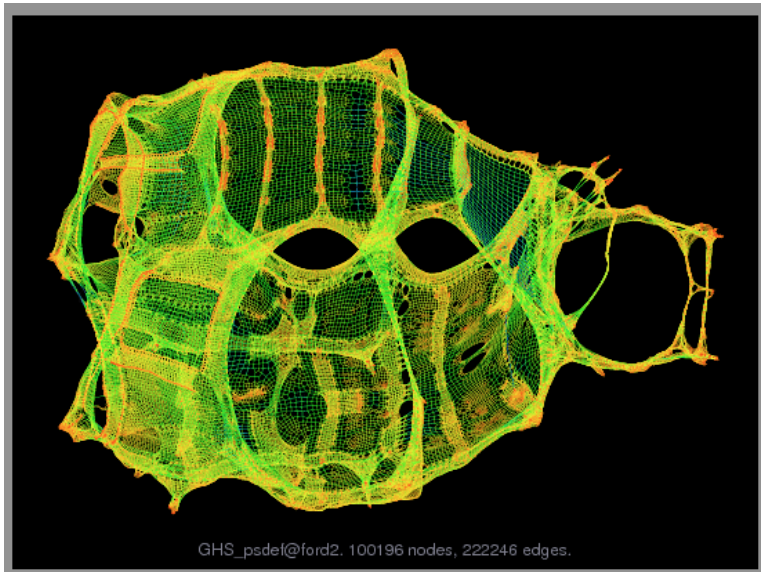
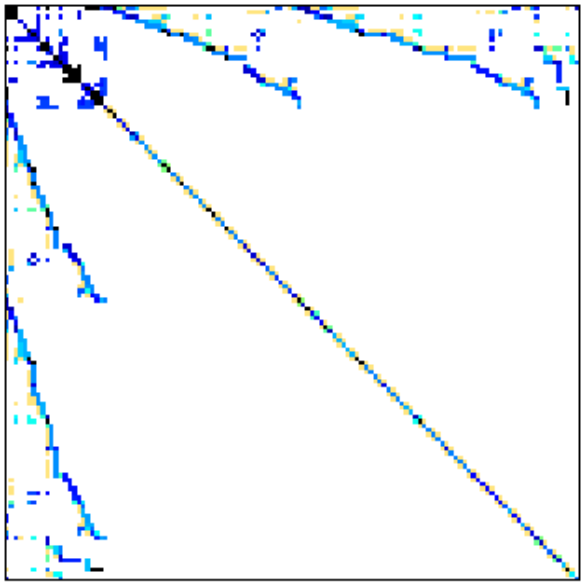


Figure : Its undirected graph

Examples from Tim Davis's Sparse Matrix Collection,
`http://www.cise.ufl.edu/research/sparse/matrices/`

Sparse matrices and graphs

- Semiconductor simulation matrix from Steve Hamm, Motorola, Inc. circuit with no parasitics, $n = 105676$, $nnz(A) = 513072$



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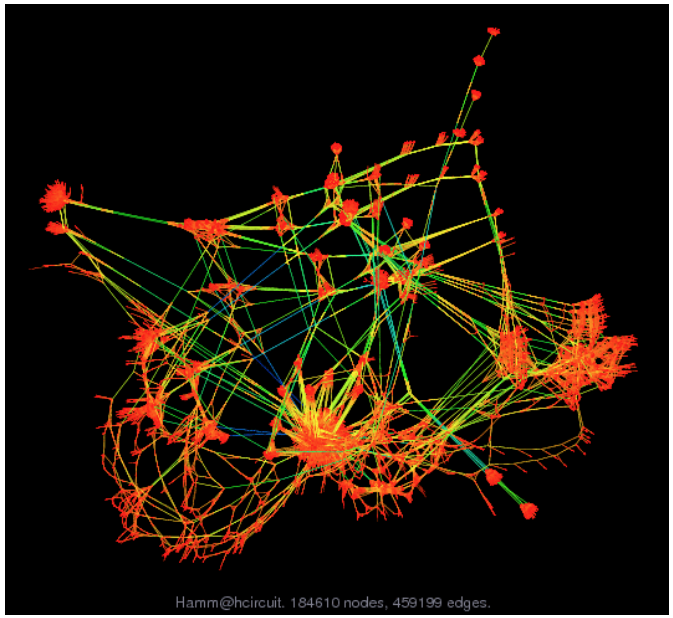

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Sparse linear solvers

Direct methods of factorization

- For solving $Ax = b$, least squares problems
  - Cholesky, LU, QR, LDL^T factorizations
- Limited by fill-in/memory consumption and scalability

Iterative solvers

- For solving $Ax = b$, least squares, $Ax = \lambda x$, SVD
- When only multiplying A by a vector is possible
- Limited by accuracy/convergence

Hybrid methods

As domain decomposition methods

Plan

Sparse linear solvers

Krylov subspace methods

- Conjugate gradient method

Iterative solvers that reduce communication

Krylov subspace methods

Solve $Ax = b$ by finding a sequence $x_1, x_2, ..., x_k$ that minimizes some measure of error over the corresponding spaces

$$x_0 + \mathcal{K}_i(A, r_0), \quad i = 1, ..., k$$

.

They are defined by two conditions:

1. Subspace condition: $x_k \in x_0 + \mathcal{K}_k(A, r_0)$
2. Petrov-Galerkin condition: $r_k \perp \mathscr{L}_k$

$$\iff (r_k)^t y = 0, \quad \forall \quad y \in \mathscr{L}_k$$

where

- x_0 is the initial iterate, r_0 is the initial residual,
- $\mathcal{K}_k(A, r_0) = span\{r_0, Ar_0, A^2 r_0, ..., A^{k-1} r_0\}$ is the Krylov subspace of dimension k,
- $\mathscr{L}_k$ is a well-defined subspace of dimension k.

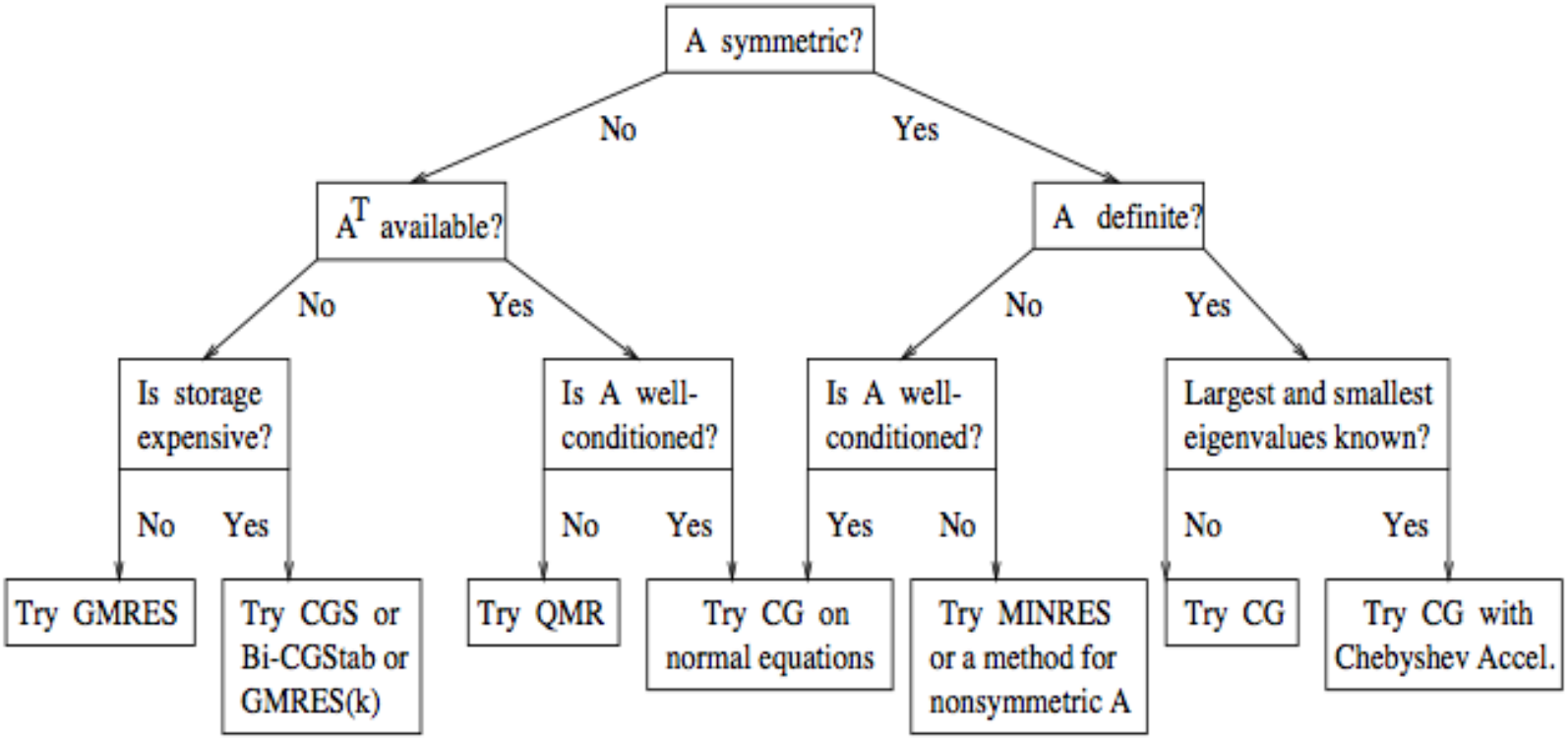
One of Top Ten Algorithms of the 20th Century

From SIAM News, Volume 33, Number 4:
Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of Krylov subspace iteration methods.

- Russian mathematician Alexei Krylov writes first paper, 1931.
- Lanczos - introduced an algorithm to generate an orthogonal basis for such a subspace when the matrix is symmetric.
- Hestenes and Stiefel - introduced CG for SPD matrices.

Other Top Ten Algorithms: Monte Carlo method, decompositional approach to matrix computations (Householder), Quicksort, Fast multipole, FFT.

Choosing a Krylov method



All methods (GMRES, CGS,CG…) depend on SpMV (or variations…)

See www.netlib.org/templates/Templates.html for details

Source slide: J. Demmel

Conjugate gradient (Hestenes, Stieffel, 52)

- A Krylov projection method for SPD matrices where $\mathscr{L}_k = \mathcal{K}_k(A, r_0)$.
- Finds $x^* = A^{-1}b$ by minimizing the quadratic function

$$\begin{aligned} \phi(x) &= \frac{1}{2}(x)^t Ax - b^t x \\ \bigtriangledown\phi(x) &= Ax - b = 0 \end{aligned}$$

- After j iterations of CG,

$$||x^* - x_j||_A \leq 2||x - x_0||_A \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^j,$$

where x_0 is starting vector, $||x||_A = \sqrt{x^T Ax}$ and $\kappa(A) = |\lambda_{max}(A)|/|\lambda_{min}(A)|$.

Conjugate gradient

- Computes A-orthogonal search directions by conjugation of the residuals

$$\left\{ \begin{array}{lcl} p_1 & = & r_0 = - \bigtriangledown \phi(x_0) \\ p_k & = & r_{k-1} + \beta_k p_{k-1} \end{array} \right. \quad (1)$$

- At k-th iteration,

$$x_k = x_{k-1} + \alpha_k p_k = argmin_{x \in x_0 + \mathcal{K}_k(A, r_0)} \phi(x)$$

where α_k is the step along p_k.

- CG algorithm obtained by imposing the orthogonality and the conjugacy conditions

$$\begin{array}{rcl} r_k^T r_i & = & 0, \text{for all } i \neq k, \\ p_k^T A p_i & = & 0, \text{for all } i \neq k. \end{array}$$

CG algorithm

Algorithm 1 The CG Algorithm

$r_0 = b - Ax_0$, $\rho_0 = ||r_0||_2^2$, $p_1 = r_0$, $k = 1$
while ($\sqrt{\rho_k} > \epsilon||b||_2$ and $k < k_{max}$) **do**
    if $(k \neq 1)$ **then**
        $\beta_k = (r_{k-1}, r_{k-1})/(r_{k-2}, r_{k-2})$
        $p_k = r_{k-1} + \beta_k p_{k-1}$
    end if
    $\alpha_k = (r_{k-1}, r_{k-1})/(Ap_k, p_k)$
    $x_k = x_{k-1} + \alpha_k p_k$
    $r_k = r_{k-1} - \alpha_k Ap_k$
    $\rho_k = ||r_k||_2^2$
    $k = k + 1$
end while

Challenge in getting efficient and scalable solvers

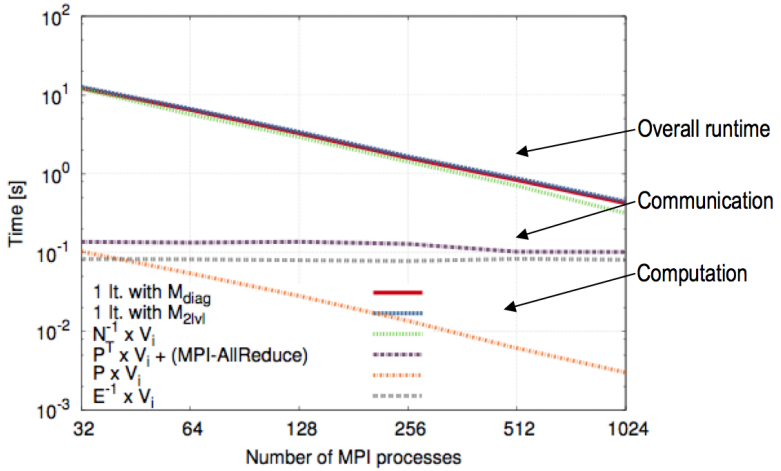
- A Krylov solver finds x_{k+1} from $x_0 + \mathcal{K}_{k+1}(A, r_0)$ where

$$\mathcal{K}_{k+1}(A, r_0) = span\{r_0, Ar_0, A^2 r_0, ..., A^k r_0\},$$

  such that the Petrov-Galerkin condition $b - Ax_{k+1} \perp \mathscr{L}_{k+1}$ is satisfied.
- Does a sequence of k SpMVs to get vectors $[x_1, ..., x_k]$
- Finds best solution x_{k+1} as linear combination of $[x_1, ..., x_k]$

Typically, each iteration requires

- Sparse matrix vector product
  $\rightarrow$ point-to-point communication
- Dot products for orthogonalization
  $\rightarrow$ global communication



Map making, with R. Stompor, M. Szydlarski
Results obtained on Hopper, Cray XE6, NERSC

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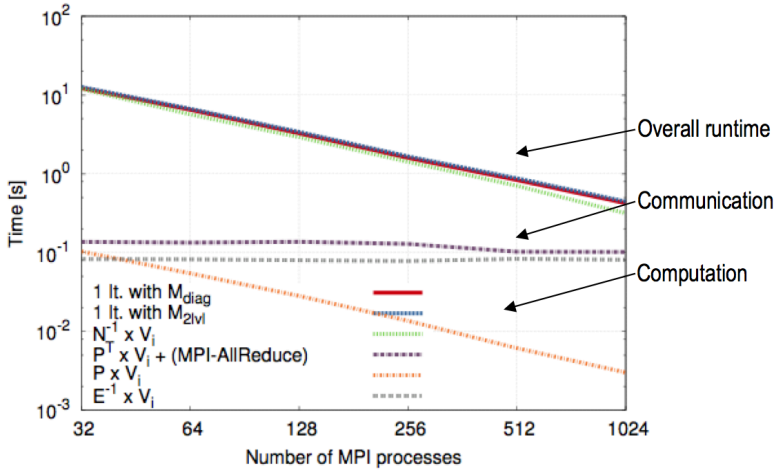

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Ways to improve performance

- Improve the performance of sparse matrix-vector product.
- Improve the performance of collective communication.
- Change numerics - reformulate or introduce Krylov subspace algorithms to:
  - reduce communication,
  - increase arithmetic intensity - compute sparse matrix-set of vectors product.
- Use preconditioners to decrease the number of iterations till convergence.

Plan

Sparse linear solvers

Krylov subspace methods

Iterative solvers that reduce communication

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Iterative solvers that reduce communication

Communication avoiding based on s-step methods

- Unroll k iterations, orthogonalize every k steps.
- A factor of $O(k)$ less messages and bandwidth in sequential.
- A factor of $O(k)$ less messages in parallel (same bandwidth).

Enlarged Krylov methods

- Decrease the number of iterations to decrease the number of global communication.
- Increase arithmetic intensity.

Other approaches available in the litterature, but not presented here.

CA solvers based on s-step methods: main idea

To avoid communication, unroll k-steps, ghost necessary data,

- generate a set of vectors W for the Krylov subspace $\mathcal{K}_k(A, r_0)$,
- (A)-orthogonalize the vectors using a communication avoiding orthogonalization algorithm (e.g. TSQR(W)).

References

- Van Rosendale '83, Walker '85, Chronopoulous and Gear '89, Erhel '93, Toledo '95, Bai, Hu, Reichel '91 (Newton basis), Joubert and Carey '92 (Chebyshev basis), etc.
- Recent references: G. Atenekeng, B. Philippe, E. Kamgnia (to enable multiplicative Schwarz preconditioner), J. Demmel, M. Hoemmen, M. Mohiyuddin, K. Yellick (to minimize communication, next slides), Carson, Demmel, Knight (CA and other Krylov solvers, preconditioners)

CA-GMRES

GMRES: find x in $span\{b, Ab, ..., A^k b\}$ minimizing $||Ax - b||_2$
Cost of k steps of standard GMRES vs new GMRES

Standard GMRES
 for i=1 to k
  w = A · v(i-1)
  MGS(w, v(0),...,v(i-1))
  update v(i), H
 endfor
 solve LSQ problem with H

Sequential: #words_moved =
  O(k·nnz) from SpMV
 + O(k^2·n) from MGS
Parallel: #messages =
  O(k) from SpMV
 + O(k^2 · log p) from MGS

Source of following 11 slides: J. Demmel

CA-GMRES

GMRES: find x in $span\{b, Ab, ..., A^k b\}$ minimizing $||Ax - b||_2$
Cost of k steps of standard GMRES vs new GMRES

Standard GMRES
for i=1 to k
w = A · v(i-1)
MGS(w, v(0),...,v(i-1))
update v(i), H
endfor
solve LSQ problem with H

Communication-avoiding GMRES
W = [v, Av, A^2v, ... , A^kv]
[Q,R] = TSQR(W) ... "Tall Skinny QR"
Build H from R, solve LSQ problem

Sequential: #words_moved =
O(k·nnz) from SpMV
+ O(k^2·n) from MGS
Parallel: #messages =
O(k) from SpMV
+ O(k^2 · log p) from MGS

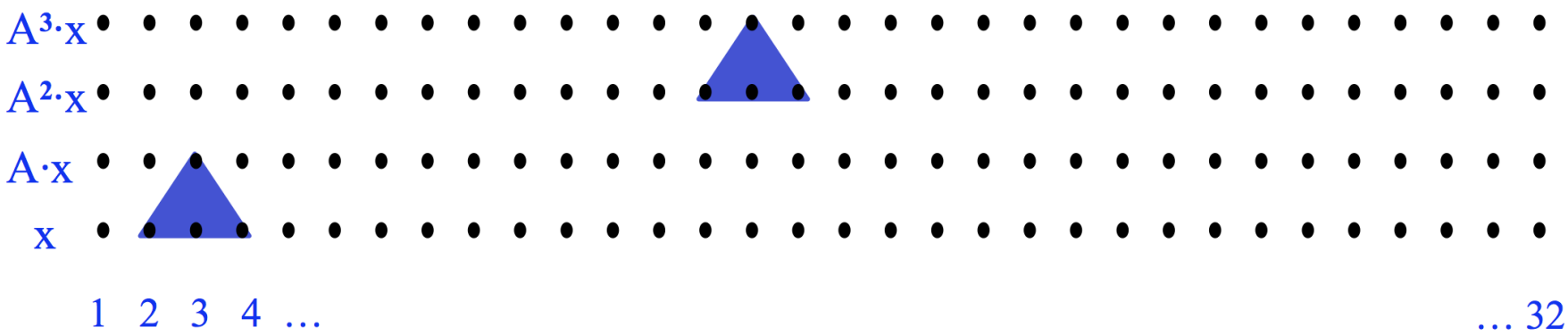
Sequential: #words_moved =
O(nnz) from SpMV
+ O(k·n) from TSQR
Parallel: #messages =
O(1) from computing W
+ O(log p) from TSQR

Source of following 11 slides: J. Demmel

Matrix Powers Kernel

- Generate the set of vectors $\{Ax, A^2x, \ldots A^kx\}$ in parallel
- Ghost necessary data to avoid communication
- Example: A tridiagonal, $n = 32$, $k = 3$
- Shaded triangles represent data computed redundantly

$$Ax = \begin{pmatrix} * & * & & & & & \\ * & * & * & & & & \\ & * & * & * & & & \\ & & * & * & * & & \\ & & & \ddots & \ddots & \ddots & \end{pmatrix} \cdot \begin{pmatrix} * \\ * \\ * \\ * \\ \vdots \end{pmatrix} = \begin{pmatrix} * \\ * \\ * \\ * \\ \vdots \end{pmatrix}$$



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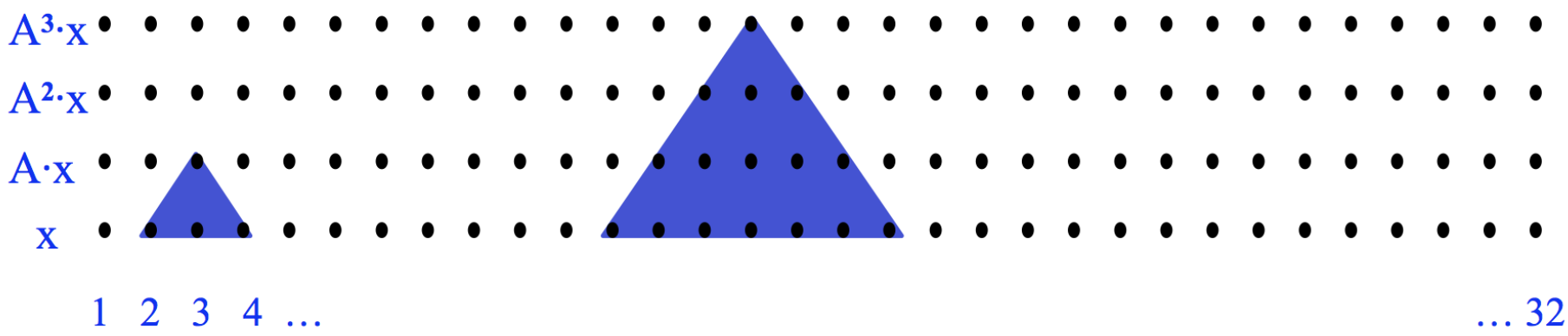

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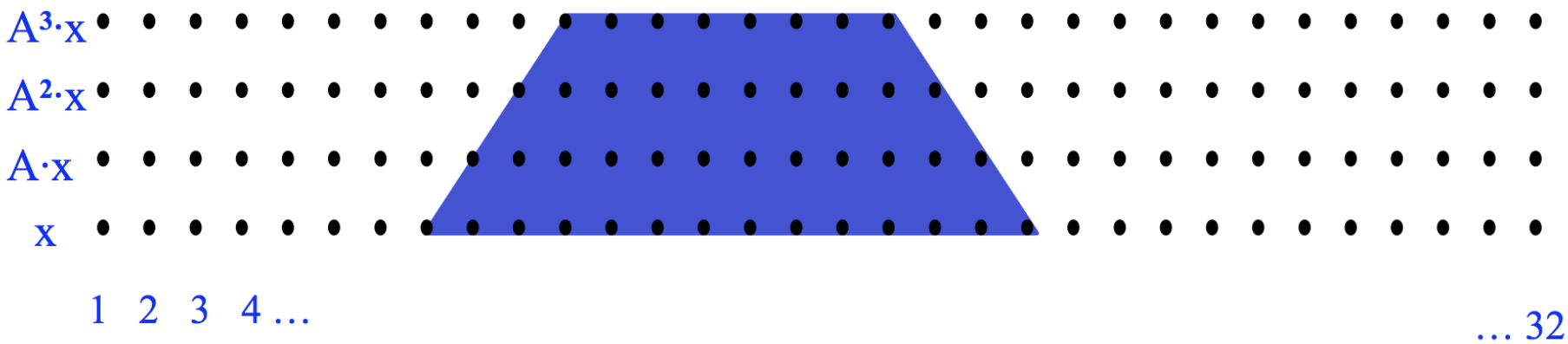

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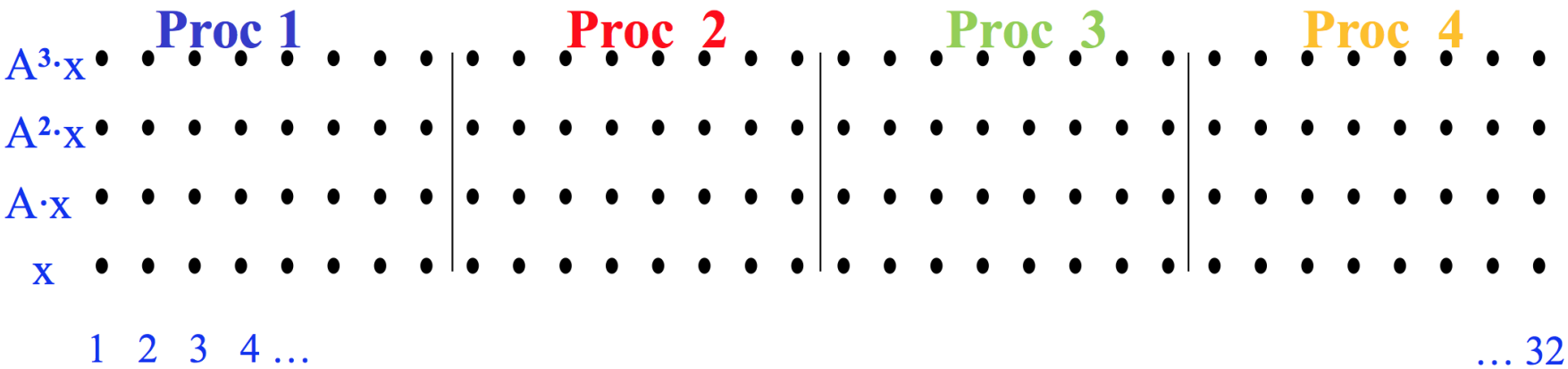

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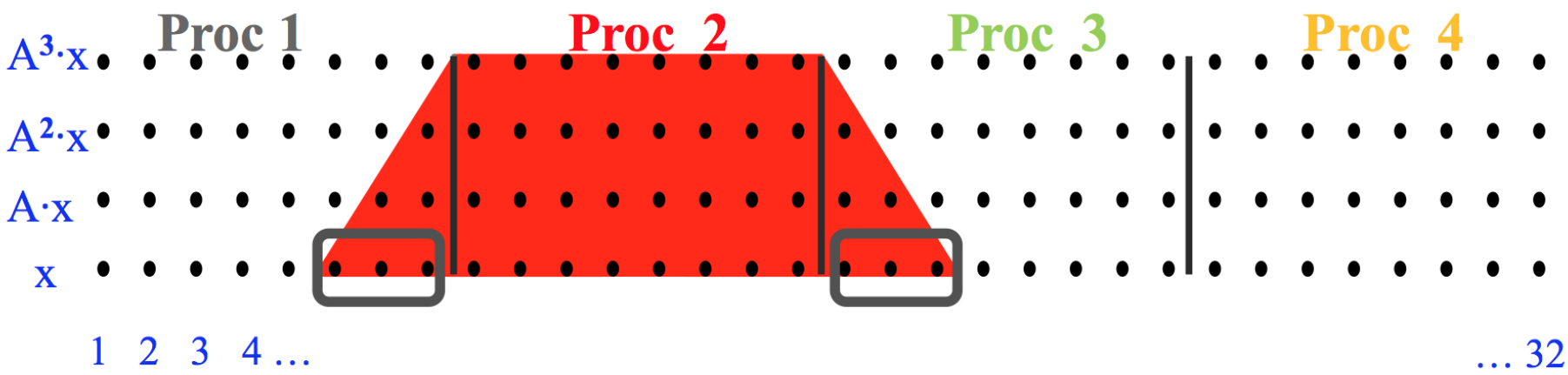

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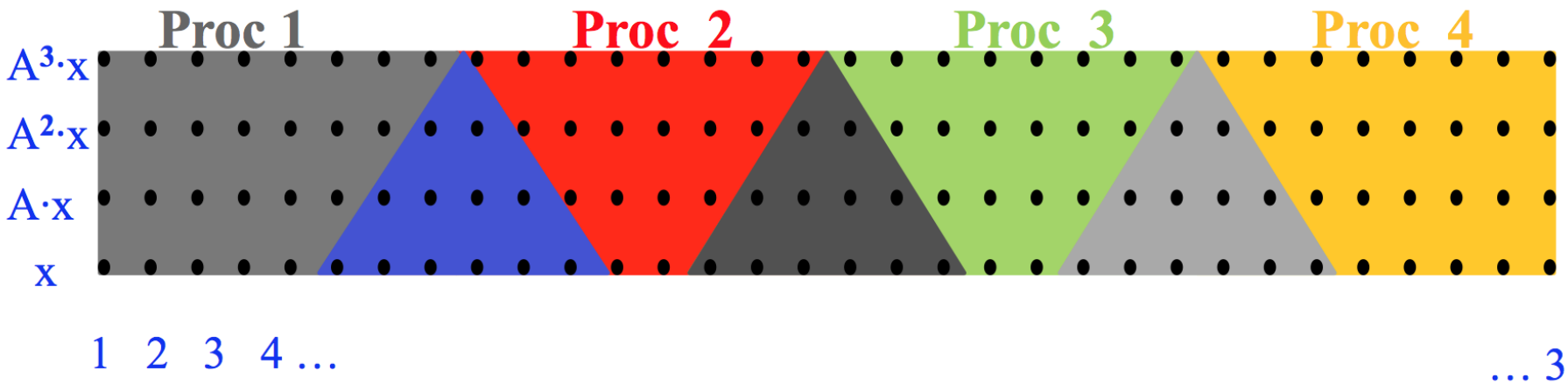
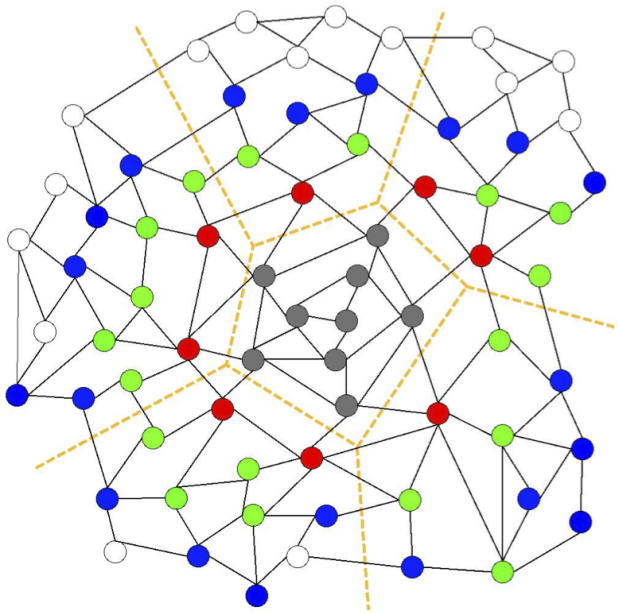


Matrix Powers Kernel (contd)

Ghosting works for structured or well-partitioned unstructured matrices, with modest surface-to-volume ratio.

- Parallel: block-row partitioning based on (hyper)graph partitioning,
- Sequential: top-to-bottom processing based on traveling salesman problem.



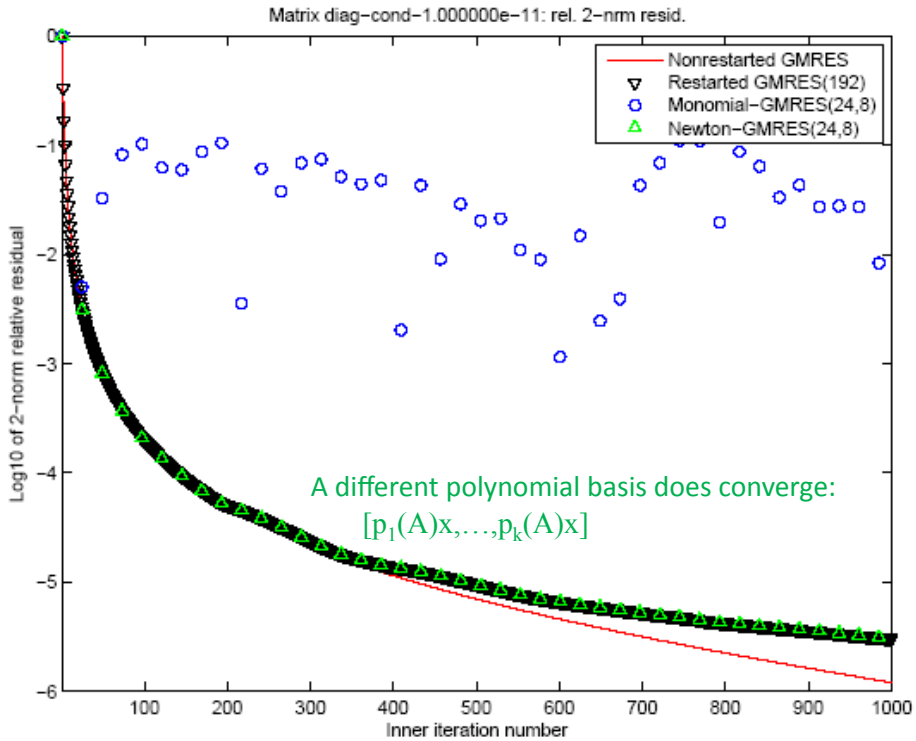
Challenges and research opportunities

Length of the basis k is limited by

- Size of ghost data
- Loss of precision

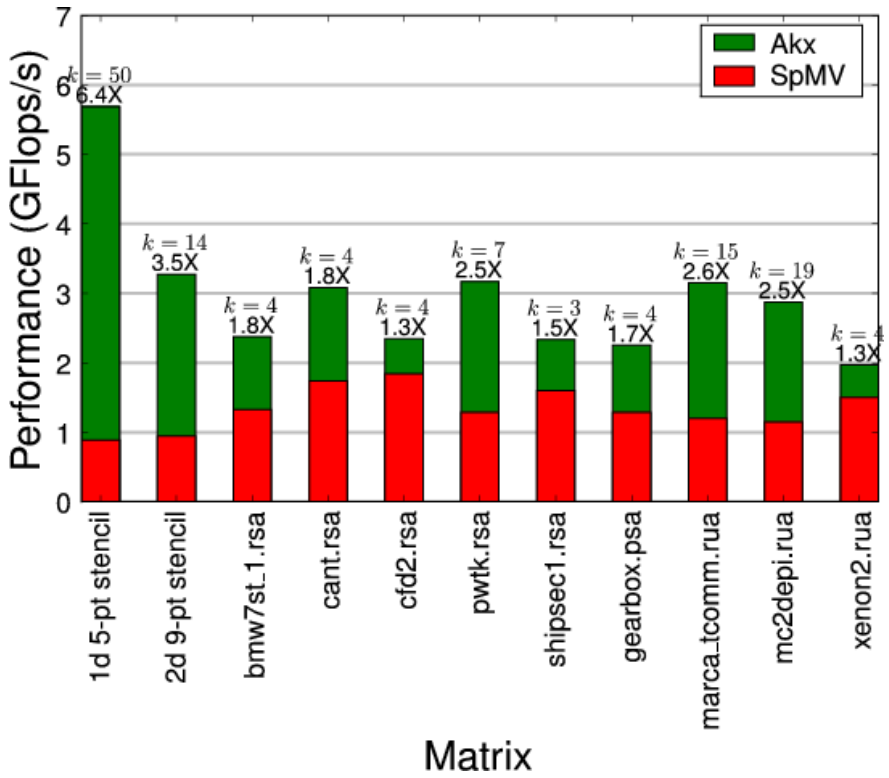
Preconditioners: lots of recent work

- Highly decoupled preconditioners: Block Jacobi
- Hierarchical, semiseparable matrices (M. Hoemmen, J. Demmel)
- CA-ILU0, deflation (Carson, Demmel, Knight)

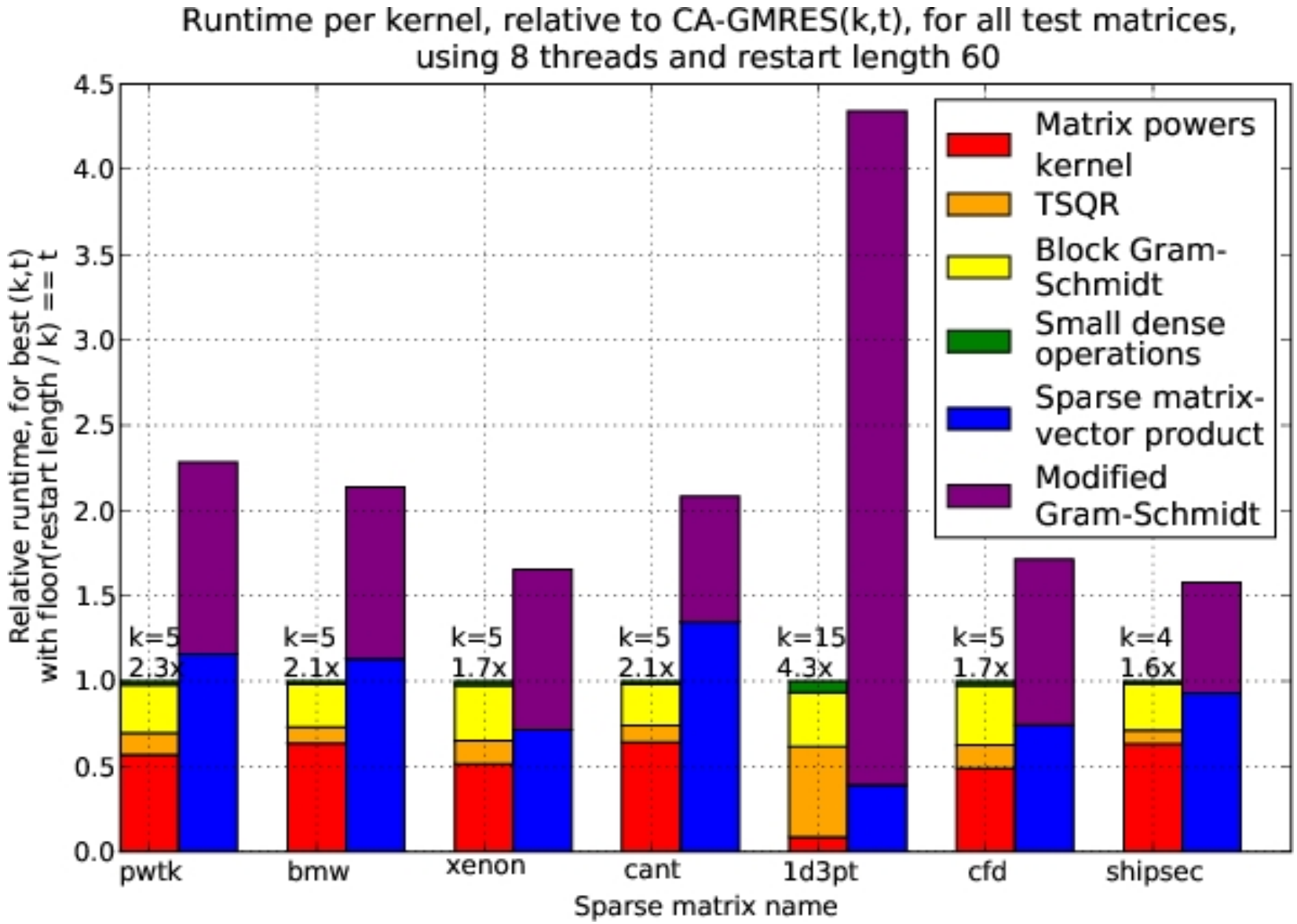


Performance

- Speedups on Intel Clovertown (8 cores), data from [Demmel et al., 2009]
- Used both optimizations:
  - sequential (moving data from DRAM to chip)
  - parallel (moving data between cores on chip)

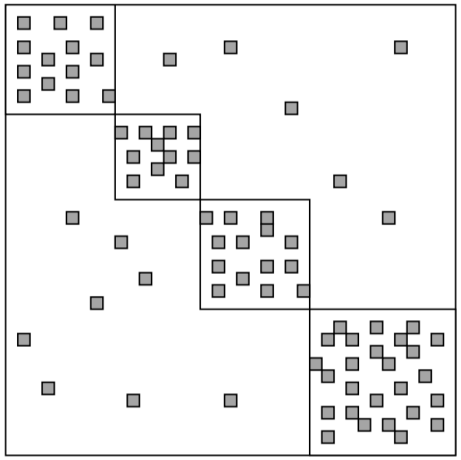


Performance (contd)



Enlarged Krylov methods [Grigori et al., 2014a]

- Partition the matrix into t domains
- split the residual r_{k-1} into t vectors corresponding to the t domains,



$$r_0 \rightarrow T(r_0) = \begin{bmatrix} * & 0 & & 0 \\ \vdots & \vdots & & \vdots \\ * & 0 & & 0 \\ 0 & * & & 0 \\ \vdots & \vdots & & \vdots \\ 0 & * & & 0 \\ & & \ddots & \\ 0 & 0 & & * \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & * \end{bmatrix}$$

- generate t new basis vectors, obtain an enlarged Krylov subspace

$$\mathscr{K}_{t,k}(A, r_0) \quad = \quad span\{T_s(r_0), AT_s(r_0), A^2 T_s(r0), ..., A^{k-1} T_s(r_0)\}$$

- search for the solution of the system $Ax = b$ in $\mathscr{K}_{t,k}(A, r_0)$

Properties of enlarged Krylov subspaces

- The Krylov subspace $\mathcal{K}_k(A, r_0)$ is a subset of the enlarged one

$$\mathcal{K}_k(A, r_0) \subset \mathscr{K}_{t,k}(A, r_0)$$

- For all $k < k_{max}$ the dimensions of $\mathscr{K}_{t,k}$ and $\mathscr{K}_{t,k+1}$ are stricltly increasing by some number i_k and i_{k+1} respectively, where

$$t \geq i_k \geq i_{k+1} \geq 1.$$

- The enlarged subspaces are increasing subspaces, yet bounded.

$$\mathscr{K}_{t,1}(A, r_0) \subsetneq \ldots \subsetneq \mathscr{K}_{t,k_{max}-1}(A, r_0) \subsetneq \mathscr{K}_{t,k_{max}}(A, r_0) = \mathscr{K}_{t,k_{max}+q}(A, r_0), \forall q > 0$$

Properties of enlarged Krylov subspaces: stagnation

- Let $\mathcal{K}_{p_{max}} = \mathcal{K}_{p_{max}+q}$ and $\mathscr{K}_{t,k_{max}} = \mathscr{K}_{t,k_{max}+q}$ for $q > 0$. Then

$$k_{max} \leq p_{max}.$$

- The solution of the system $Ax = b$ belongs to the subspace $x_0 + \mathscr{K}_{t,k_{max}}$.

Enlarged Krylov subspace methods based on CG

Defined by the subspace $\mathscr{K}_{t,k}$ and the following two conditions:

1. Subspace condition: $x_k \in x_0 + \mathscr{K}_{t,k}$
2. Orthogonality condition: $r_k \perp \mathscr{K}_{t,k}$

- At each iteration, the new approximate solution x_k is found by minimizing $\phi(x) = \frac{1}{2}(x)^t Ax - b^t x$ over $x_0 + \mathscr{K}_{t,k}$:

$$\phi(x_k) = min\{\phi(x), \forall x \in x_0 + \mathscr{K}_{t,k}(A, r_0)\}$$

Convergence analysis

Given

- A is an SPD matrix, x^* is the solution of $Ax = b$
- $||\overline{e}_k||_A = ||x^* - \overline{x}_k||_A$ is the k^{th} error of CG
- $||e_k||_A = ||x^* - x_k||_A$ is the k^{th} error of enlarged methods
- CG converges in $\overline{K}$ iterations

Result

Enlarged Krylov methods converge in K iterations, where $K \leq \overline{K} \leq n$.

$$||e_k||_A = ||x^* - x_k||_A \leq ||\overline{e}_k||_A$$

LRE-CG: Long Recurrence Enlarged CG

- Use the entire basis to approximate the new solution
- $Q_k = [W_1 W_2 \ldots W_k]$ is an $n \times tk$ matrix containing the basis vectors of $\mathscr{K}_{t,k}$
- At each k^{th} iteration, approximate the solution as

$$x_k = x_{k-1} + Q_k \alpha_k$$

such that

$$\phi(x_k) = min\{\phi(x), \forall x \in x_0 + \mathscr{K}_{t,k}\}$$

- Either x_k is the solution, or t new basis vectors and the new approximation $x_{k+1} = x_k + Q_{k+1}\alpha_{k+1}$ are computed.

Related work

- Block Krylov methods (O'Leary 1980): solve systems with multiple rhs

$$AX = B,$$

by searching for an approximate solution $X_k \in X_0 + \mathscr{K}_k(A, R_0)$,

$$\mathscr{K}_k(A, R_0) = block - span\{R_0, AR_0, A^2R_0, ..., A^{k-1}R_0\}.$$

- coopCG (Bhaya et al, 2012): solve one system by starting with t different initial guesses, equivalent to solving

$$AX = b * ones(1, t)$$

where X_0 is a block-vector containing the t initial guesses.

Classical CG *vs.* Enlarged CG derived from Block CG

Algorithm 2 Classic CG

$r_0 = b - Ax_0$
$p_1 = \frac{r_0}{\sqrt{r_0^t A r_0}}$
while $||r_{k-1}||_2 > \varepsilon ||b||_2$ **do**
  $\alpha_k = p_k^t r_{k-1}$
  $x_k = x_{k-1} + p_k \alpha_k$
  $r_k = r_{k-1} - A p_k \alpha_k$
  $p_{k+1} = r_k - p_k (p_k^t A r_k)$
  $p_{k+1} = \frac{p_{k+1}}{\sqrt{p_{k+1}^t A p_{k+1}}}$
end while

Algorithm 3 ECG(Odir)

$R_0 = T(b - Ax_0)$
$P_1 = \text{A-orthonormalize}(R_0)$
while $|| \sum_{i=1}^{t} R_k^{(i)} ||_2 < \varepsilon ||b||_2$ **do**
  $\alpha_k = P_k^t R_{k-1}$ ▷ $t \times t$
  $X_k = X_{k-1} + P_k \alpha_k$ ▷ $n \times t$
  $R_k = R_{k-1} - A P_k \alpha_k$ ▷ $n \times t$
  $P_{k+1} = AP_k - P_k(P_k^t AAP_k) - P_{k-1}(P_{k-1}^t AAP_k)$ ▷ $n \times t$
  $P_{k+1} = \text{A-orthonormalize}(P_{k+1})$
end while
$x = \sum_{i=1}^{t} X_k^{(i)}$ ▷ $n \times 1$

- EK-CG based on Orthodir (Lanczos formula) [Ashby et al., 1990]
- More stable than Orthomin [OLeary., 1980], $P_{k+1} = R_k - P_k(P_k^t A R_k)$.

Classical CG *vs.* Enlarged CG derived from Block CG

Algorithm 4 Classic CG

$r_0 = b - Ax_0$
$p_1 = \frac{r_0}{\sqrt{r_0^t A r_0}}$
while $||r_{k-1}||_2 > \varepsilon ||b||_2$ **do**
  $\alpha_k = p_k^t r_{k-1}$
  $x_k = x_{k-1} + p_k \alpha_k$
  $r_k = r_{k-1} - A p_k \alpha_k$
  $p_{k+1} = r_k - p_k (p_k^t A r_k)$
  $p_{k+1} = \frac{p_{k+1}}{\sqrt{p_{k+1}^t A p_{k+1}}}$
end while

messages per iteration
O(1) from SpMV +
O(log P) from dot prod + norm

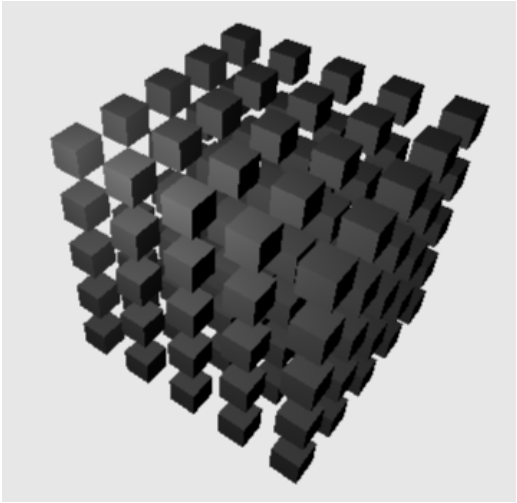
Algorithm 5 ECG(Odir)

$R_0 = T(b - Ax_0)$
$P_1 = \text{A-orthonormalize}(R_0)$
while $|| \sum_{i=1}^{t} R_k^{(i)} ||_2 < \varepsilon ||b||_2$ **do**
  $\alpha_k = P_k^t R_{k-1}$ ▷ $t \times t$
  $X_k = X_{k-1} + P_k \alpha_k$ ▷ $n \times t$
  $R_k = R_{k-1} - A P_k \alpha_k$ ▷ $n \times t$
  $P_{k+1} = AP_k - P_k(P_k^t AAP_k) - P_{k-1}(P_{k-1}^t AAP_k)$ ▷ $n \times t$
  $P_{k+1} = \text{A-orthonormalize}(P_{k+1})$
end while
$x = \sum_{i=1}^{t} X_k^{(i)}$ ▷ $n \times 1$

messages per iteration
O(1) from SpMV +
O(log P) from BCGS + A-ortho

Test cases: boundary value problem

3D Skyscraper Problem - SKY3D



$$
\begin{aligned}
-div(\kappa(x)\nabla u) &= f \ in\ \Omega \\
u &= 0 \ on\ \partial\Omega_D \\
\frac{\partial u}{\partial n} &= 0 \ on\ \partial\Omega_N
\end{aligned}
$$

discretized on a 3D grid , where

$$
\kappa(x) = \begin{cases} 10^3 * ([10 * x_2] + 1), if\ [10 * x_i] = 0 mod(2),\ i = 1, 2, 3, \\ 1, \qquad\qquad\qquad\qquad\qquad\qquad otherwise. \end{cases}
$$

3D Anisotropic layers - ANI3D

- Ω divided into 10 layers parallel to $z = 0$, of size 0.1
- in each layer, the coefficients are constants (κ_x equal to 1, 10^2 or 10^4, $\kappa_y = 10\kappa_x$, $\kappa_z = 1000\kappa_x$).

Test cases (contd)

Linear elasticity 3D problem

$$
\begin{aligned}
\operatorname{div}(\sigma(u)) + f &= 0 && \text{on } \Omega, \\
u &= u_D && \text{on } \partial\Omega_D, \\
\sigma(u) \cdot n &= g && \text{on } \partial\Omega_N,
\end{aligned}
$$

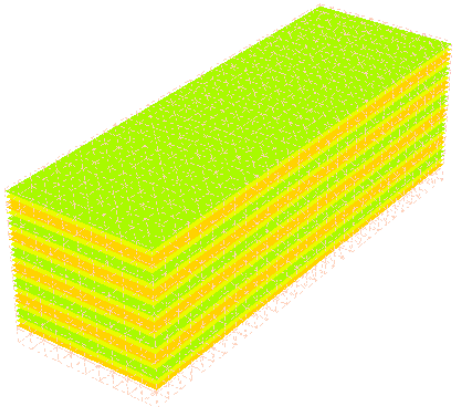


Figure : The distribution of Young's modulus

- $u \in \mathbb{R}^d$ is the unknown displacement field, f is some body force.
- Young's modulus E and Poisson's ratio ν take two values, $(E_1, \nu_1) = (2 \cdot 10^{11}, 0.25)$, and $(E_2, \nu_2) = (10^7, 0.45)$.
- Cauchy stress tensor $\sigma(u)$ is given by Hooke's law, defined by E and ν.

Test cases

Matrices

Generated with FreeFem++.

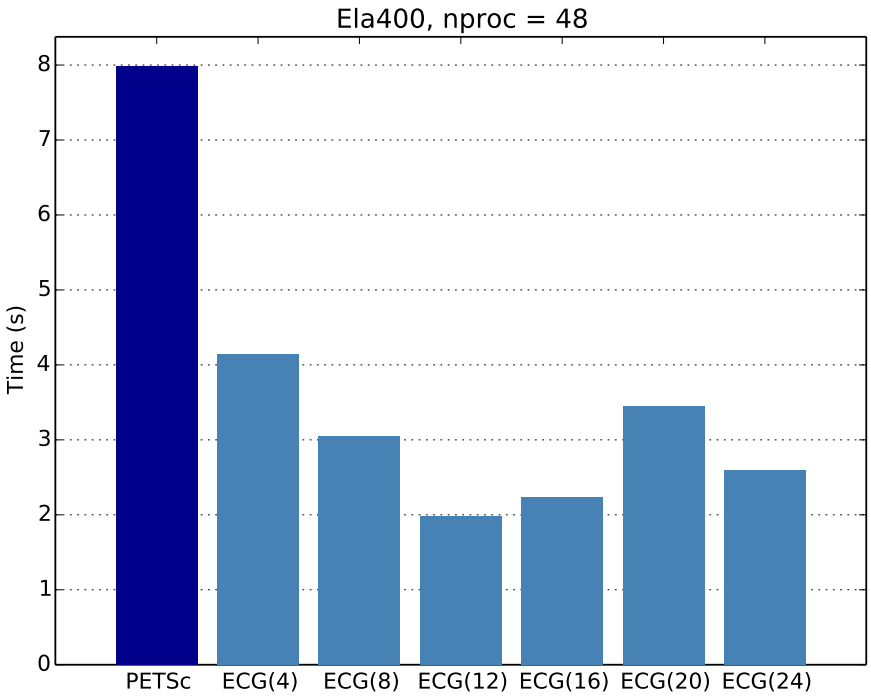
matrix	$n(A)$	$nnz(A)$	Description
SKY3D	8000	53600	Skyscraper
ANI3D	8000	53600	Anisotropic Layers
ELAST3D	11253	373647	Linear Elasticity P1 FE

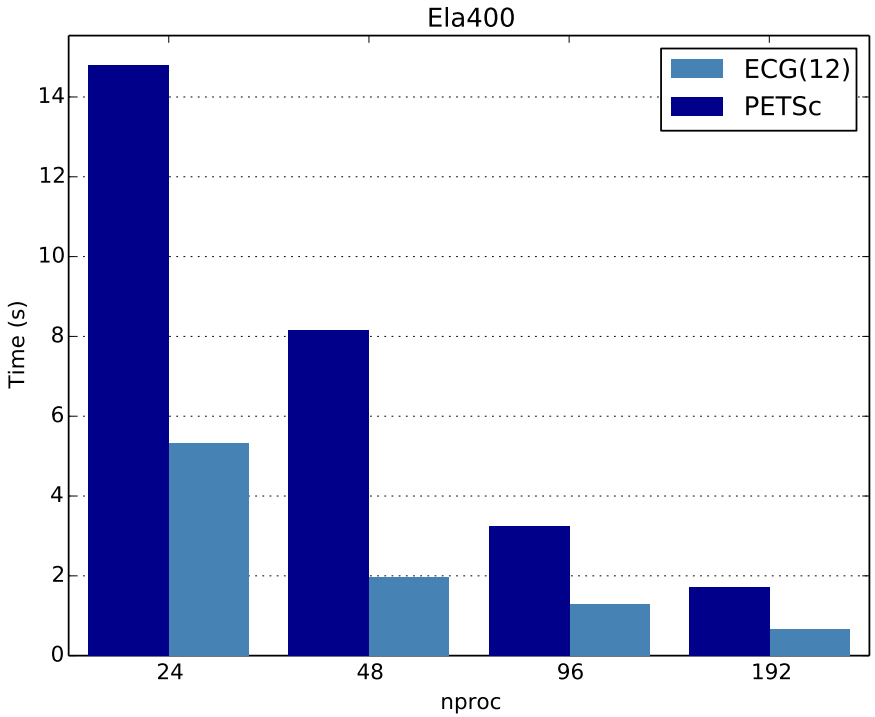
Convergence of different CG versions

Pa	CG Iter	CG Err	SRE-CG Iter	SRE-CG Err
SKY3D				
8	902	1E-5	211	1E-5
16	902	1E-5	119	9E-6
32	902	1E-5	43	4E-6
ANI3D				
2	4187	4e-5	875	7e-5
4	4146	4e-5	673	8e-5
8	4146	4e-5	449	1e-4
16	4146	4e-5	253	2e-4
32	4146	4e-5	148	2e-4
64	4146	4e-5	92	1e-4
ELAST3D				
2	1098	1e-7	652	1e-7
4	1098	1e-7	445	1e-7
8	1098	1e-7	321	8e-8
16	1098	1e-7	238	4e-8
32	1098	1e-7	168	5e-8
64	1098	1e-7	116	1e-8

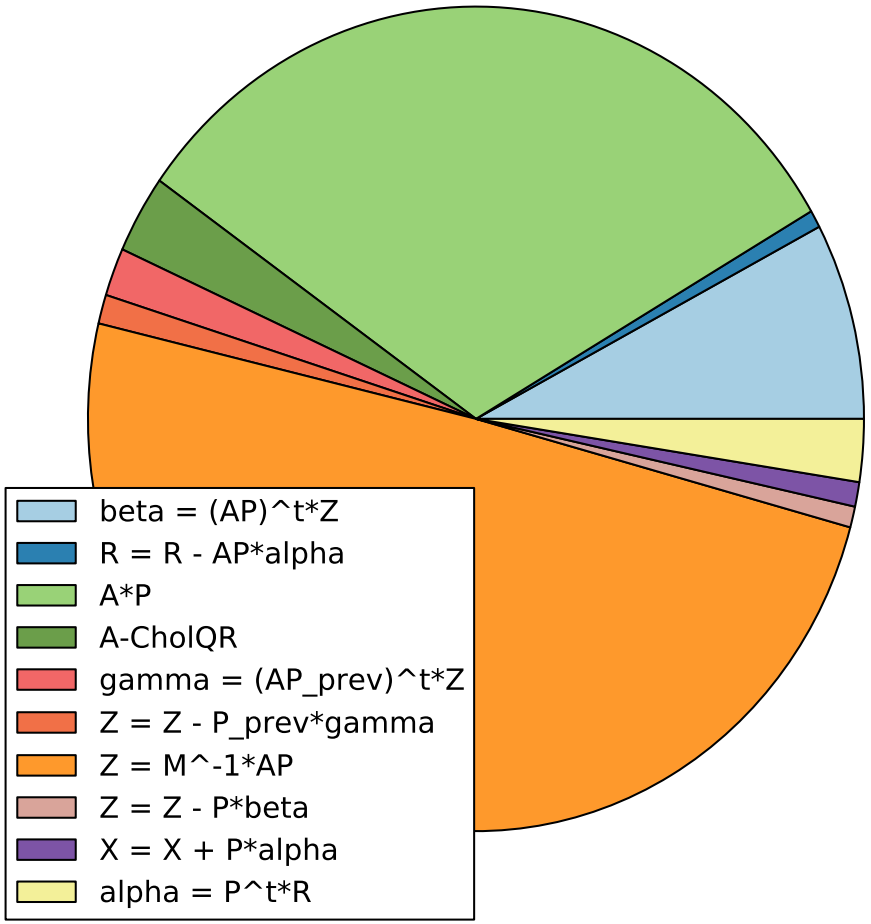
Comparison with PETSc

- Run on MeSU (UPMC cluster) $\rightarrow$ 24 cpus by node
- Compiled with Intel Suite 15, Petsc 3.7.4
- Results from [Grigori and Tissot, 2017]





Detailed profiling (source slide O. Tissot)



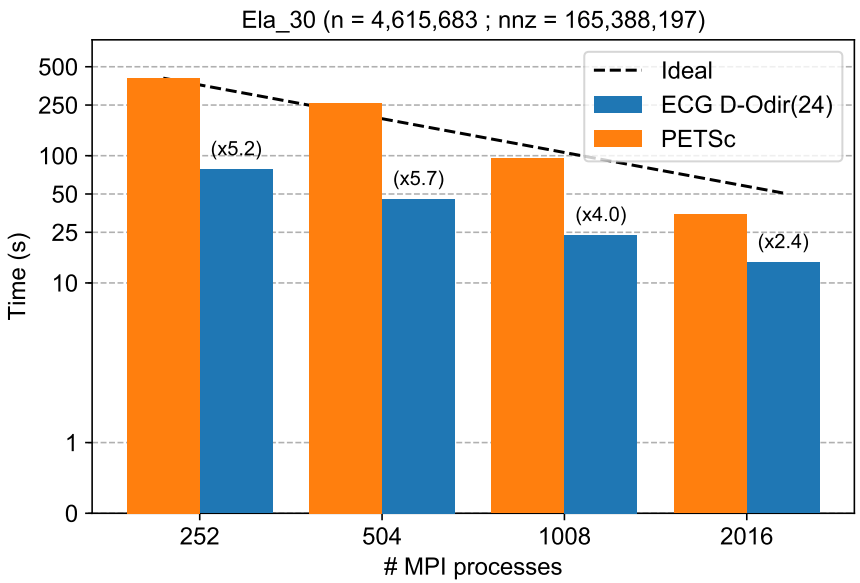
- Ela400 on 96 cores
- Orthodir ECG(12)
- Around 50% of the time spent in applying the preconditioner
- Around 30% of the time spent in Sparse Matrix-Matrix

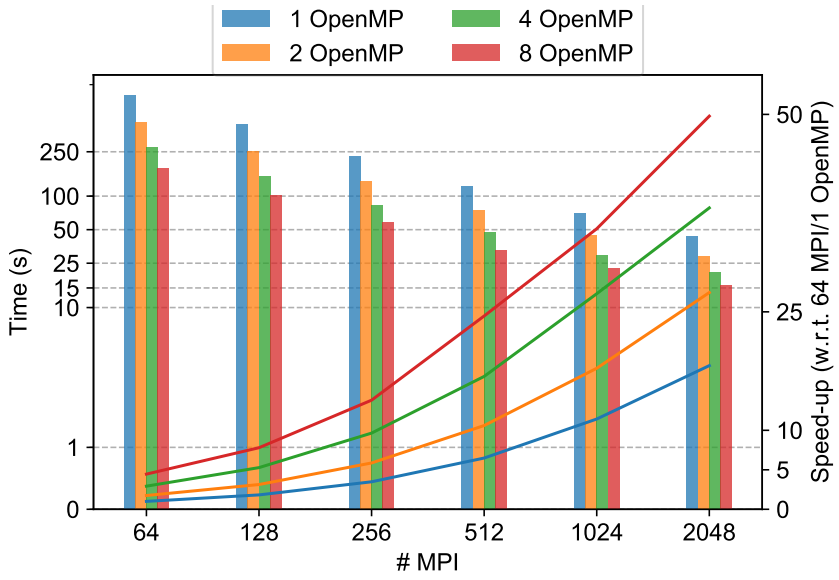
Method	iter	time (s)	time/iter
ECG(12)	318	1.3	4.1×10^{-3}
PETSc	5198	3.3	6.3×10^{-4}

Table : Comparison with PETSc PCG. PETSc iteration is 6.5 times faster than ECG(12) one. MKL-Pardiso has a strange behaviour with multiple rhs n our experiments: 1 rhs solve is 3 times faster than 2 rhs solve.

Comparison with PETSc

- Run on MeSU (UPMC cluster) $\rightarrow$ 24 cpus by node
- Compiled with Intel Suite 15, Petsc 3.7.4
- Results from [Grigori and Tissot, 2017]





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