Krylov subspace methods and preconditioners

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Plan

Sparse linear solvers
- Sparse matrices and graphs
- Classes of linear solvers

Krylov subspace methods
- Conjugate gradient method

Enlarged Krylov methods
- Definition and properties
- Numerical and parallel performance results

Preconditioned Krylov subspace methods
- One level Additive Schwarz methods
- Two level preconditioners

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.

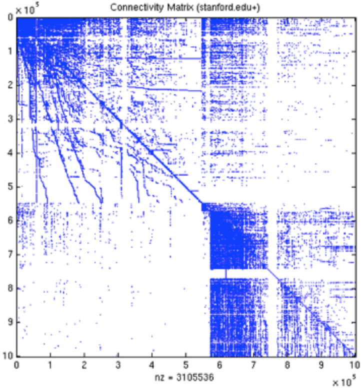


Figure: Nonzero structure of the matrix

Sparse matrices and graphs

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

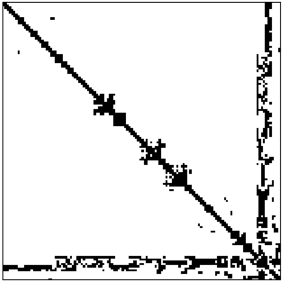


Figure: Nonzero structure of the matrix

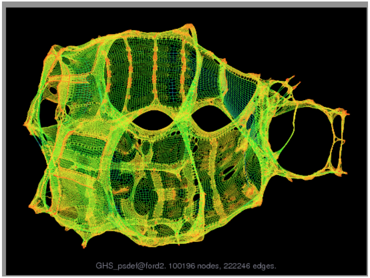


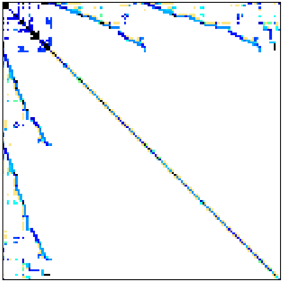
Figure: Its undirected graph

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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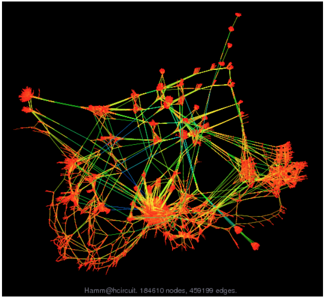

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Sparse linear solvers

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

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: $r_k \perp \mathscr{L}_k$

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

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.

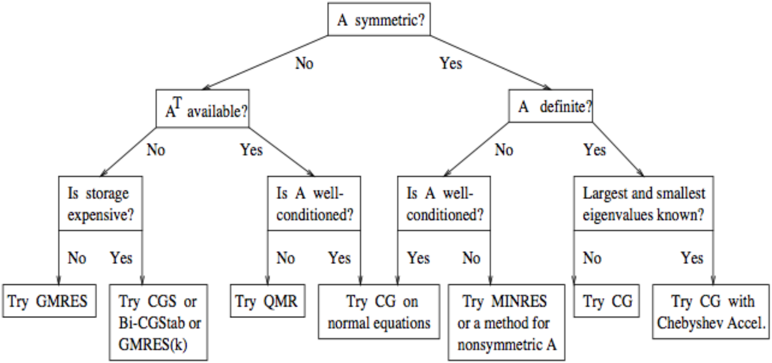
One of Top Ten Algorithms of the 20th Century

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

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

- After j iterations of CG,

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

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

$$\begin{cases} p_1 & = & r_0 = -\bigtriangledown \phi(x_0) \\ p_k & = & r_{k-1} + \beta_k p_{k-1} \end{cases} \quad (2)$$

- At k-th iteration,

$$\begin{aligned} p_k &= r_{k-1} + \beta_k p_{k-1} && (3) \\ x_k &= x_{k-1} + \alpha_k p_k = argmin_{x \in x_0 + \mathcal{K}_k(A, r_0)} \phi(x) && (4) \\ r_k &= r_{k-1} - \alpha_k A p_k && (5) \end{aligned}$$

where α_k is the step along p_k.

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

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

CG derivation

Since we have $x_k = x_{k-1} + \alpha_k p_k$ we obtain

$$r_k = r_{k-1} - \alpha_k A p_k \text{ and } (r_k, r_{k-1}) = 0 \text{ hence}$$
$$r_{k-1}^T r_{k-1} - \alpha_k r_{k-1}^T A p_k = 0 \implies \alpha_k = \frac{(r_{k-1}, r_{k-1})}{(Ap_k, r_{k-1})}$$

Since we have $p_k = r_{k-1} + \beta_k p_{k-1}$,

$$(Ap_k, r_{k-1}) = (Ap_k, p_k - \beta_k p_{k-1}) = (Ap_k, p_k) \implies \alpha_k = \frac{(r_{k-1}, r_{k-1})}{(Ap_k, p_k)}$$

Since $p_k = r_{k-1} + \beta_k p_{k-1}$ is A-orthogonal to p_{k-1} we obtain

$$\beta_k = -\frac{(r_{k-1}, Ap_{k-1})}{(p_{k-1}, Ap_{k-1})} \text{ and } Ap_{k-1} = \frac{1}{\alpha_{k-1}}(r_{k-1} - r_k) \implies \beta_k = \frac{(r_{k-1}, r_{k-1})}{(r_{k-2}, r_{k-2})}$$

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
  $\alpha_k = (r_{k-1}, r_{k-1})/(Ap_k, p_k)$
  $x_k = x_{k-1} + \alpha_k p_k$
  $r_k = r_{k-1} - \alpha_k A p_k$
  $\rho_k = ||r_k||_2^2$
  $k = k + 1$
end while

Properties of CG

- The directions $p_1, \ldots p_n$ are A-conjugate, the following properties are satisfied:

$$\begin{aligned} (Ap_k, p_j) &= 0, \text{ for all } k, j, k \neq j \\ (r_k, r_j) &= 0, \text{ for all } k, j, k \neq j \\ (p_k, r_j) &= 0, \text{ for all } k, j, k < j \end{aligned}$$

- The Krylob subspace is spanned by the residuals and the search directions:

$$\mathcal{K}_k(A, r_0) = \text{span}\{r_0, r_1, ..., r_{k-1}\} = \text{span}\{p_0, p_1, ..., p_{k-1}\}$$

Adviced exercice: prove the above relations, e.g. by using recurrence on equations (3), (4), (5).
We do not prove (4) and (1), the proofs are not required for the exam. The proofs can be found in [Saad, 2003]

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

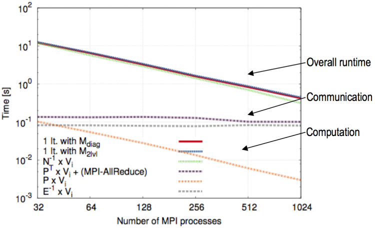
$$\mathcal{K}_{k+1}(A, r_0) = span\{r_0, Ar_0, A^2 r_0, ..., A^k r_0\},$$

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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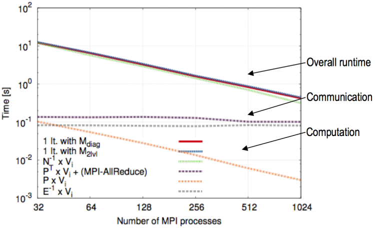

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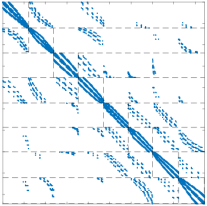
Ways to improve performance

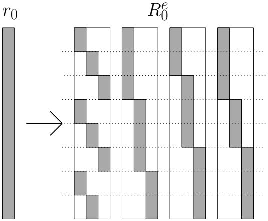
- Improve the performance of sparse matrix-vector product.
- Improve the performance of collective communication.
- Change numerics - reformulate or introduce Krylov subspace algorithms to:
  - reduce communication,
  - increase arithmetic intensity - compute sparse matrix-set of vectors product.
- Use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

Plan

Enlarged Krylov methods [LG, Moufawad, Nataf, 14]

- Partition the matrix into N domains
- Split the residual r_0 into t vectors corresponding to the N domains, obtain R_0^e,





- Generate t new basis vectors, obtain an **enlarged** Krylov subspace

$$\mathcal{K}_{t,k}(A, r_0) = \text{span}\{R_0^e, AR_0^e, A^2 R_0^e, ..., A^{k-1} R_0^e\}$$

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

Properties of enlarged Krylov subspaces

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

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

- For all $k < k_{max}$ the dimensions of $\mathcal{K}_{t,k}$ and $\mathcal{K}_{t,k+1}$ 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.

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

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

Enlarged Krylov subspace methods based on CG

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

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

- 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 $x_0 + \mathcal{K}_{t,k}$:

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

- Can be seen as a particular case of a block Krylov method
  - $AX = S(b)$, such that $S(b)ones(t,1) = b$; $R_0^e = AX_0 - S(b)$
  - Orthogonality condition involves the block residual $R_k \perp \mathcal{K}_{t,k}$

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Related work

- Block Krylov methods [O'Leary, 1980]: solve systems with multiple rhs

$$AX = B,$$

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

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

  - coopCG (Bhaya et al, 2012): solve one system by starting with t different initial guesses
  - BRRHS-CG [Nikishin and Yeremin, 1995]: use a block method with t-1 random right hand sides

- Multiple preconditioners
  - GMRES with multiple preconditioners [Greif, Rees, Szyld, 2011]
  - AMPFETI [Rixen, 97], [Gosselet et al, 2015]

- And to reduce communication: s-step methods, pipelined methods

Convergence analysis

Given

- A is an SPD matrix, x^* is the solution of $Ax = b$
- $||x^* - \overline{x}_k||_A$ is the k^{th} error of CG
- $||x^* - x_k||_A$ is the k^{th} error of ECG

Result

CG

$$||x^* - \overline{x}_k||_A \leq 2||x^* - x_0||_A \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k$$

where $\kappa = \frac{\lambda_{max}(A)}{\lambda_{min}(A)}$

ECG

$$||x^* - x_k||_A \leq C||x^* - x_0||_A \left(\frac{\sqrt{\kappa_t}-1}{\sqrt{\kappa_t}+1}\right)^k$$

where $\kappa_t = \frac{\lambda_{max}(A)}{\lambda_t(A)}$

C is a const indpdt. of k, dpdt. of t

From here on, results on ECG obtained with O. Tissot.
Proof of convergence of ECG not required for exam, it can be found in [Grigori and Tissot, 2019].

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

Algorithm 2 Classical CG

$p_1 = r_0(r_0^\top A r_0)^{-1/2}$
while $||r_{k-1}||_2 > \varepsilon ||b||_2$ **do**
    $\alpha_k = p_k^\top r_{k-1}$
    $x_k = x_{k-1} + p_k \alpha_k$
    $r_k = r_{k-1} - A p_k \alpha_k$
    $z_{k+1} = r_k - p_k(p_k^\top A r_k)$
    $p_{k+1} = z_{k+1}(z_{k+1}^\top A z_{k+1})^{-1/2}$
end while

Cost per iteration

$\#$ flops $= O(\frac{n}{P}) \leftarrow$ BLAS 1 & 2
$\#$ words $= O(1)$
$\#$ messages $= O(1)$ from SpMV $+$ $O(logP)$ from dot prod $+$ norm

Algorithm 3 ECG

$P_1 = R_0^e(R_0^{e\top} A R_0^e)^{-1/2}$
while $|| \sum_{i=1}^{\top} R_k^{(i)} ||_2 < \varepsilon ||b||_2$ **do**
    $\alpha_k = P_k^\top R_{k-1}$ ▷ $t \times t$ matrix
    $X_k = X_{k-1} + P_k \alpha_k$
    $R_k = R_{k-1} - A P_k \alpha_k$
    Construct Z_{k+1} s.t. $Z_{k+1}^\top A P_i = 0, \forall i \leq k$
    $P_{k+1} = Z_{k+1}(Z_{k+1}^\top A Z_{k+1})^{-1/2}$
end while
$x = \sum_{i=1}^{\top} X_k^{(i)}$

Cost per iteration

$\#$ flops $= O(\frac{nt^2}{P}) \leftarrow$ BLAS 3
$\#$ words $= O(t^2) \leftarrow$ Fit in the buffer
$\#$ messages $= O(1)$ from SpMV $+$ $O(logP)$ from A-ortho

Construction of the search directions P_{k+1}

1 Construct Z_{k+1} s.t. $Z_{k+1}^\top AP_i = 0$, $\forall i \leq k$ by using:

1.a **Orthomin** as in block CG [O'Leary., 1980] and original CG method [Hestenes and Stiefel., 1952]:

$$Z_{k+1} = R_k - P_k(P_k^\top AR_k)$$

1.b or **Orthodir** as in ECG [Grigori et al., 2016], based on Lanczos formula [Ashby et al., 1990]:

$$Z_{k+1} = AP_k - P_k(P_k^\top AAP_k) - P_{k-1}(P_{k-1}^\top AAP_k)$$

2 A-orthonormalize P_{k+1}, using e.g. A Cholesky QR:

$$P_{k+1} = Z_{k+1}(Z_{k+1}^\top AZ_{k+1})^{-1/2}$$

Orthomin (Omin)	**Orthodir (Odir)**
→ Cheaper	→ More expensive
→ In practice breakdowns	→ In practice no breakdowns

Orthomin (Omin) versus Orthodir (Odir)

Both rely on same projection process

- $\hat{X}_k = \tilde{X}_k$ and $\hat{R}_k = \tilde{R}_k$
- !! $\hat{P}_k \neq \tilde{P}_k$ and $\hat{Z}_k \neq \tilde{Z}_k$

- With a tilde $\rightarrow$ Omin variables
- With a hat $\rightarrow$ Odir variables

Proposition

Assume no breakdown occurred, then there exists orthogonal matrix δ_k st:

$$\tilde{P}_k = \hat{P}_k \delta_k$$

$$\tilde{Z}_{k+1} = -\hat{Z}_{k+1} \delta_k \tilde{\alpha}_k, \text{ where } \tilde{\alpha}_k = \tilde{P}_k^T \tilde{R}_{k-1}$$

- Generalization of result in [Ashby et al., 1990]; explicit link between Lanczos and CG
- When k is large, $||\tilde{\alpha}_k||_2$ becomes small, hence $||\tilde{Z}_{k+1}||_2 < ||\hat{Z}_{k+1}||_2$
- The conditioning of $\tilde{Z}_{k+1}^\top A \tilde{Z}_{k+1}$ can be worse than that of $\hat{Z}_{k+1}^\top A \hat{Z}_{k+1}$!

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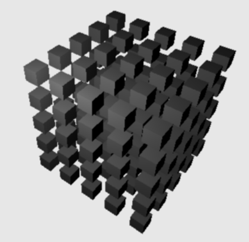
Test cases: boundary value problem

2D and 3D Skyscraper Problem - SKY2D,3D



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

discretized on a 3D grid , where

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

Test cases (contd)

Linear elasticity 3D problem

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

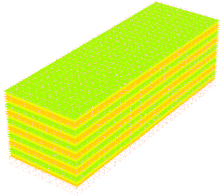


Figure: The distribution of Young's modulus

- $u \in \mathbb{R}^d$ 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.

Matrices Generated with FreeFem++ (F. Hecht, Sorbonne Université)
Linear Elasticity discretized using $\mathbb{P}_1$ FE, $1600 \times Y \times Y$ grid

Enlarged CG: numerical results

- Block Jacobi preconditioner (1024 blocks)
- Stopping criterion 10^{-6}, initial block size 32
- BRRHS-CG: block method with $t-1$ random rhs

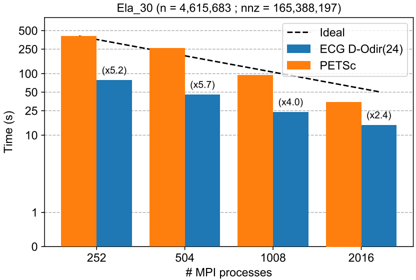
matrix	$n(A)$	$nnz(A)$
SKY2D	10,000	49,600
Ela3D100	36,663	1,231,497
Ela2D200	80,802	964,800

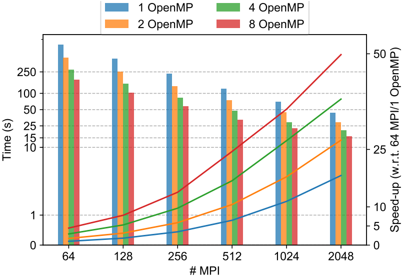
		PCG	BRRHS-CG		ECG	
	red. size	iter	iter	$\dim(\mathcal{K}_{32,k})$	iter	$\dim(\mathcal{K}_{32,k})$
SKY2D	×	655	61	1952	57	1824
	✓	655	61	1739	59	1546
Ela3D100	×	955	102	3264	109	3488
	✓	955	102	3093	116	2384
Ela2D200	×	4551	255	8160	253	8096
	✓	4551	258	7331	266	6553

Enlarged CG: parallel performance

- Stopping criterion 10^{-5}, blocks Jacobi = #MPI
- Performance study on:
  – Kebnekaise (Suede), Intel Xeon (Broadwell), 28 MPI process/node
  – Cori NERSC, Intel KNL, 68 cores each

	D-Odir(24)		CG	
# MPI	# iter	res	# iter	res
252	513	1.3E-4	13,626	1.3E-4
504	531	1.9E-4	15,819	1.9E-4
1,008	606	2.6E-4	17,023	2.7E-4
2,016	696	2.6E-4	19,047	2.7E-4





Plan

Sparse linear solvers

Krylov subspace methods

Enlarged Krylov methods

Preconditioned Krylov subspace methods
- One level Additive Schwarz methods
- Two level preconditioners

Preconditioned Krylov subspace methods

- Solve by using iterative methods

$$Ax = b.$$

- Convergence depends on $\kappa(A)$ and the eigenvalue distribution (for SPD matrices).
- To accelerate convergence, solve

$$M^{-1}Ax = M^{-1}b,$$

where
  - M approximates well the inverse of A and/or
  - improves $\kappa(A)$, the condition number of A.
- Ideally, we would like to bound $\kappa(A)$, independently of the size of the matrix A.

Additive Schwarz: notations

Solve $M^{-1}Ax = M^{-1}b$, where $A \in \mathbb{R}^{n \times n}$ is SPD

For $\mathcal{N} = \{1, \ldots, n\}$, let $\mathcal{N}_i \subset \mathcal{N}$ for $i = 1 \ldots N$ be the subset of DOF of subdomain i, referred to as Ω_i, possibly with overlap. We define:

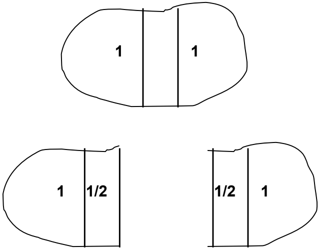
- The restriction operator $R_i \in \mathbb{R}^{n_i \times n}$, $R_i = I_n(\mathcal{N}_i, :)$.
- The prolongation operator, $R_i^T \in \mathbb{R}^{n \times n_i}$

- The matrix associated to domain i, $A_i \in \mathbb{R}^{n_i \times n_i}$,

$$A_i = R_i A R_i^T$$

- The algebraic partition of unity $(D_i)_{1 \le i \le N}$,

$$I_n = \sum_{i=1}^{N} R_i^T D_i R_i$$



Additive and Restrictive Additive Schwarz methods

- Original idea from Schwarz algorithm at the continuous level (Schwarz 1870)
- Restricted Additive Schwarz (Cai & Sarkis 1999) defined as

$$M_{RAS}^{-1} := \sum_{i=1}^{N} R_i^T D_i A_i^{-1} R_i$$

- Symmetric formulation, Additive Schwarz (1989) defined as

$$M_{AS}^{-1} := \sum_{i=1}^{N} R_i^T A_i^{-1} R_i$$

- In practice, RAS more efficient than AS

Two level preconditioners

Given a coarse subspace $V_0 \in \mathbb{R}^{n \times n_0}$ and Z its basis, $V_0 = \text{span } Z$, let $R_0 = Z^T$, the coarse grid $R_0 A R_0^T$.
The two level AS preconditioner is

$$M_{AS,2}^{-1} := R_0^T \left(R_0 A R_0^T\right)^{-1} R_0 + \sum_{i=1}^{N} R_i^T \left(A_i\right)^{-1} R_i$$

Let k_c be minimum number of distinct colors so that $\left(span\{R_i^T\}\right)_{1 \le i \le N}$ of the same color are mutually A-orthogonal. The following holds (e.g. Chan and Mathew 1994)

$$\lambda_{max}(M_{AS,2}^{-1} A) \le k_c + 1$$

Convergence theory

Results from e.g. [Chan and Mathew, 1994, Dolean et al., 2015].

$$M_{AS,2}^{-1}A := \sum_{i=0}^{N} R_i^T (A_i)^{-1} R_i A = \sum_{i=0}^{N} P_i, \text{ where } P_i = R_i^T (A_i)^{-1} R_i A$$

P_i are orthogonal projection matrices in the A inner product since

$$\begin{aligned} P_i P_i &= R_i^T (A_i)^{-1} R_i A R_i^T (A_i)^{-1} R_i A = R_i^T (A_i)^{-1} R_i A = P_i \\ A P_i &= A R_i^T (A_i)^{-1} R_i A = P_i^T A \end{aligned}$$

Recall that $a(u,v) = v^T A u$ and $||P_i|| \leq 1$.

$$\begin{aligned} \lambda_{max}(M_{AS,2}^{-1}A) &= \sup_{u \in \mathbb{R}^n} \frac{a(M_{AS,2}^{-1}Au, u)}{a(u,u)} \\ &= \sup_{u \in \mathbb{R}^n} \sum_{i=0}^{N} \frac{a(P_i u, u)}{||u||_a^2} = \sup_{u \in \mathbb{R}^n} \sum_{i=0}^{N} \frac{a(P_i u, P_i u)}{||u||_a^2} \\ &\leq \sum_{i=0}^{N} \sup_{u \in \mathbb{R}^n} \frac{a(P_i u, P_i u)}{||u||_a^2} \leq N+1 \end{aligned}$$

Convergence theory (contd)

If we define a-orthogonal projectors

$$\tilde{P}_i = \sum_{j \in \Theta_i} P_j, \text{ for } i = 1, \dots k_c$$

where Θ_i is a set of indices with the same color (that is the indices denoting disjoint subdomains). We can apply the same reasoning and obtain

$$\lambda_{max}(M_{AS,2}^{-1} A) \leq k_c + 1$$

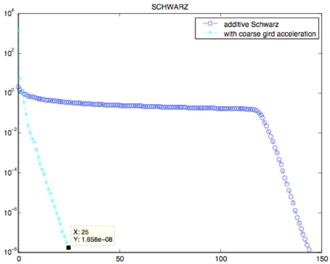
How to compute the coarse subspace $V_0 = \text{span } Z$

- Nicolaides 87 (CG): kernel of the operator (constant vectors) for a Poisson like problem works well

$$Z \quad := \quad \left(R_i^T D_i R_i 1\right)_{i=1:N}$$

Z defined as in (Nicolaides 1987):

$$Z = \begin{pmatrix} 1_{\Omega_1} & & & \\ & 1_{\Omega_2} & & \\ & & \ddots & \\ & & & 1_{\Omega_N} \end{pmatrix}$$



Courtesy of F. Nataf

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- Other early references: [Morgan 92] (GMRES), [Chapman, Saad 92], [Kharchenko, Yeremin 92], [Burrage, Ehrel, and Pohl, 93]
- Estimations of eigenvectors corresponding to smallest eigenvalues / knowledge from the physics
- Geneo [Nataf, Spillane et al]: through solving local Gen EVPs, bounds smallest eigenvalue for standard FE and bilinear forms, SPD input matrix

subd	dofs	AS	AS-ZEM (V_0)	GenEO (V_0)
4	1452	79	54 (24)	16 (46)
8	29040	177	87 (48)	16 (102)
16	58080	378	145 (96)	16 (214)

V_0: size of the coarse space
AS-ZEM Nicolaides with rigid body motions, 6 per subd
Results for 3D elasticity problem provided by F. Nataf

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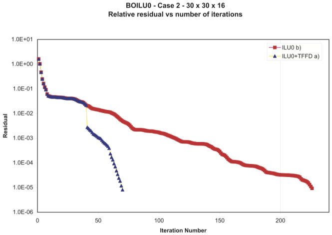
The need for two level preconditioners

- When solving complex linear systems arising, e.g. from large discretized systems of PDEs with strongly heterogeneous coefficients (high contrast, multiscale).

  - Flow in porous media
  - Elasticity problems
  - CMB data analysys (no PDE)



- Most of the existing preconditioners lack robustness
  - wrt jumps in coefficients / partitioning into irregular subdomains, e.g. one level DDM methods (block Jacobi, RAS), incomplete LU
  - A few small eigenvalues hinder the convergence of iterative methods

Using deflation to deal with low frequency modes

In the unified framework of [Tang et al., 2009], let :

$$P := I - AZE^{-1}Z^T, \quad E := Z^T AZ$$

where

- Z is the deflation subspace matrix of full rank
- E is the coarse grid correction, a small dense invertible matrix
- P is the deflation matrix, $PAZ = 0$

Usage in different classes of preconditioners

- DDM - Z and Z^T are the restriction and prolongation operators based on subdomains, E is a coarse grid, P is a subspace correction
- Deflation - Z contains the vectors to be deflated
- Multigrid - interpretation possible

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Example of preconditioner

$$P_{2lvl}^{-1} = M^{-1}P + ZE^{-1}Z^T,$$

where M is the first level preconditioner (eg based on block Jacobi).

- $P_{2lvl}^{-1}AZ = Z$
- The small eigenvalues are shifted to 1.
- P_{2lvl} is not SPD, even when A is, better choices available, but more expensive.

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Two level preconditioners (contd)

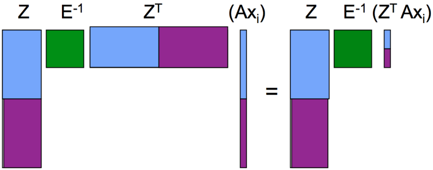
Computing the preconditioner requires

- Deflation subspace Z, which can be formed by
  - Eigenvectors corresponding to smallest eigenvalues - from previous linear systems solved with different right hand sides, etc.
  - Using knowledge from the physics, partition of the unity, etc.
- Computing AZ and $E = Z^T AZ$.

Applying the preconditioner at each iteration requires

- Computing $y = ZE^{-1}Z^T(Ax_i) = ZE^{-1}Z^Tv$

  $\Rightarrow$ involves collective communication when computing Z^Tv, and solving a linear system with E.



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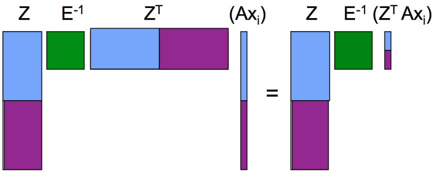

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