

Spectral Schur complement techniques for symmetric eigenvalue problems

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Supercomputing Institute

- 1 Introduction
- 2 The domain decomposition framework
- 3 Solving the spectral Schur complement eigenvalue problem
 - Computing more than one eigenpairs
- 4 Experiments
- 5 Conclusion

Introduction

The symmetric eigenvalue problem

$$Ax^{(i)} = \lambda_i x^{(i)}, \quad i = 1, \dots, n,$$

where $A \in \mathbb{R}^{n \times n}$ is symmetric, $x^{(i)} \in \mathbb{R}^n$ and $\lambda_i \in \mathbb{R}$. A pair $(\lambda_i, x^{(i)})$ is an *eigenpair* of A .

Focus

- 1 Compute, up to a tolerance tol , all eigenpairs $(\lambda_i, x^{(i)})$ located inside the interval $[\alpha, \beta]$ where $\alpha, \beta \in \mathbb{R}$ and $\lambda_1 \leq \alpha, \beta \leq \lambda_n$.
- 2 Given a shift $\zeta \in \mathbb{R}$, find the k (λ, x) pairs closest to ζ .

How to compute a few eigenpairs of A ?

- 1 Typically: Lanczos on A or $\rho(A - \sigma I)$, $\sigma \in \mathbb{C}$
- 2 In this talk we consider Schur complement eigenvalue solvers

Schur complement eigenvalue solvers (I)

Block matrix representation

Consider matrix A written as

$$A = \begin{pmatrix} B & E \\ E^T & C \end{pmatrix}$$

where $B \in \mathbb{R}^{d \times d}$, $E \in \mathbb{R}^{d \times s}$ and $C \in \mathbb{R}^{s \times s}$, $n = d + s$.

Let $x = [u^T, y^T]^T$, $u \in \mathbb{R}^d$, $y \in \mathbb{R}^s$, assume $\lambda \notin \Lambda(B)$

Solution of $(A - \lambda I)x = 0$ is transformed to:

- 1 Solve $(B - \lambda I)u = -Ey$
- 2 Solve $S(\lambda)y = 0$

where

$$S(\lambda) = C - \lambda I - E^T(B - \lambda I)^{-1}E,$$

is the **spectral Schur complement matrix**

Some references on spectral Schur complements

- Component Mode Synthesis and Automated Multi-Level Substructuring (AMLS) [BeLe] for the analysis of frequency response
 - Substructuring techniques (domain decomposition)
 - Approximate y by linearizing $S(\lambda) \rightarrow$ Generalized eig. problem with pencil $(S(0), S'(0))$
 - Approximate u by approximating $-(B - \lambda I)^{-1} E y$
 - Perform a Rayleigh-Ritz projection
 - AMLS is a multilevel extension of CMS (combined with mode truncation)
 - Typically: fast computation but modest accuracy
- Other work: Abramov and Chishov (spectral Schur complements), Lui (Kron's method),...

Not Schur complement based, but of similar nature

Hybridized Raviart-Thomas approximation of 2nd order elliptic eigenvalue problems [Coc]

- The original eigenvalue problem is condensed by hybridization
- Result: transformation to a non-linear, but smaller eigenvalue problem
- Lower energy modes can be recovered accurately
- Solving the non-linear eigenvalue problem:
 - First solve a perturbed (linearized) version to obtain accurate approximations
 - Exploit Newton's method (or RQI) to refine each approximate eigenvalue

HDG approximation of 2nd order elliptic eigenvalue problems [Gop]

- Similar framework with the Raviart-Thomas approximation
- Covers a narrower effective spectrum but can be benefited by postprocessing

In this talk we concentrate on Schur complement eigenvalue solvers from a **domain decomposition** viewpoint and contribute:

- 1 A numerical scheme based on Newton root-finding procedures
- 2 An extension of current understanding regarding Schur complement eigenvalue solvers
- 3 An implementation of the proposed scheme in distributed computing environments

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Partitioning of the domain (Metis, Scotch,...)

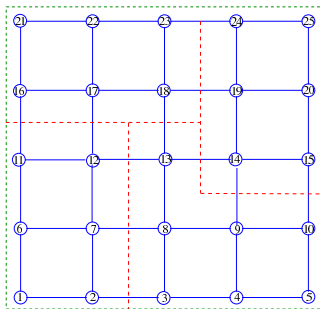


Figure: An edge-separator

- Goal: Partition a discretized domain in p subdomains
- Two main approaches to partition a graph:
 - Edge-separator (vertex-based partitioning)
 - Vertex-separator (edge-based partitioning)
- After partitioning, three types of unknowns:
 - interior unknowns
 - local interface unknowns
 - external interface unknowns
- The i 'th subdomain has d_i interior unknowns and s_i local interface unknowns

The local viewpoint in each subdomain

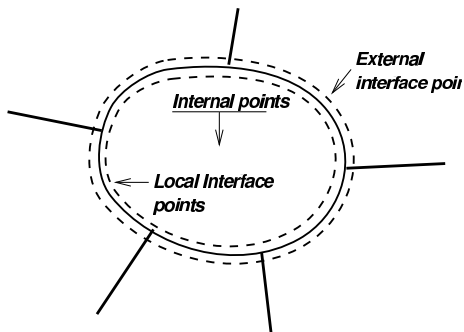


Figure: Local viewpoint

Equation $(A - \lambda I)x = 0$ can be written locally as

$$\underbrace{\begin{pmatrix} B_i - \lambda I & \hat{E}_i \\ \hat{E}_i^T & C_i - \lambda I \end{pmatrix}}_{A_i} \underbrace{\begin{pmatrix} u_i \\ y_i \end{pmatrix}}_{x_i} + \left(\sum_{j \in N_i} E_{ij} y_j \right) = 0.$$

- $B_i \in \mathbb{R}^{d_i \times d_i}$: coupling between interior variables
- $\hat{E}_i \in \mathbb{R}^{d_i \times s_i}$: coupling between interior/loc. interface variables
- $C_i \in \mathbb{R}^{s_i \times s_i}$: coupling between local interface variables
- N_i : set of indices for subdomains that are neighbors to the i 'th subdomain
- $E_{ij} \in \mathbb{R}^{s_i \times s_j}$: coupling among subdomains i and j

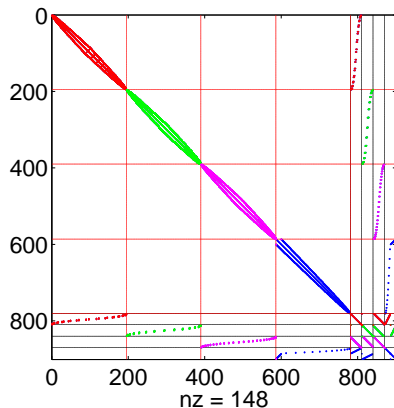
Global reordering of the eigenvalue problem

Stack interior variables u_1, u_2, \dots, u_p into u , then interface variables y_1, y_2, \dots, y_p to y , and reorder A so that interior variables are numbered before interface ones:

$$\begin{pmatrix} B_1 & & & E_1 \\ & B_2 & & E_2 \\ & & \ddots & \vdots \\ & & & B_p & E_p \\ E_1^\top & E_2^\top & \dots & E_p^\top & C \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_p \\ y \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_p \\ y \end{pmatrix}$$

where $E_i = [0_{d_i, \ell_i}, \hat{E}_i, 0_{d_i, \nu_i}]$, with $\ell_i = \sum_{j=1}^{i-1} s_j$, $\nu_i = \sum_{j=i+1}^p s_j$.

Example with $p = 4$ (different color \rightarrow different subdomain):



Notation: write as

$$A = \begin{pmatrix} B & E \\ E^\top & C \end{pmatrix}$$

The spectral Schur complement

- Eliminating the u_i 's we get

$$S(\lambda)y = \begin{pmatrix} S_1(\lambda) & E_{12} & \cdots & E_{1p} \\ E_{21} & S_2(\lambda) & \cdots & E_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ E_{p1} & E_{p2} & \cdots & S_p(\lambda) \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix} = 0$$

with $S_i(\lambda) = C_i - \lambda I - E_i^\top (B_i - \lambda I)^{-1} E_i$.

- Interface problem (non-linear):

$$S(\lambda)y = 0$$

- Top parts can be recovered as $u_i = -(B_i - \lambda I)^{-1} E_i y$

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Spectral Schur complement revisited

Our viewpoint:

- Find $\sigma \in \mathbb{R}$ such that

$$\mu(\sigma) = 0,$$

where $\mu(\sigma)$ denotes the smallest ($|\cdot|$) eigenvalue of $S(\sigma)$.

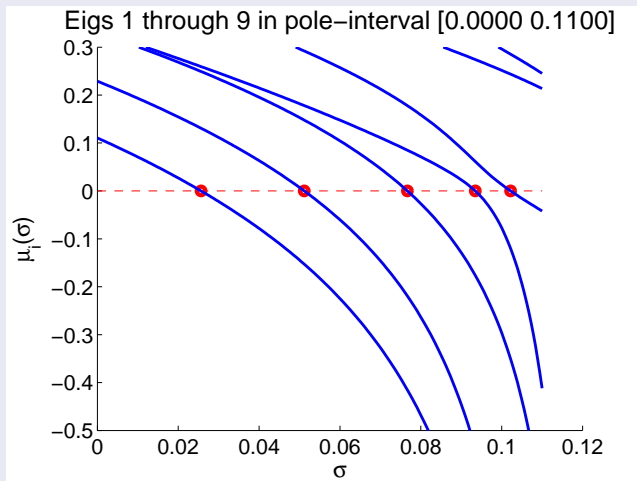
- We can treat $\mu(\sigma)$ as a function \rightarrow root-finding problem
- Bisection: slow. Newton: fast, but needs the derivative
- Other functions are possible, e.g. $\mu(\sigma) = \det[S(\sigma)]$ (Lui) \rightarrow not very practical

Eigenbranches

- For each σ : $S(\sigma)y^{(i)}(\sigma) = \mu_i(\sigma)y^{(i)}(\sigma)$, $i = 1, \dots, s$ (in sorted ascending algebraic order)
- Each $\mu_i(\sigma)$ is a function of σ (we call it an *eigenbranch*)
- The eigenvalues of B are the poles of the eigenbranches

Eigenbranches – illustration

An example for a discretized 2D Laplacian



Basic algorithm - Newton's scheme

Derivative of $\mu_i(\sigma)$

- Eigenbranch $\mu_i(\sigma)$ is analytic for any $\sigma \notin \Lambda(B)$ with

$$\frac{d\mu_i(\sigma)}{d\sigma} = \frac{(S'(\sigma)y^{(i)}(\sigma), y^{(i)}(\sigma))}{(y^{(i)}(\sigma), y^{(i)}(\sigma))} = -1 - \frac{\|(B - \sigma I)^{-1} E y^{(i)}(\sigma)\|_2^2}{\|y^{(i)}(\sigma)\|_2^2}.$$

where

$$S'(\sigma) = -I - E^\top (B - \sigma I)^{-2} E.$$

Algorithm 3.1

- 1: Select σ , tol
- 2: **repeat**
- 3: Compute $\mu(\sigma) =$ Smallest eigenvalue in modulus of $S(\sigma)$
- 4: along with associated unit eigenvector $y(\sigma)$
- 5: Set $\eta := \|(B - \sigma I)^{-1} E y(\sigma)\|_2$, and $\sigma := \sigma + \mu(\sigma)/(1 + \eta^2)$
- 6: **until** $|\mu(\sigma)| \leq \text{tol}$

“Chasing” an eigenbranch using Newton’s iteration

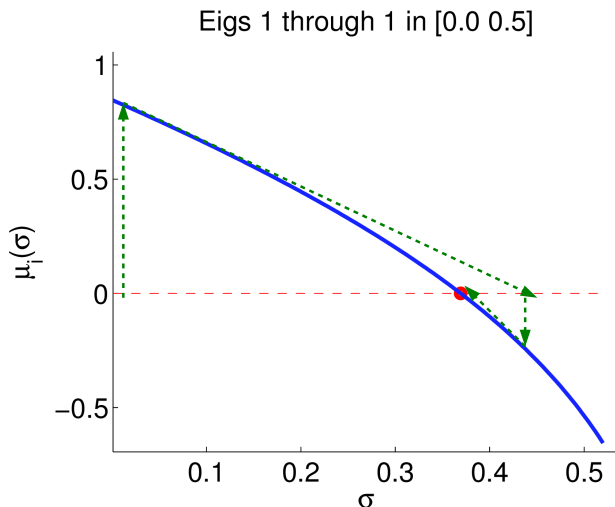


Figure: Computing the algebraically smallest eigenvalue of a 2D Laplacian

Computing $(\mu(\sigma), y(\sigma))$ – the main computational kernel!

- Perfect setting for a form of (inexact) inverse iteration (MINRES, GMRES)
- Alternatively, the Lanczos algorithm can be used
- Note that $\mu'(\sigma)$ is upper-bounded by -1 and its computation is entirely local across the subdomains

Residual of the approximation + connection with RQ

It can be shown that

$$\|(A - \sigma I)\hat{x}(\sigma)\| = |\mu(\sigma)|$$

where $\hat{x}(\sigma) = [-(B - \sigma I)^{-1}Ey(\sigma); y(\sigma)]$ is the approximate eigenvector, and the Newton update also is the Rayleigh quotient,

$$\sigma = \rho(A, \hat{x}(\sigma)).$$

Eigenbranches across the poles (I)

Let (θ_j, v_j) , $j = 1, \dots, d$ be the eigenpairs of B . We re-write:

$$S(\sigma) = C - \sigma I - E^T(B - \sigma I)E = C - \sigma I - \sum_{j=1}^d \frac{w_j w_j^T}{\theta_j - \sigma}, \quad \text{with} \quad w_j \equiv E^T v_j.$$

Analysis (assume θ_k , $1 \leq k \leq d$, is a simple pole)

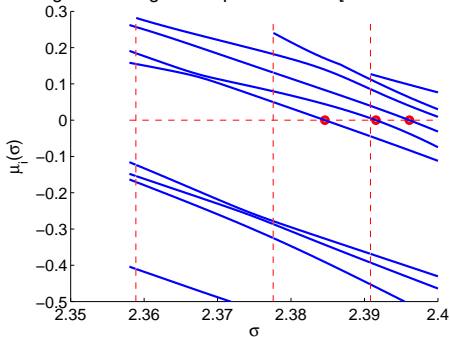
We have

$$\mu_j(\sigma) = \min_{\mathcal{U}^j, \dim(\mathcal{U}^j)=j} \max_{r \in \mathcal{U}^j} \rho(\sigma, r), \quad \rho(\sigma, r) = \frac{(S(\sigma)r, r)}{(r, r)}.$$

- As $\sigma \rightarrow \theta_k^-$, one eigenbranch $(\mu_1(\sigma))$ will descend to $-\infty$
- However, if $r \perp w_k \rightarrow$ eigenbranches $\mu_2(\sigma), \dots, \mu_s(\sigma)$ are well defined and converge to the eigenvalues of an operator which is orthogonal to w_k

Eigenbranches across the poles (II)

Eigs 26 through 32 in pole-interval [2.3580 2.4000]



Eigs 1 through 2 in [0.0 0.5]

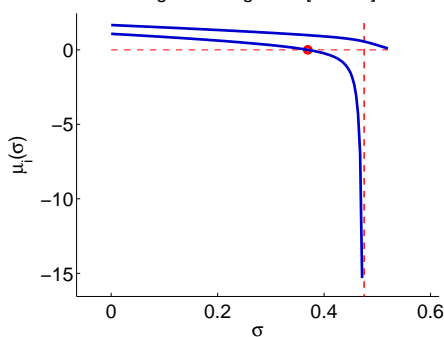


Figure: Behavior of a few eigenbranches as they cross a pole. Red circles: eigenvalues of A (roots). Dashed lines: eigenvalues of B (poles) Left: Eigenbranches $\mu_{26}, \dots, \mu_{32}$ in an interval not containing their poles. Right: Eigenbranches $\mu_1(\sigma)$ and $\mu_2(\sigma)$ as σ approaches the pole of $\mu_1(\sigma)$.

A branch-hopping scheme

Algorithm 3.2 – “Chasing” more than one eigenvalues

```
1: Given  $a, b$ . Select  $\sigma = a$ 
2: while  $\sigma < b$  do
3:   Compute  $S(\sigma)\mu(\sigma) = \mu(\sigma)y(\sigma)$ 
4:   if  $|\mu(\sigma)| \leq \text{tol}$  then
5:     Obtain  $\mu(\sigma) =$  smallest positive eigenvalue of  $S(\sigma)$ 
6:   end if
7:   Compute derivative and update  $\sigma$  as in Algorithm 3.1
8: end while
```

- Algorithm 3.2 assumes that we move rightwards; can be trivially modified for the case where we move leftwards.

Short illustration - the branch-hopping scheme

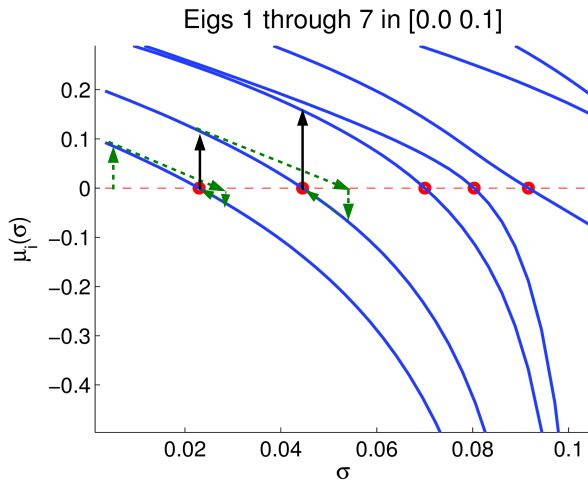


Figure: Computing the few smallest eigenvalues for the same 2D Laplacian

Effects of p in convergence – illustration

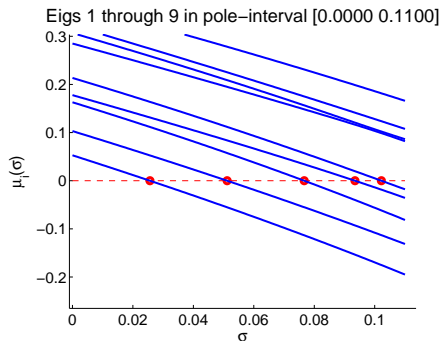
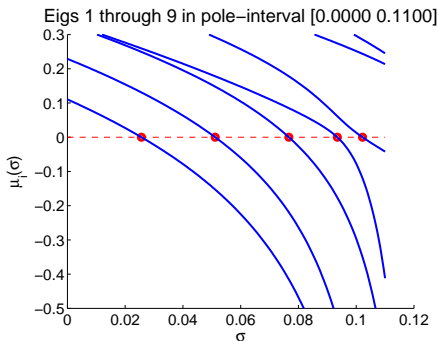


Figure: The shape of eigenbranches $\mu_1(\sigma), \dots, \mu_9(\sigma)$. Left: $p = 4$. Right: $p = 16$.

Effects of p in convergence – eigenvalues of B as p varies

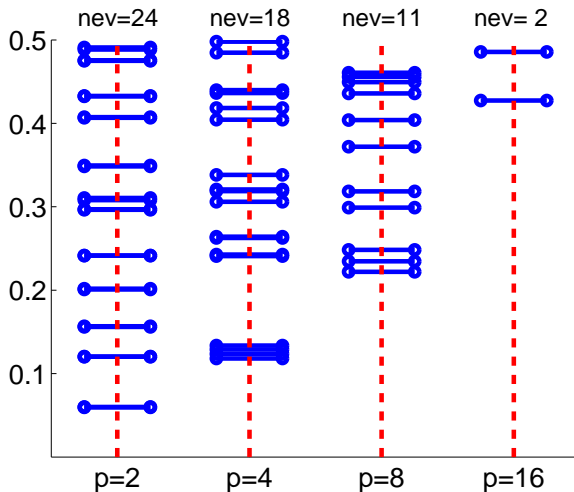


Figure: Monitoring the few smallest eigenvalues of B in a fixed interval as p varies.

A few more considerations

Multiple eigenvalues

Multiple eigenvalue $\lambda \rightarrow$ multiple (with the same degree of multiplicity) zero eigenvalue of $S(\lambda)$.

Misconvergence

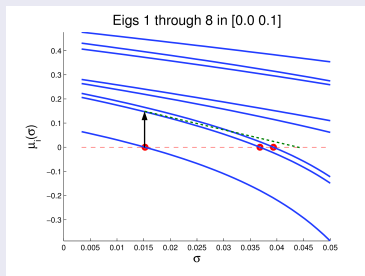


Figure: An example of misconvergence.

It is possible to misconverge when the root of the eigenbranch is close to its pole. To deal with this (potential) issue:

- Standard tool: inertia
- Have “better linear” eigenbranches
- Post-process new σ by inverse iteration

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Computational system

- Tests performed on Itasca Linux cluster @ MSI
- Each node is a two-socket, quad-core 2.8 GHz Intel Xeon X5560 “Nehalem EP” with 24 GB of system memory
- Interconnection: 40-gigabit QDR InfiniBand (IB)

Test matrices

- Tests on 3D discretized Laplacians (7pt. st. – FD) lying on the unit cube
- Dirichlet boundary conditions
- We use n_x , n_y , n_z to denote the number of nodes along each dimension
- tol for each eigenpair set to $1e - 8$
- *Software*: PETSc C++ (METIS+CHOLMOD)

Qualitative behavior of Alg 3.2 on a few 3D Laplacians

		$[\alpha, \beta] := [0, 0.5]$		$[\alpha, \beta] := [2, 2.2]$		$[\alpha, \beta] := [4.1, 4.2]$	
		#Eigvls	It	#Eigvls	It	#Eigvls	It
n = 21 × 20 × 19							
# of subdomains (p)	2	35	60	82	152	127	360
	4		43		130		172
	8		35		116		152
	16		39		96		148
n = 41 × 20 × 19							
# of subdomains (p)	2	72	210	154	342	209	424
	4		170		292		314
	8		154		273		310
	16		138		241		300
n = 41 × 40 × 20							
# of subdomains (p)	2	160	385	319	703	472	802
	4		354		540		647
	8		296		502		592
	16		270		451		533

Convergence of Alg. 3.2

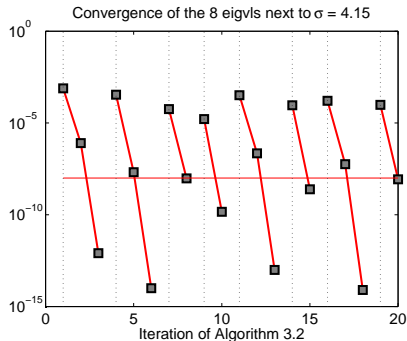
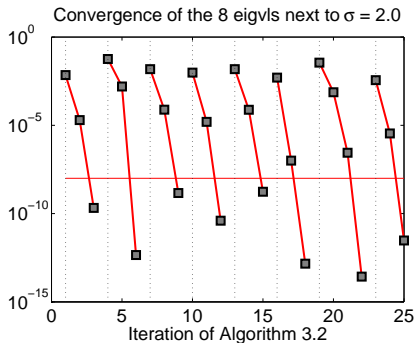


Figure: Rel. res. for a few consecutive eigenvalues. Left: $n_x = 21$, $n_y = 20$ and $n_z = 19$. Right: $n_x = 41$, $n_y = 20$ and $n_z = 19$.

Combining Alg. 3.1 with inverse iteration

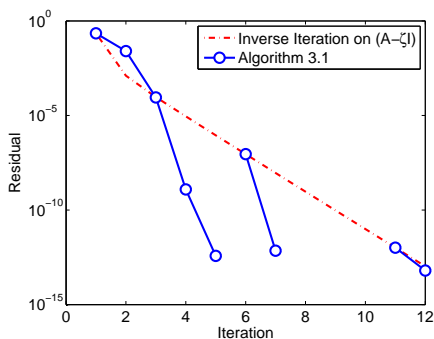
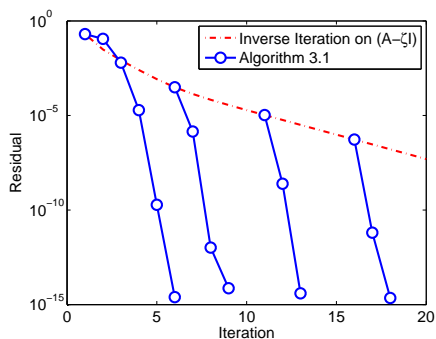


Figure: Convergence behavior for computing the eigenpair closest to ζ when combining inverse iteration and Newton's method. Left: $\zeta = 0.0$. Right: $\zeta = 3.0$.

Experiments in distributed computing environments

Performing the Matrix-Vector product with $S(\zeta)$

- 1 MV multiplication with $C - \sigma I$ (non-local),
- 2 MV multiplication with E and E^T (local),
- 3 system solution with $B - \sigma I$ (local),

Comparisons against residual inverse iteration (RI)

- RI: Similar to inverse iteration but with fixed inner tolerance
- Computation of $(\mu(\sigma), y(\sigma))$ is performed inexactly
- We use MINRES as the iterative solver
- Each subdomain is handled by a separate MPI process

Table: Computing $k = 1$ and $k = 5$ eigenvalues next to ζ for a $41 \times 40 \times 39$ 3D Laplacian. For the case where $\zeta \neq 0$, the starting shift for each particular eigenpair computation in Newton's scheme was provided by first performing three steps of inexact Inverse Iteration. Times are listed in seconds.

$n = 41 \times 40 \times 39$							
(p, k)	s	$\zeta = 0.0$			$\zeta = 0.1$ (19)		
		T_{NT}	lt	T_{RI}	T_{NT}	lt	T_{RI}
(16,1)	15423	0.21	3	0.10	1.07	4	1.32
(16,5)	- -	1.39	15	0.62	5.85	19	7.77
(32,1)	20037	0.06	3	0.03	0.27	2	0.90
(32,5)	- -	0.32	14	0.19	1.52	14	4.86
(64,1)	24789	0.09	3	0.04	0.14	3	0.66
(64,5)	- -	0.44	14	0.21	1.01	15	3.51

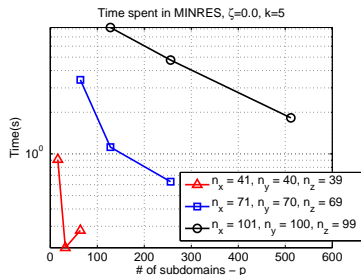
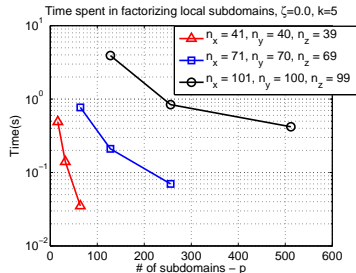
Table: Computing $k = 1$ and $k = 5$ eigenvalues next to ζ for a $71 \times 70 \times 69$ 3D Laplacian. For the case where $\zeta \neq 0$, the starting shift for each particular eigenpair computation in Newton's scheme was provided by first performing three steps of inexact Inverse Iteration. Times are listed in seconds.

n = 71 × 70 × 69								
(p, k)	s	$\zeta = 0.0$			$\zeta = 0.1$ (137)			
		T_{NT}	It	T_{RI}	T_{NT}	It	T_{RI}	
(64,1)	83358	0.80	3	0.61	15.4	2	15.9	
(64,5)	- -	4.20	14	3.22	80.4	10	79.9	
(128,1)	108508	0.19	3	0.32	3.12	2	8.41	
(128,5)	- -	1.25	14	1.71	15.1	10	38.5	
(256,1)	136159	0.10	3	0.27	5.99	2	12.7	
(256,5)	- -	0.68	13	1.45	25.3	10	51.7	

Table: Computing $k = 1$ and $k = 5$ eigenvalues next to ζ for a $101 \times 100 \times 99$ 3D Laplacian. For the case where $\zeta \neq 0$, the starting shift for each particular eigenpair computation in Newton's scheme was provided by first performing three steps of inexact Inverse Iteration. Times are listed in seconds.

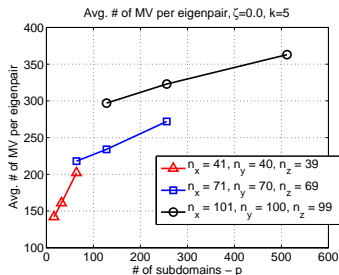
$n = 101 \times 100 \times 99$							
(p, k)	s	$\zeta = 0.0$			$\zeta = 0.1$ (439)		
		T_{NT}	It	T_{RI}	T_{NT}	It	T_{RI}
(128,1)	230849	2.73	3	2.02	48.1	3	93.3
(128,5)	- -	13.2	15	10.3	233.2	16	472.1
(256,1)	293626	1.10	3	1.61	23.4	3	62.4
(256,5)	- -	5.80	14	8.32	129.2	16	301.5
(512,1)	369663	0.62	2	0.99	32.4	2	75.3
(512,5)	- -	3.01	12	5.71	168.9	12	322.9

Time breakdown



For the case $\zeta = 0.0$, $k = 5$:

- 1 Time to factorize $B - \sigma I$
- 2 Time spent on solving linear systems
- 3 Avg. of MINRES iters per eigenpair



A comparison with ARPACK

Table: Computing $k = 1$ and $k = 5$ eigenvalues next to ζ with the proposed Newton scheme and ARPACK. The discretization selected as $n_x = 71$, $n_y = 70$, and $n_z = 69$. Times are listed in seconds. **Newton's scheme is using 8 cores.**

(p, k)	$\zeta = 0.0$		$\zeta = 0.1$ (137)	
	T_{NT}	T_{ARP}	T_{NT}	T_{ARP}
(64,1)	5.5	35.4	170.0	351.5
(128,1)	3.4	–	105.1	–
(256,1)	5.3	–	122.5	–
(64,5)	28.3	94.1	884.7	416.3
(128,5)	15.3	–	532.3	–
(256,5)	25.9	–	605.3	–

Contents

- 1 Introduction
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Conclusion

In this talk

- We presented a Schur complement eigenvalue solver that focuses solely on the interface problem region
- Eigenvalue branches of the SSC \rightarrow Newton's method
- Potential for 2-D level parallelism
- Ultimately, k eigenpairs are computed at the cost of one

Considerations

- Use subspace acceleration
- Solution of generalized eigenvalue problems
- Combine with an efficient mechanism to obtain initial guesses (AMLS?)
- Use Newton's method on a higher-order approximation of $S(\lambda)$

Misconvergence

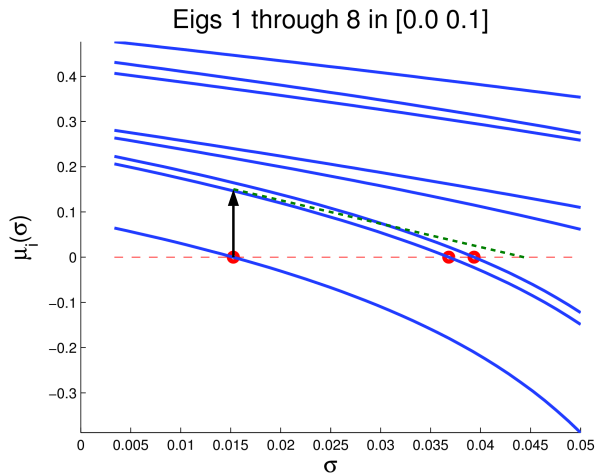


Figure: An example of misconvergence.

Table: Computing $k = 1$ and $k = 5$ eigenvalues next to ζ for a 801×800 2D Laplacian. For the case where $\zeta \neq 0$, the starting shift for each particular eigenpair computation in Newton's scheme was provided by first performing three steps of inexact Inverse Iteration. Times are listed in seconds.

n = 801 × 800							
(p, k)	s	$\zeta = 0.0$			$\zeta = 0.01$ (488)		
		T_{NT}	It	T_{RI}	T_{NT}	It	T_{RI}
(64,1)	24945	1.09	3	1.25	37.4	2	156.4
(64,5)	- -	5.95	15	6.98	198.7	12	775.1
(128,1)	36611	0.27	2	0.67	24.0	2	75.4
(128,5)	- -	1.31	9	3.82	125.0	11	382.1
(256,1)	52319	0.22	2	0.48	11.2	2	44.9
(256,5)	- -	1.59	9	2.73	61.3	10	231.6

Table: Computing $k = 1$ and $k = 5$ eigenvalues next to ζ for a 1001×1000 2D Laplacian. For the case where $\zeta \neq 0$, the starting shift for each particular eigenpair computation in Newton's scheme was provided by first performing three steps of inexact Inverse Iteration. Times are listed in seconds.

n = 1001 × 1000							
(p, k)	s	$\zeta = 0.0$			$\zeta = 0.01$ (764)		
		T_{NT}	It	T_{RI}	T_{NT}	It	T_{RI}
(128,1)	46073	0.42	3	1.03	95.3	2	102.1
(128,5)	- -	2.84	15	5.33	482.7	10	532.1
(256,1)	65780	0.27	2	0.64	54.2	2	73.4
(256,5)	- -	1.35	10	3.32	281.3	9	381.4
(512,1)	93440	0.25	2	0.58	49.4	2	58.1
(512,5)	- -	1.42	10	3.21	256.7	10	312.8

Eigenbranches across the poles (III)

Let θ_k^- be a simple eigenvalue of B and define

$$S_k(\sigma) = C - \sigma I - \sum_{j=1, j \neq k}^d \frac{w_j w_j^T}{\theta_j - \sigma}, \quad \rho_k(\sigma, r) = \frac{(S_k(\sigma)r, r)}{(r, r)}$$

In the following we assume that $\sigma \in [\sigma_0, \theta_k]$ where $[\sigma_0, \theta_k)$ contains no eigenvalues of B .

As $\sigma \rightarrow \theta_k^-$, for any $j > 1$, we have

$$\mu_j(\sigma) = \rho(\sigma, y^{(j)}(\sigma)) = \rho_k(\sigma, y^{(j)}(\sigma)) - \frac{(y^{(j)}(\sigma)^T w_k)^2}{\theta_k - \sigma},$$

and since $\rho_k(\sigma, y^{(j)}(\sigma))$ is bounded, we get $\lim_{\sigma \rightarrow \theta_k^-} w_k^T y^{(j)}(\sigma) = 0$.

Eigenbranches across the poles (IV)

Let

$$P_k = I - w_k w_k^T / (w_k^T w_k) = I - \hat{w}_k \hat{w}_k^T.$$

Multiplying $S(\sigma)y^{(j)}(\sigma) = \mu_j(\sigma)y^{(j)}(\sigma)$ by P_k from the left yields

$$P_k S_k(\sigma) P_k y^{(j)}(\sigma) - \mu_j(\sigma) P_k y^{(j)}(\sigma) = -P_k S_k(\sigma) (\hat{w}_k^T y^{(j)}(\sigma)) \hat{w}_k.$$

Therefore, the eigenpair $(\mu_j(\sigma), P_k y^{(j)}(\sigma))$ converges to an eigenpair of $P_k S_k(\theta_k) P_k$, which is a trivial extension of $S_{k,|}(\sigma) = [P_k S_k(\sigma) P_k]_{|_{w_k^\perp}}$.