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The EVSL package for symmetric eigenvalue problems

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First:

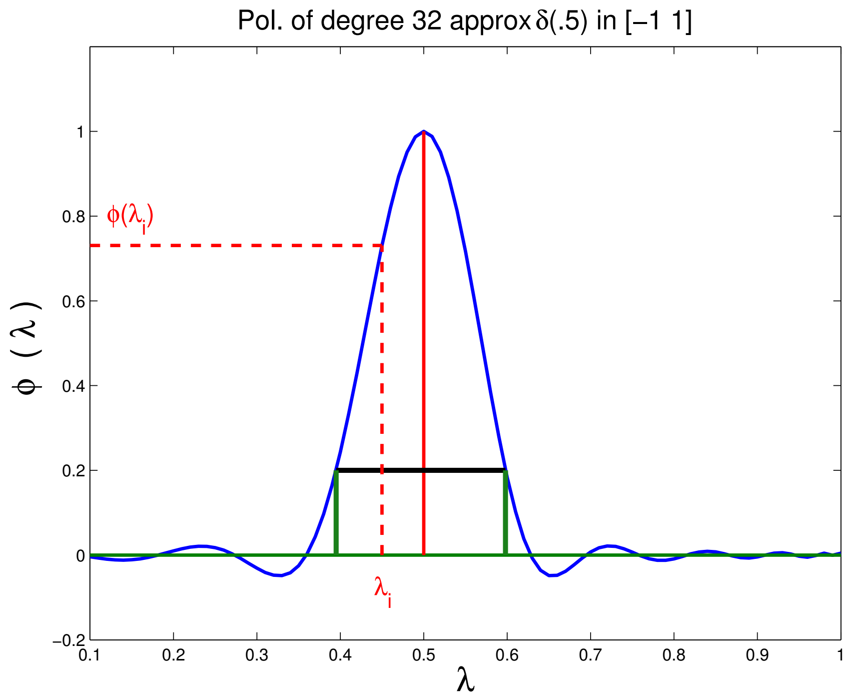
- **Joint work with Ruipeng Li, Yuanzhe Xi, and Luke Erlandson**
- **Application side: collaboration with Jia Shi, Maarten V. de Hoop (Rice)**
- **Support: NSF**

“Spectrum Slicing”

- Context: very large number of eigenvalues to be computed
- Goal: compute spectrum by slices by applying filtering
- Apply Lanczos or Subspace iteration to problem:

$$\phi(A)u = \mu u$$

$\phi(t) \equiv$ a polynomial or rational function that enhances wanted eigenvalues

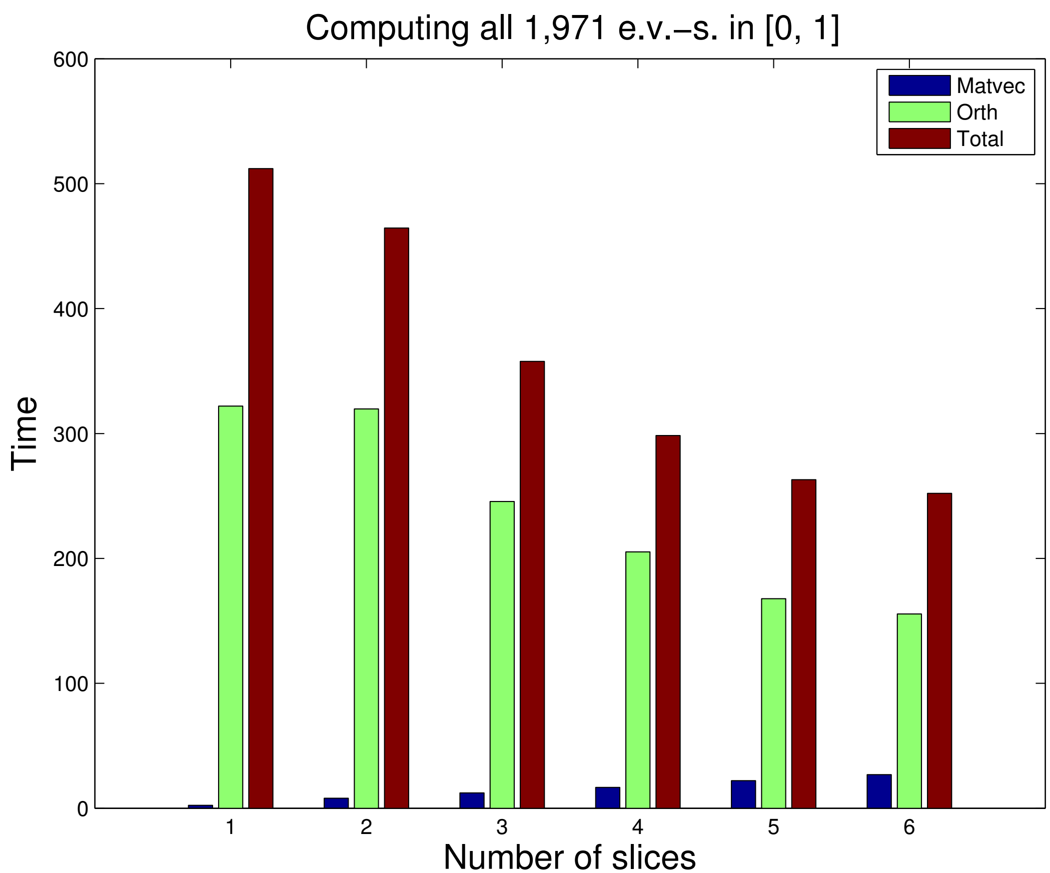


Rationale. Eigenvectors on both ends of wanted spectrum need not be orthogonalized against each other :

➤ Idea: Get the spectrum by ‘slices’ or ’windows’ [e.g., a few hundreds or thousands of pairs at a time]

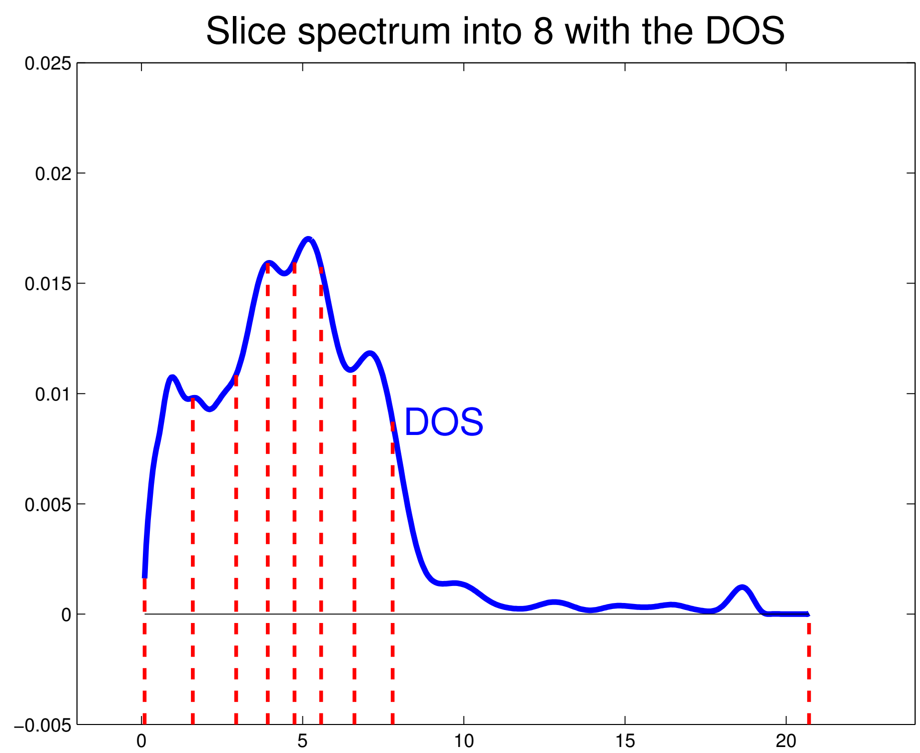
➤ Note: Orthogonalization cost can be very high if we do not slice the spectrum

Illustration: All eigenvalues in [0, 1] of a 49^3 Laplacean



Note: This is a small pb. in a scalar environment. Effect likely much more pronounced in a fully parallel case.

How do I slice my spectrum?



Answer: Use the spectral density, aka, 'Density Of States' (DOS)

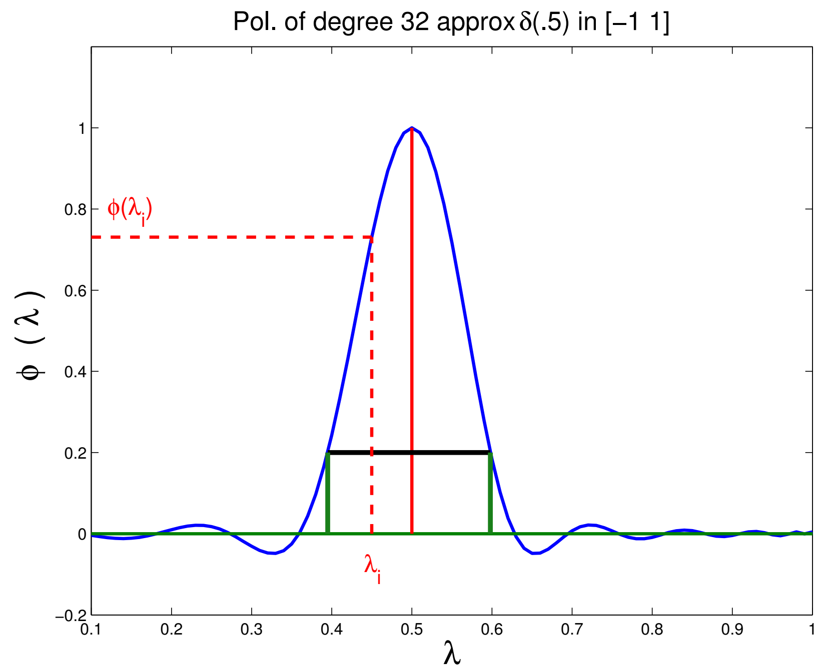
➤ DOS inexpensive to compute

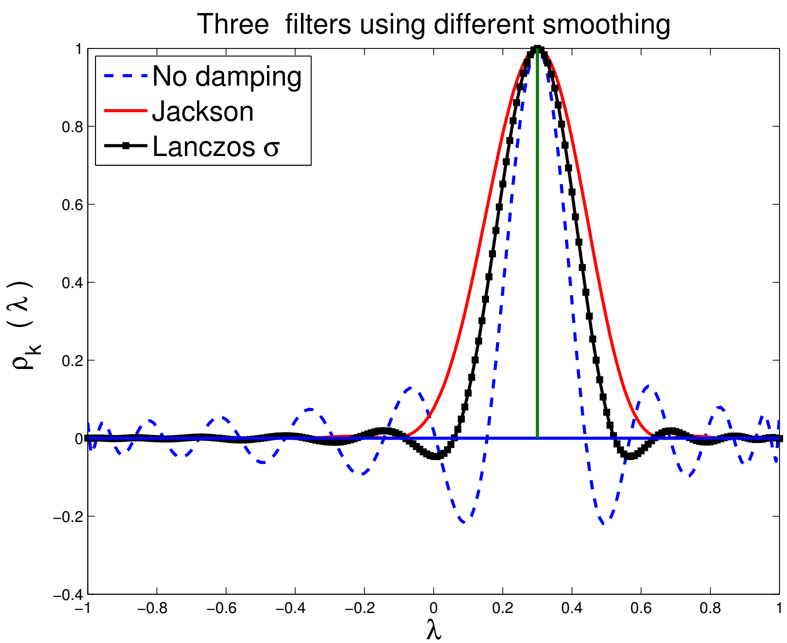
➤ We must have:

$$\int_{t_i}^{t_{i+1}} \phi(t)dt = \frac{1}{n_{slices}} \int_a^b \phi(t)dt$$

Polynomial filtering: The δ-Dirac function approach

➤ Obtain the LS approximation to the $\delta-$ Dirac function – Centered at some point (TBD) inside interval. $\longrightarrow$





$\longleftarrow$ Damping: Jackson, Lanczos σ damping, or none.

'The soul of a new filter' – A few technical details

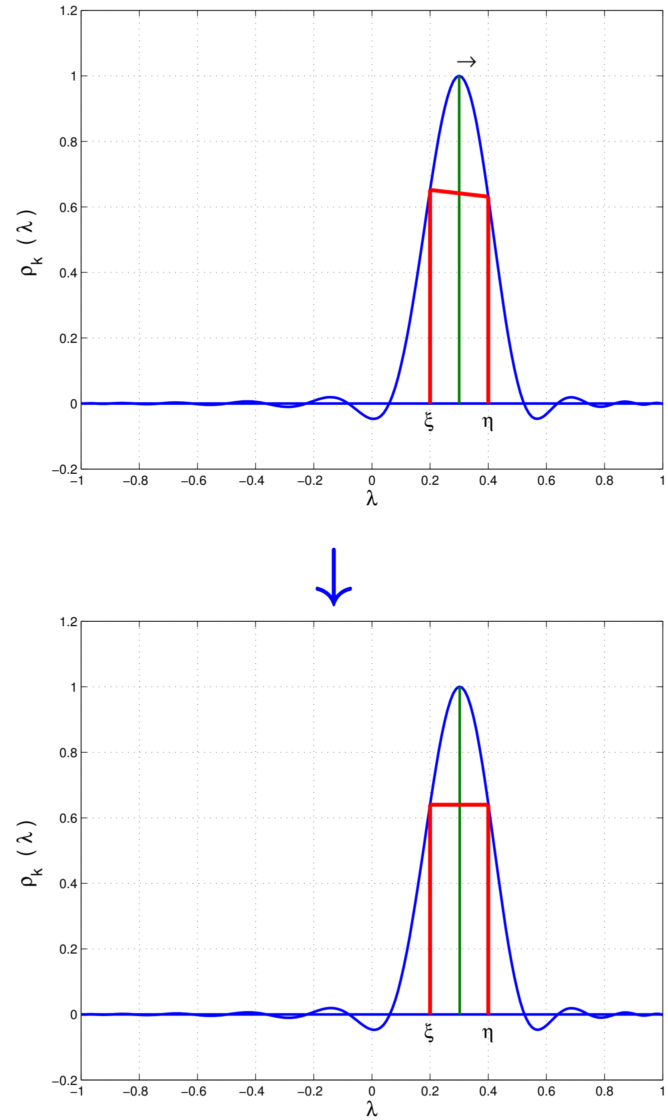
Issue # one: 'balance the filter'

➤ To facilitate the selection of *'wanted'* eigenvalues [Select $\boldsymbol{\lambda}$'s such that $\rho(\boldsymbol{\lambda}) >$ bar] we need to ...

➤ ... find γ so that $\rho(\boldsymbol{\xi}) - \rho(\boldsymbol{\eta}) = 0$

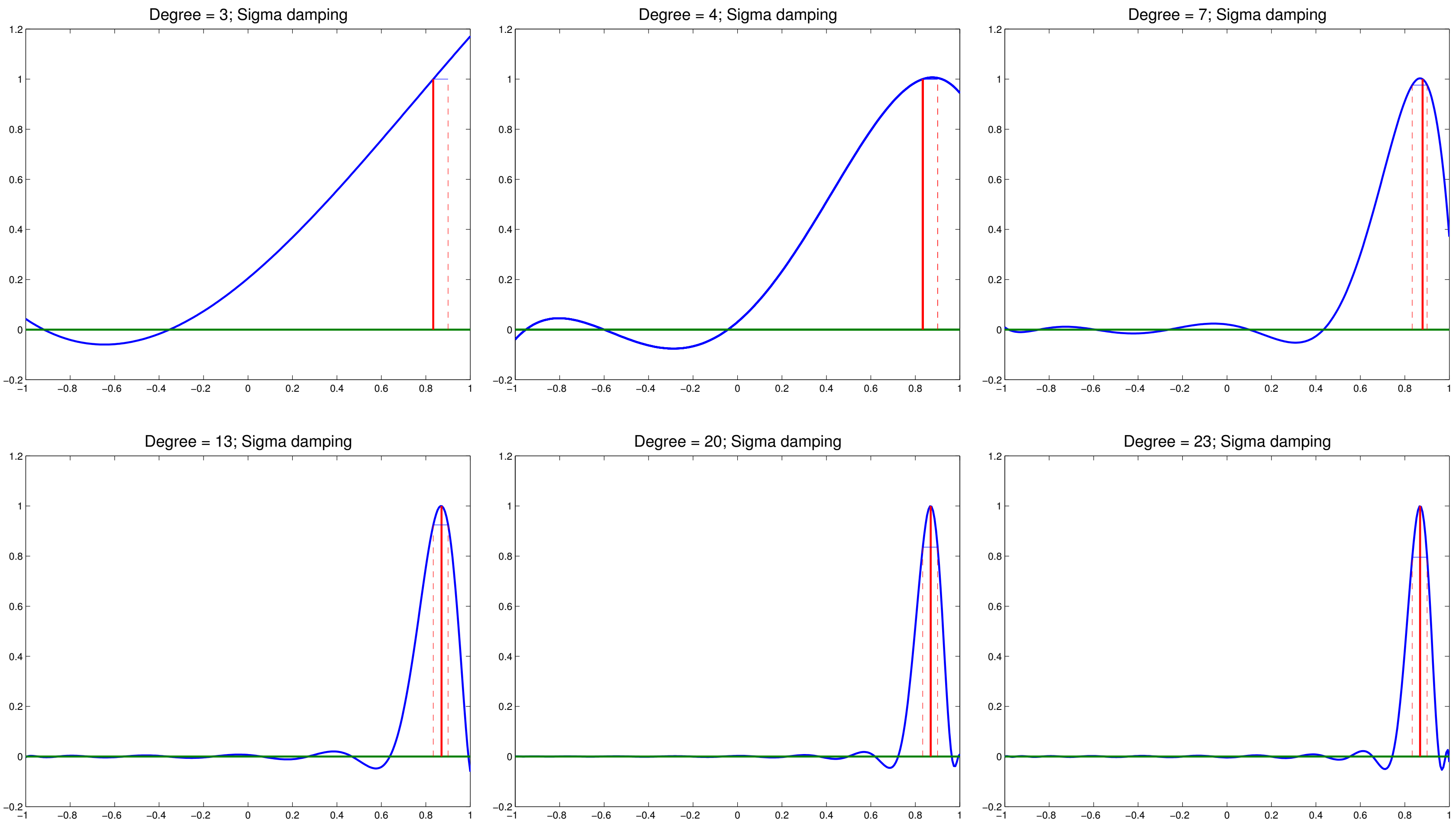
Procedure: Solve the equation $\rho_\gamma(\boldsymbol{\xi}) - \rho_\gamma(\boldsymbol{\eta}) = 0$ with respect to γ, accurately.

Use Newton scheme



Issue # two: Determine degree & polynomial (automatically)

Start low then increase degree until value (s) at the boundary (ies) become small enough - Exple for [0.833, 0.907..]



Which Projection: Lanczos,w/o restarts, Subspace iteration,..

Options:

➤ Subspace iteration: quite appealing in some applications (e.g., electronic structure): Can re-use previous subspace.

➤ Simplest: (+ most efficient) Lanczos without restarts

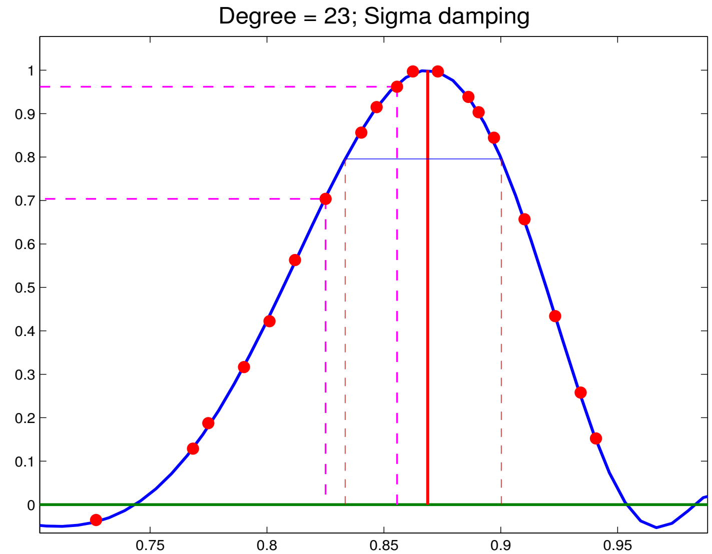
➤ Lanczos with Thick-Restarting [TR Lanczos, Stathopoulos et al ’98, Wu & Simon’00]

➤ Crucial tool in TR Lanczos: deflation (’Locking’)

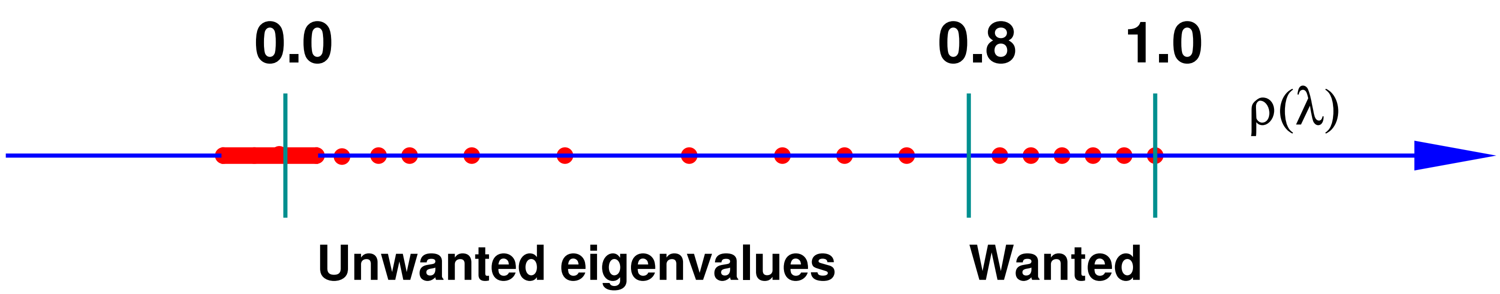
Main idea: *Keep extracting eigenvalues in interval $[\xi, \eta]$ until none are left [remember: deflation]*

➤ If filter is good: Can catch all eigenvalues in interval thanks to deflation + Lanczos.

Polynomial filtered Lanczos: No-Restart version

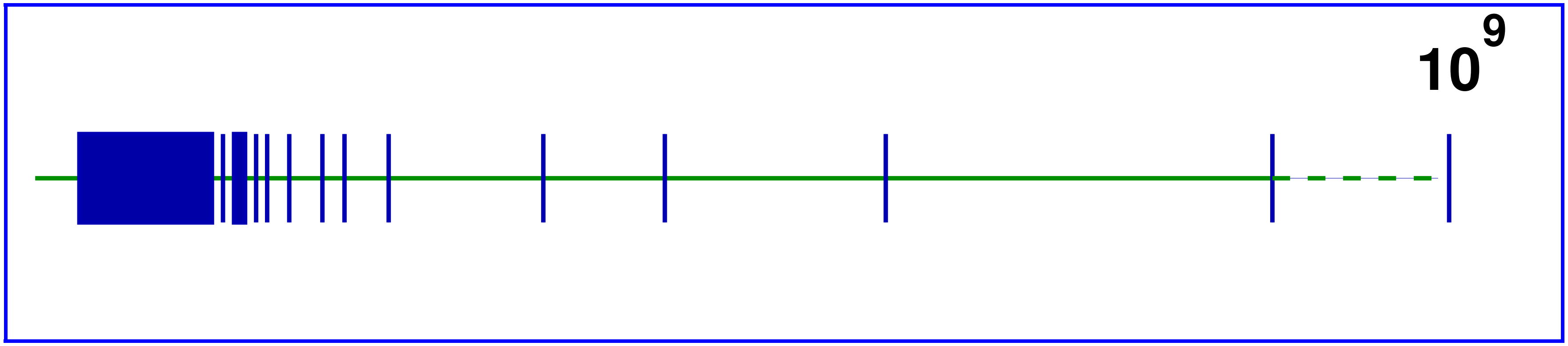


- Use Lanczos with full reorthogonalization on $\rho(A)$. Eigenvalues of $\rho(A)$: $\rho(\lambda_i)$
- Accept if $\rho(\lambda_i) \geq \texttt{bar}$
- Ignore if $\rho(\lambda_i) < \texttt{bar}$



Rational filters: Why?

➤ Consider a spectrum like this one:



➤ Polynomial filtering utterly ineffective for this case

➤ Second issue: situation when Matrix-vector products are expensive

➤ Generalized eigenvalue problems.

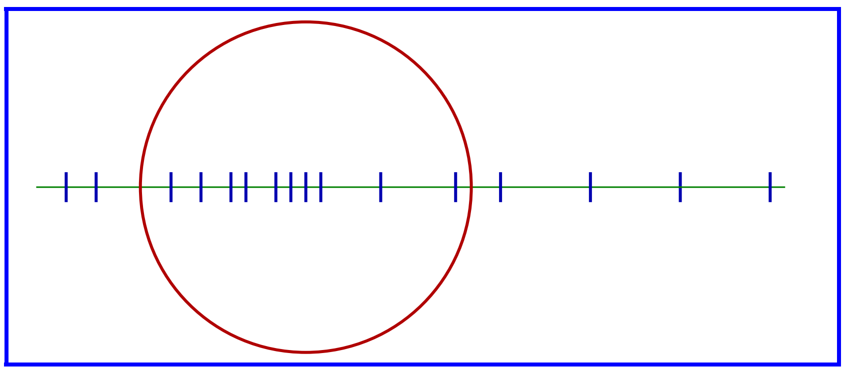
- Alternative is to use rational filters:

$$\phi(z) = \sum_j \frac{\alpha_j}{z-\sigma_j}$$

$$\phi(A) = \sum_j \alpha_j (A - \sigma_j I)^{-1}$$

$\rightarrow$ We now need to solve linear systems

- Tool: Cauchy integral representations of spectral projectors



$$P = \frac{-1}{2i\pi} \int_\Gamma (A - sI)^{-1} ds$$

- Numer. integr. $P \rightarrow \tilde{P}$
- Use Krylov or S.I. on $\tilde{P}$

- Sakurai-Sugiura approach [Krylov]

- FEAST [Subs. iter.] (E. Polizzi)

The Gauss viewpoint: Least-squares rational filters

- Given: poles $\sigma_1, \sigma_2, \cdots, \sigma_p$
- Related basis functions $\phi_j(z) = \frac{1}{z-\sigma_j}$

Find $\phi(z) = \sum_{j=1}^{p} \alpha_j \phi_j(z)$ that minimizes

$$\int_{-\infty}^{\infty} w(t)|h(t) - \phi(t)|^2 dt$$

- $h(t)$ = step function $\chi_{[-1,1]}$.
- $w(t)$= weight function.

For example $a = 10$, $\beta = 0.1$

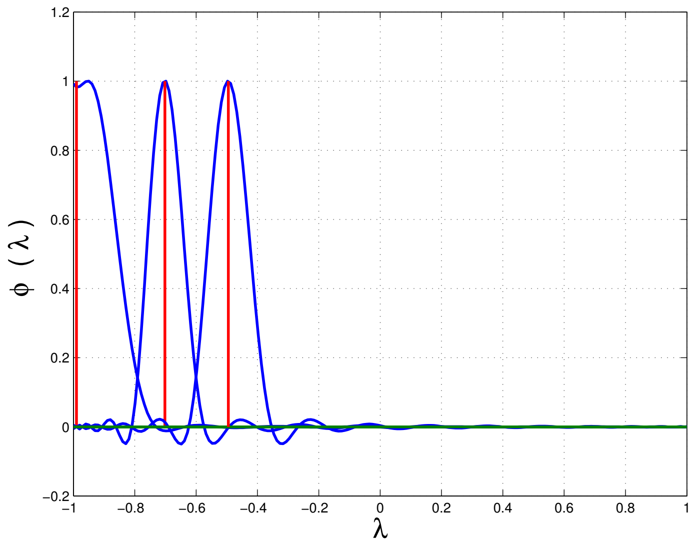
$$w(t) = \begin{cases} 0 \text{ if } & |t| > a \\ \beta \text{ if } & |t| \le 1 \\ 1 \text{ else} & \end{cases}$$

- Many advantages

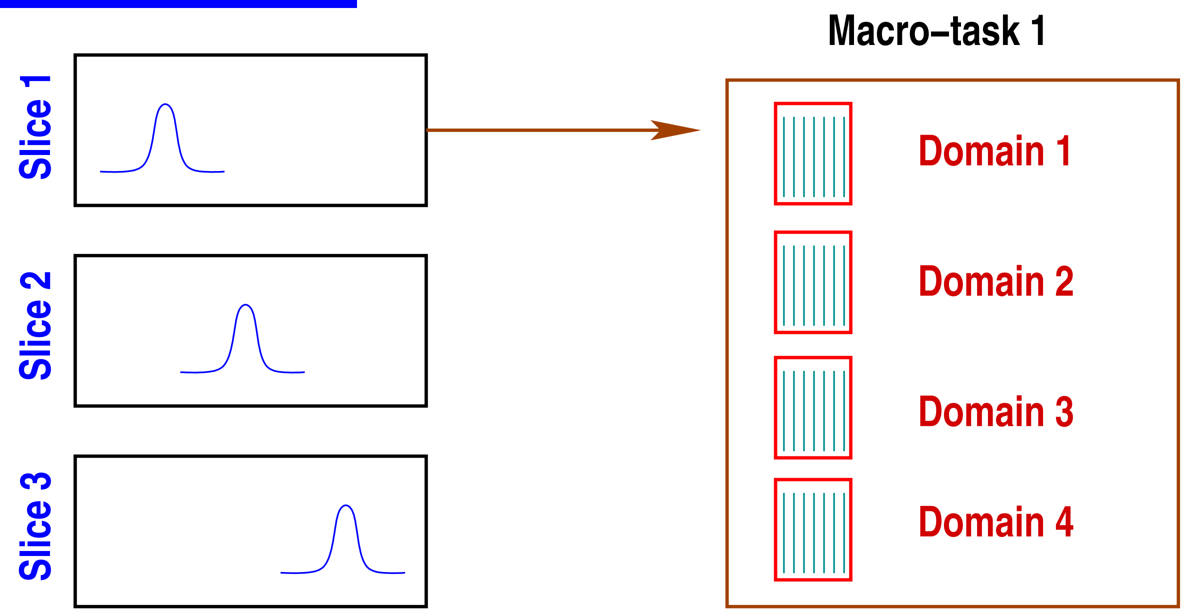
Spectrum Slicing and the EVSL project

- EVSL package now at version 1.1.x
- Uses polynomial and rational filtering: Each can be appealing in different situations.

Spectrum slicing: Invokes Kernel Polynomial Method or Lanczos quadrature to cut the overall interval containing the spectrum into small sub-intervals.

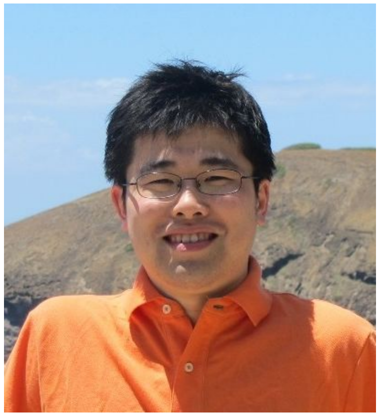


Levels of parallelism



The two main levels of parallelism in EVSL

EVSL Main Contributors (version 1.1.0+) & Support



- Ruipeng Li
LLNL

- Yuanzhe Xi
Post-doc (UMN)

- Luke Erlandson
UG Intern (UMN)

➤ Work supported by NSF (also past work: DOE)

➤ See web-site for details:

`http://www-users.cs.umn.edu/~saad/software/EVSL/`

EVSL: current status & plans

Version _1.0 Released in Sept. 2016

- Matrices in CSR format (only)
- Standard Hermitian problems (no generalized)
- Spectrum slicing with KPM (Kernel Polynomial Meth.)
- Trivial parallelism across slices with OpenMP
- Methods:
  - Non-restart Lanczos – polynomial & rational filters
  - Thick-Restart Lanczos – polynomial & rational filters
  - Subspace iteration – polynomial & rational filters

Version _1.1.x V_1.1.0 Released back in August 2017.

- general `matvec` [passed as function pointer]
- $\boldsymbol{Ax = \lambda Bx}$
- Fortran (03) interface.
- Spectrum slicing by Lanczos and KPM
- Efficient Spectrum slicing for $\boldsymbol{Ax = \lambda Bx}$ (no solves with $\boldsymbol{B}$).

Version _1.2.x pEVSL – In progress

- Fully parallel version [MPI + openMP]

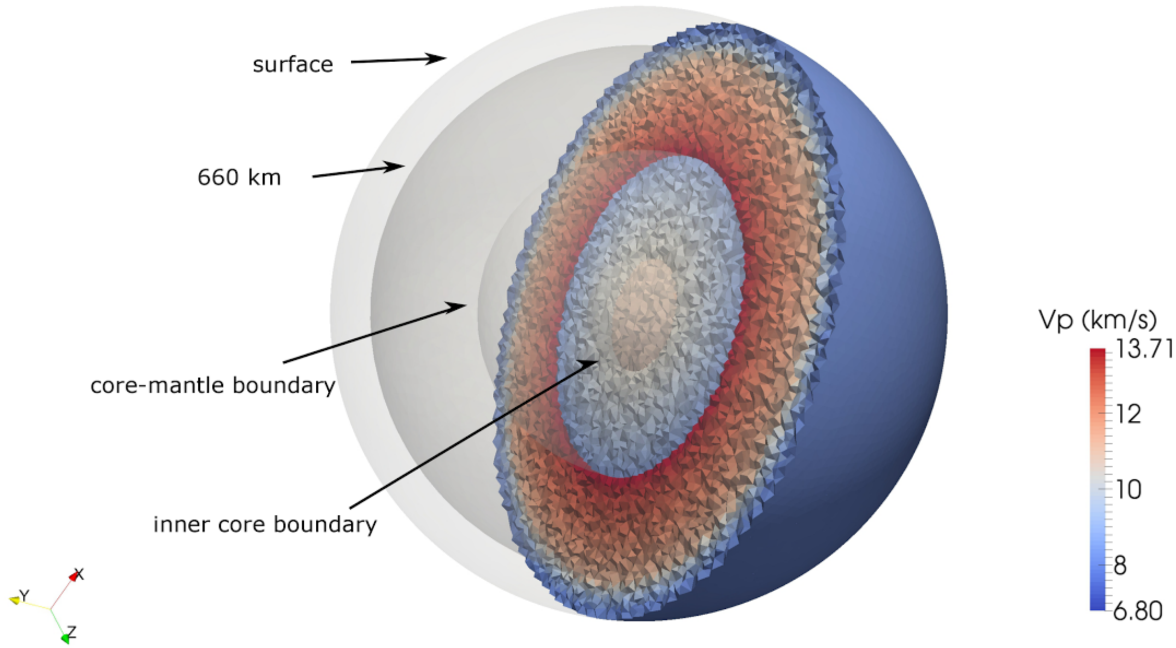
Spectrum slicing and the EVSL package

- All eigenvalues in $[0,\ 1]$ of of a 49^3 discretized Laplacian
- eigs(A,1971,'sa'): 14830.66 sec
- Solution: Use DOS to partition $[0,\ 1]$ into 5 slices
- Polynomial filtering from EVSL on Mesabi MSI, 23 threads/slice

$[a_i, a_{i+1}]$	# eigs	CPU time (sec)			max residual
		matvec	orth.	total	
$[0.00000, 0.37688]$	386	1.31	18.26	28.66	2.5×10^{-14}
$[0.37688, 0.57428]$	401	3.28	38.25	56.75	8.7×10^{-13}
$[0.57428, 0.73422]$	399	4.69	36.47	56.73	1.7×10^{-12}
$[0.73422, 0.87389]$	400	5.97	38.60	61.40	6.6×10^{-12}
$[0.87389, 1.00000]$	385	6.84	36.16	59.45	4.3×10^{-12}

➤ Grand tot. = 263 s. Time for slicing the spectrum: 1.22 sec.

Computing the Earth normal modes



- Collaborative effort: Rice-UMN:
  J. Shi, R. Li, Y. Xi, YS, and M. V. De Hoop
- FEM model leads to a generalized eigenvalue problem:

$$\begin{bmatrix} A_s & & E_{fs} \\ & 0 & A_d \\ E_{fs}^T & A_d^T & A_p \end{bmatrix} \begin{bmatrix} u^s \\ u^f \\ p^e \end{bmatrix} = \omega^2 \begin{bmatrix} M_s & & \\ & M_f & \\ & & 0 \end{bmatrix} \begin{bmatrix} u^s \\ u^f \\ p^e \end{bmatrix}$$

- Want all eigen-values/vectors inside a given interval
- Issue 1: ‘mass’ matrix has a large null space..
- Issue 2: interior eigenvalue problem
- Solution for 1: change formulation of matrix problem [eliminate p^e ...]

➤ New formulation :

$$\underbrace{\left\{\begin{pmatrix} A_s & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} E_{fs} \\ A_d \end{pmatrix} A_p^{-1} \begin{pmatrix} E_{fs}^T & A_d^T \end{pmatrix}\right\}}_{\widehat{A}} \begin{pmatrix} u^s \\ u^f \end{pmatrix} =$$

$$\omega^2 \underbrace{\begin{pmatrix} M_s & 0 \\ 0 & M_f \end{pmatrix}}_{\widehat{M}} \begin{pmatrix} u^s \\ u^f \end{pmatrix}$$

➤ Use polynomial filtering – need to solve with $\widehat{M}$ but ...

- ... severe scaling problems if direct solvers are used

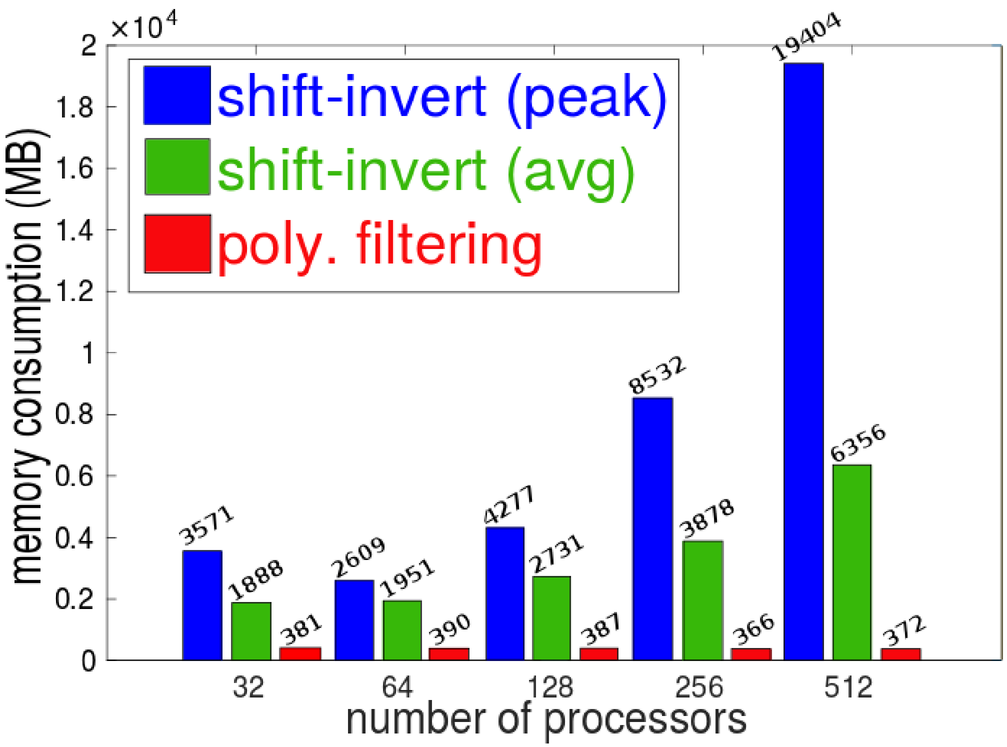
Hence:

➤ Replace action of M^{-1} by a low-deg. polynomial in M [to avoid direct solvers]

➤ Memory : parallel shift-invert and polynomial filtering

Machine: Comet, SDSC

Matrix size	# Proc.s
$\mathbf{591,303}$	32
$\mathbf{1,157,131}$	64
$\mathbf{2,425,349}$	128
$\mathbf{4,778,004}$	256
$\mathbf{9,037,671}$	512



Recent: weak calability test for different solid (Mars-like) models on TACC Stampede2

nn/np	Mat-size	Av (ms)	$\leftarrow$ Eff.	Mv (ms)	$\leftarrow$ Eff.	$M^{-1}v$ (μs)	$\leftarrow$ Eff.
2/96	1,038,084	1760	1.0	495	1.0	0.01044	1.0
4/192	2,060,190	1819	0.960	568	0.865	0.0119	0.870
8/384	3,894,783	1741	0.948	571	0.813	0.0119	0.825
16/768	7,954,392	1758	0.959	621	0.763	0.0129	0.774
32/1536	15,809,076	1660	1.009	572	0.824	0.0119	0.834
64/3072	31,138,518	1582	1.043	566	0.820	0.0117	0.837
128/6144	61,381,362	1435	1.133	546	0.838	0.0113	0.851
256/12288	120,336,519	1359	1.173	592	0.757	0.01221	0.774

Conclusion

- `EVSL` code available here: [Current version: version 1.1.1]

  `www.cs.umn.edu/~saad/software/EVSL`

- `EVSL` Also on github (development)

Plans: (1) Release fully parallel code; (2) Block versions; (3) Iterative solvers for rational filt.; (4) Nonhermitian case;

- Earth modes calculations done with fully parallel code
  $\longrightarrow$ Not quite ready for distribution

A final note: Scalability issues with parallel direct solvers ...

- ... Needed: iterative solvers for the highly indefinite case