Beyond AMLS: Domain decomposition with rational filtering

Vassilis Kalantzis (joint work with Yuanzhe Xi and Yousef Saad)

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Acknowledgments

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U.S. DEPARTMENT OF ENERGY

Contents

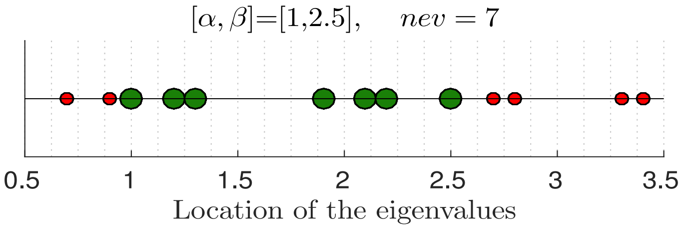
The algebraic generalized eigenvalue problem

The symmetric generalized eigenvalue problem is formally defined as

$$Ax = \lambda Mx.$$

Matrices A and M are assumed sparse and symmetric, while M is also SPD.

- The pencil (A, M) has n eigenpairs which we will denote by $\left(\lambda_i, x^{(i)}\right), \ i = 1, \ldots, n$.
- We are only interested in computing those eigenpairs $\left(\lambda_i, x^{(i)}\right)$ for which $\lambda_i \in [\alpha, \beta]$.
- We will denote the number of eigenvalues which satisfy the above property by 'nev'.

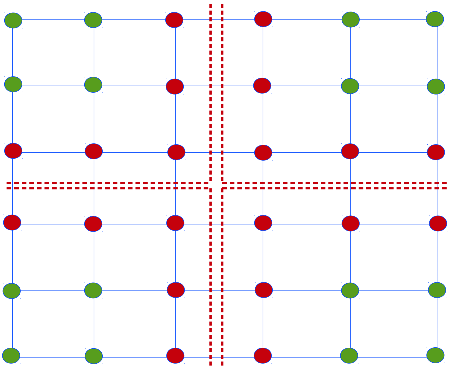


Contents

Reordering equations/unknowns ($p \geq 2$ subdomains)

$$A = \begin{pmatrix} B_1 & & & & E_1 \\ & B_2 & & & E_2 \\ & & \ddots & & \vdots \\ & & & B_p & E_p \\ E_1^T & E_2^T & \cdots & E_p^T & C \end{pmatrix},$$

$$M = \begin{pmatrix} M_B^{(1)} & & & & M_E^{(1)} \\ & M_B^{(2)} & & & M_E^{(2)} \\ & & \ddots & & \vdots \\ & & & M_B^{(p)} & M_E^{(p)} \\ \left(M_E^{(1)}\right)^T & \left(M_E^{(2)}\right)^T & \cdots & \left(M_E^{(p)}\right)^T & M_C \end{pmatrix}.$$



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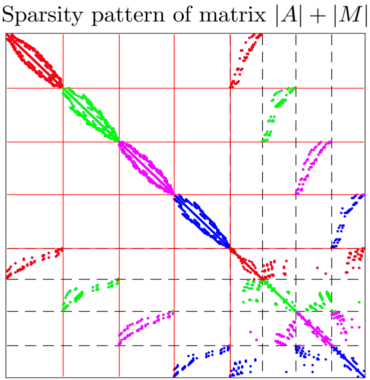
Notation: write as

$$A = \begin{pmatrix} B & E \\ E^T & C \end{pmatrix}, M = \begin{pmatrix} M_B & M_E \\ M_E^T & M_C \end{pmatrix},$$

$$x^{(i)} = \begin{pmatrix} u^{(i)} \\ y^{(i)} \end{pmatrix} = \begin{pmatrix} u_1^{(i)} \\ \vdots \\ u_p^{(i)} \\ y_1^{(i)} \\ \vdots \\ y_p^{(i)} \end{pmatrix}.$$

An example of the sparsity pattern of A and M for $p = 4$

$$A = \begin{pmatrix} B & E \\ E^T & C \end{pmatrix} = \begin{pmatrix} B_1 & & & & E_1 \\ & B_2 & & & E_2 \\ & & \ddots & & \vdots \\ & & & B_p & E_p \\ E_1^T & E_2^T & \cdots & E_p^T & C \end{pmatrix}$$



Invariant subspaces from a Schur complement viewpoint

$$(A - \lambda_i M)x^{(i)} = \begin{pmatrix} B - \lambda_i M_B & E - \lambda_i M_E \\ E^T - \lambda_i M_E^T & C - \lambda_i M_C \end{pmatrix} \begin{pmatrix} u^{(i)} \\ y^{(i)} \end{pmatrix} = 0.$$

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$$\left[C - \lambda_i M_C - \underbrace{(E - \lambda_i M_E)^T (B - \lambda_i M_B)^{-1} (E - \lambda_i M_E)}_{\text{block-diagonal}} \right] y^{(i)} = 0,$$

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To compute the eigenpairs $\left(\lambda_i, x^{(i)}\right)_{i=1,\dots,nev}$

Perform a Rayleigh-Ritz projection onto $\mathcal{Z} = \mathcal{U} \oplus \mathcal{Y}$:

$$\mathcal{Y} = \mathrm{span}\left\{ y^{(i)} \right\}_{i=1,\dots,nev},$$

$$\mathcal{U} = \mathrm{span}\left\{ -(B - \lambda_i M_B)^{-1} (E - \lambda_i M_E) y^{(i)} \right\}_{i=1,\dots,nev}.$$

Contents

Rational filtering

- We consider the following rational filter

$$\rho(\zeta) = \sum_{\ell=1}^{2N_c} \frac{\omega_\ell}{\zeta - \zeta_\ell} \approx \underbrace{\frac{1}{2\pi i} \int_{\Gamma_{[\alpha,\beta]}} \frac{1}{\nu - \zeta} d\nu}_{I_{[\alpha,\beta]}(\zeta)}$$

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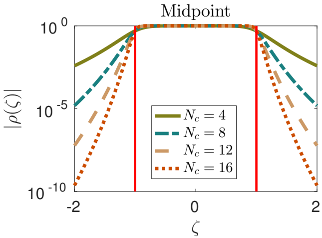

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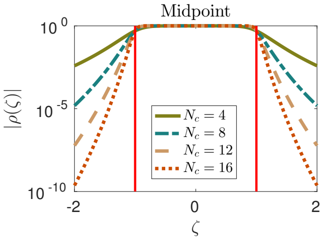

- It is possible to apply $\rho(.)$ to (A, M):

$$\rho(M^{-1}A) = 2\Re e \left\{ \sum_{\ell=1}^{N_c} \omega_\ell (A - \zeta_\ell M)^{-1} M \right\}.$$

  - Examples: FEAST (Subspace Iteration), Sakurai-Sugiura (Moments-based).
  - Krylov projection schemes are also possible (RF-KRYLOV).

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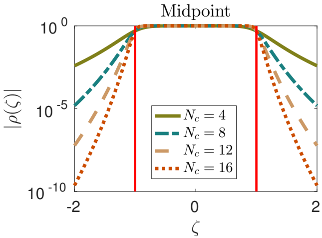

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  - Examples: FEAST (Subspace Iteration), Sakurai-Sugiura (Moments-based).
  - Krylov projection schemes are also possible (RF-KRYLOV).
- Our idea: Decouple application of $\rho(\zeta)$ to interior/interface variables.
- Potential advantages:
  1. Reduced use of complex arithmetic.
  2. Orthonormalization of shorter vectors (interface variables).
  3. Faster convergence.

Summary of the proposed technique

- Our goal is to construct a subspace $\mathcal{Z} = \mathcal{U} \oplus \mathcal{Y}$ to perform a Rayleigh-Ritz projection onto.
- Recall that, ideally,

$$\mathcal{Y} = \mathrm{span}\left\{ y^{(i)} \right\}_{i=1,\ldots,nev},$$

$$\mathcal{U} = \mathrm{span}\left\{ -(B - \lambda_i M_B)^{-1}(E - \lambda_i M_E) y^{(i)} \right\}_{i=1,\ldots,nev}.$$

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The technique proposed in this talk:

1. Constructs $\mathcal{Y}$ by applying the rational filter $\rho(\zeta)$ to the interface region (Schur complement matrices).
2. Uses the above subspace to construct $\mathcal{U}$. This step is performed in real arithmetic and is embarrassingly parallel.

How to approximate $\mathrm{span}\left\{y^{(1)}, \ldots, y^{(nev)}\right\}$ (I)

Let $\zeta \in \mathbb{C}$ and define

$$B_\zeta = B - \zeta M_B, \quad E_\zeta = E - \zeta M_E, \quad C_\zeta = C - \zeta M_C,$$
$$S(\zeta) = C_\zeta - E_\zeta^T B_\zeta^{-1} E_\zeta.$$

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Then,

$$(A - \zeta M)^{-1} = \begin{pmatrix} B_\zeta^{-1} + B_\zeta^{-1} E_\zeta S(\zeta)^{-1} E_\zeta^T B_\zeta^{-1} & -B_\zeta^{-1} E_\zeta S(\zeta)^{-1} \\ -S(\zeta)^{-1} E_\zeta^T B_\zeta^{-1} & S(\zeta)^{-1} \end{pmatrix}.$$

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The matrix inverse $(A - \zeta M)^{-1}$ can be also written as:

$$(A - \zeta M)^{-1} = \sum_{i=1}^{n} \frac{1}{\lambda_i - \zeta} x^{(i)} \left(x^{(i)}\right)^T = \sum_{i=1}^{n} \frac{1}{\lambda_i - \zeta} \begin{bmatrix} u^{(i)} \left(u^{(i)}\right)^T & u^{(i)} \left(y^{(i)}\right)^T \\ y^{(i)} \left(u^{(i)}\right)^T & y^{(i)} \left(y^{(i)}\right)^T \end{bmatrix}.$$

How to approximate span $\left\{y^{(1)},\ldots,y^{(nev)}\right\}$ (II)

Recall that

$$\rho(M^{-1}A) = 2\Re e\left\{\sum_{\ell=1}^{N_c}\omega_\ell(A-\zeta_\ell M)^{-1}M\right\}.$$

Combining alltogether we get:

$$\rho(M^{-1}A) = 2\Re e\left\{\sum_{\ell=1}^{N_c}\omega_\ell\begin{bmatrix}B_{\zeta_\ell}^{-1}+B_{\zeta_\ell}^{-1}E_{\zeta_\ell}S(\zeta_\ell)^{-1}E_{\zeta_\ell}^TB_{\zeta_\ell}^{-1} & -B_{\zeta_\ell}^{-1}E_{\zeta_\ell}S(\zeta_\ell)^{-1}\\ -S(\zeta_\ell)^{-1}E_{\zeta_\ell}^TB_{\zeta_\ell}^{-1} & \boxed{S(\zeta_\ell)^{-1}}\end{bmatrix}\right\}M$$

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$$= \sum_{i=1}^{n}\rho(\lambda_i)\begin{bmatrix} u^{(i)}\left(u^{(i)}\right)^T & u^{(i)}\left(y^{(i)}\right)^T \\ y^{(i)}\left(u^{(i)}\right)^T & \boxed{y^{(i)}\left(y^{(i)}\right)^T}\end{bmatrix}M. \quad \left(\rho(\lambda_i) = 2\Re e\left\{\sum_{\ell=1}^{N_c}\frac{\omega_\ell}{\lambda_i-\zeta_\ell}\right\}\right)$$

How to approximate $\mathrm{span}\left\{y^{(1)},\ldots,y^{(nev)}\right\}$ (III)

Equating blocks leads to:

$$2\Re e\left\{\sum_{\ell=1}^{N_c}\omega_\ell S(\zeta_\ell)^{-1}\right\}=\sum_{i=1}^{n}\rho(\lambda_i)y^{(i)}\left(y^{(i)}\right)^T.$$

Since $\rho(\lambda_1),\ldots,\rho(\lambda_{nev})\neq 0$:

$$\mathrm{span}\left\{y^{(1)},\ldots,y^{(nev)}\right\}\subseteq \mathrm{range}\left(2\Re e\left\{\sum_{\ell=1}^{N_c}\omega_\ell S(\zeta_\ell)^{-1}\right\}\right).$$

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Capture $\text{range}\left(\Re e\left\{\sum_{\ell=1}^{N_c}\omega_\ell S(\zeta_\ell)^{-1}\right\}\right)$ by a Krylov projection scheme.

How to approximate span $\{y^{(1)}, \ldots, y^{(nev)}\}$ (IV)

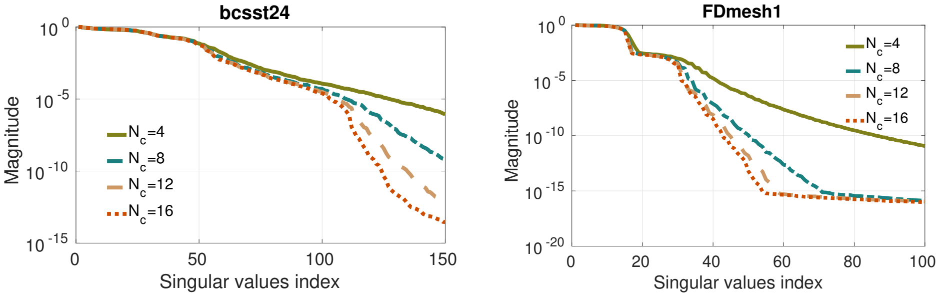

Figure: Leading singular values of $2\Re e\left\{\sum_{\ell=1}^{N_c} \omega_\ell S(\zeta_\ell)^{-1}\right\} = \sum_{i=1}^{n} \rho(\lambda_i) y^{(i)} \left(y^{(i)}\right)^T, \quad ([\alpha, \beta] = [\lambda_1, \lambda_{100}])$.

How to approximate $\text{span}\left\{y^{(1)},\ldots,y^{(nev)}\right\}$ (IV)

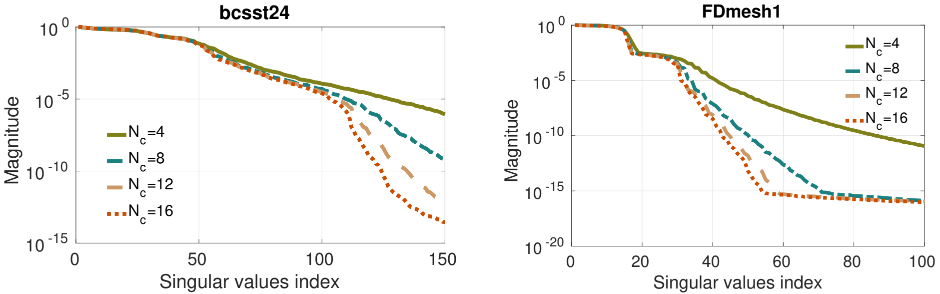

Figure: Leading singular values of $2\Re e\left\{\sum_{\ell=1}^{N_c}\omega_\ell S(\zeta_\ell)^{-1}\right\}=\sum_{i=1}^{n}\rho(\lambda_i)y^{(i)}\left(y^{(i)}\right)^T, \quad ([\alpha,\beta]=[\lambda_1,\lambda_{100}])$.

What if $\text{rank}\left(\left[y^{(1)},\ldots,y^{(nev)}\right]\right)<nev$?

Finalizing the proposed scheme (RF-DDES)

- Ideally, $\mathcal{U} = \left\{ u^{(1)}, \ldots, u^{(nev)} \right\}$, where

$$\begin{aligned} u^{(i)} &= -B_{\lambda_i}^{-1} E_{\lambda_i} y^{(i)} \\ &= -\left(B_{\lambda_i}^{-1} E_\sigma + (\lambda_i - \sigma) B_{\lambda_i}^{-1} M_E \right) y^{(i)}. \end{aligned}$$

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- We finally set $\mathcal{U} = \mathrm{span}([V, U_1, U_2])$ where

$$U_1 = -\left[B_\sigma^{-1} E_\sigma Y, \ldots, (B_\sigma^{-1} M_B)^{\psi-1} B_\sigma^{-1} E_\sigma Y \right],$$

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- V includes the eigenvectors associated with the $nev_B p$ smallest eigenvalues of (B_σ, M_B).

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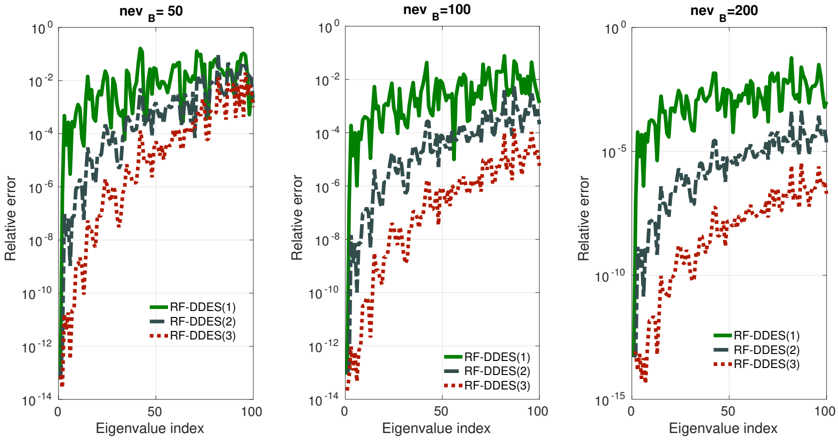
- V includes the eigenvectors associated with the $nev_B p$ smallest eigenvalues of (B_σ, M_B).
- $\left\|u^{(i)} - \hat{u}^{(i)}\right\|_{M_B} \leq \max_{\ell \geq (nev_B p)+1} O\left(\frac{(\lambda_i - \sigma)^{\psi+1}}{(\delta_\ell - \lambda_i)(\delta_\ell - \sigma)^{\psi}}\right).$

Contents

Approximation of the $nev = 100$ algebraically smallest eigenvalues of pencil qa8fk/qa8fm



A comparison of RF-KRYLOV and RF-DDES (I)

Table: Wall-clock times of RF-KRYLOV and RF-DDES using $\tau = 2, 4, 8, 16$ and $\tau = 32$ computational cores. RFD(2) and RFD(4) denote RF-DDES with $p = 2$ and $p = 4$ subdomains, respectively.

	$nev = 100$			$nev = 200$			$nev = 300$		
Matrix	RFK	RFD(2)	RFD(4)	RFK	RFD(2)	RFD(4)	RFK	RFD(2)	RFD(4)
shipsec8($\tau = 2$)	114	195	-	195	207	-	279	213	-
($\tau = 4$)	76	129	93	123	133	103	168	139	107
($\tau = 8$)	65	74	56	90	75	62	127	79	68
($\tau = 16$)	40	51	36	66	55	41	92	57	45
($\tau = 32$)	40	36	28	62	41	30	75	43	34
boneS01($\tau = 2$)	94	292	-	194	356	-	260	424	-
($\tau = 4$)	68	182	162	131	230	213	179	277	260
($\tau = 8$)	49	115	113	94	148	152	121	180	187
($\tau = 16$)	44	86	82	80	112	109	93	137	132
($\tau = 32$)	51	66	60	74	86	71	89	105	79

A comparison of RF-KRYLOV and RF-DDES (II)

Table: Wall-clock times of RF-KRYLOV and RF-DDES using $\tau = 2,\ 4,\ 8,\ 16$ and $\tau = 32$ computational cores. RFD(2) and RFD(4) denote RF-DDES with $p = 2$ and $p = 4$ subdomains, respectively.

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FDmesh2($\tau = 2$)	241	85	-	480	99	-	731	116	-
($\tau = 4$)	159	34	63	305	37	78	473	43	85
($\tau = 8$)	126	22	23	228	24	27	358	27	31
($\tau = 16$)	89	16	15	171	17	18	256	20	21
($\tau = 32$)	51	12	12	94	13	14	138	15	20
FDmesh3($\tau = 2$)	1021	446	-	2062	502	-	3328	564	-
($\tau = 4$)	718	201	281	1281	217	338	1844	237	362
($\tau = 8$)	423	119	111	825	132	126	1250	143	141
($\tau = 16$)	355	70	66	684	77	81	1038	88	93
($\tau = 32$)	177	47	49	343	51	58	706	62	82

Amount of time spent on orthonormalization

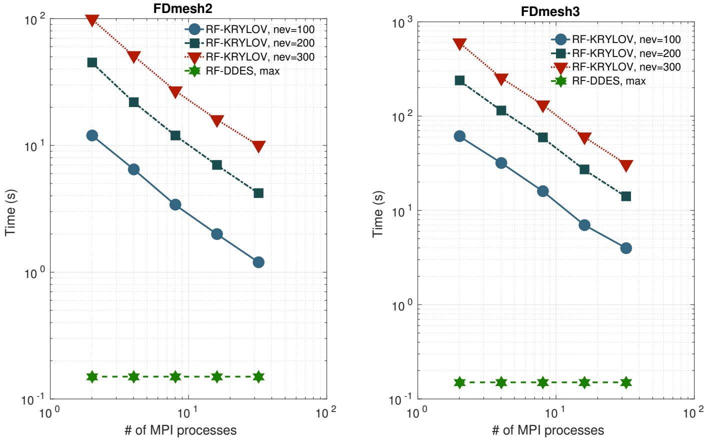

Figure: Left: "FDmesh2" ($n = 250,000$). Right: "FDmesh3" ($n = 1,000,000$).

Thank you

Questions?