Linear and Nonlinear “SP^2” Methods for Large Scale Eigenvalue Calculations

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Workshop on Recent Advances in Numerical Methods for Eigenvalue Problems
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Linear and Nonlinear “SP²” Methods for Large Scale Eigenvalue Calculations

(SP² = Structure-Preserving Subspace Projection)

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Two parts of this talk

- Part I: Linear problems
  *Algebraic Substructuring* for eigenvalue and frequency response calculations

- Part II: Nonlinear problems
  *Nonlinear Rayleigh-Ritz Iterative (NRRIT)* technique for solving nonlinear eigenvalue problems
Part I

Algebraic Substructuring for Eigenvalue and Frequency Response Calculations

joint work with

X. S. Li, C. Yang, P. Husbands, E. Ng
LBNL

W. Gao
Fudan University, China

J. H. Ko
Konkuk University, South Korea
EIG and FRA

- **EIG (eigenvalue problem)**

\[
Kq = \lambda Mq \quad \overset{\sigma}{\longrightarrow} \quad K^{\sigma}q = \lambda^{\sigma} Mq
\]

where

\[
K^{\sigma} = K - \sigma M, \quad \lambda^{\sigma} = \lambda - \sigma
\]

- **FRA (frequency response calculation)**

\[
H(\omega) = l^T(K - \omega^2 M + i\omega D)^{-1} b = l^T [\gamma_1(\omega)K^{\sigma} + \gamma_2(\omega, \sigma)M]^{-1} b
\]

\[
\uparrow
\]

\[
\sigma, \quad D = \alpha K + \beta M
\]

where

\[
\gamma_1(\omega) = 1 + i\omega \alpha
\]

\[
\gamma_2(\omega, \sigma) = -\omega^2 + \sigma + i\omega(\sigma \alpha + \beta),
\]
Substructuring methods

- Eigenvalue and frequency response calculations are ubiquitous.
- Substructuring techniques dates back to the 1960s (CMS)
- Substructuring holds great promise for solving extremely large scale problems, e.g., AMLS
- Issues as the techniques extended for broader applications:
  - Extraction of arbitrary eigenmodes
  - High frequency response calculations
  - Accuracy enhancement
  - Performance tuning
Outline of Part I

1. Substructure partition and reduction (projection)
2. **ASEIG**: eigenvalue calculation
3. **ASFRA**: frequency response calculation
4. Remarks
Substructure partition

- Single-level

\[
K^\sigma = \begin{bmatrix}
K_{11}^\sigma & K_{13}^\sigma \\
K_{22}^\sigma & K_{23}^\sigma \\
K_{31}^\sigma & K_{32}^\sigma & K_{33}^\sigma
\end{bmatrix}
\]

\[
M = \begin{bmatrix}
M_{11} & M_{13} \\
M_{22} & M_{23} \\
M_{31} & M_{32} & M_{33}
\end{bmatrix}
\]

- Multi-level (nested dissection)

![Diagram](image)

e.g., by METIS of Karypis and Kumar
Substructure reduction (projection) I.1

- Block elimination matrix $L$

$$\tilde{K}^\sigma = L^{-T} K^\sigma L^{-1} = \begin{bmatrix} K_{11}^\sigma & \hat{K}_{22}^\sigma \\ \hat{K}_{33}^\sigma & \end{bmatrix}, \quad \tilde{M} = L^{-T} M L^{-1} = \begin{bmatrix} M_{11} & \hat{M}_{13} \\ \hat{M}_{31} & M_{32} & \hat{M}_{33} \end{bmatrix}$$

- Extraction of local modes

$$S_m = \begin{bmatrix} S_1 \\ S_2 \\ S_3 \end{bmatrix} \leftarrow \begin{bmatrix} (K_{11}^\sigma, M_{11}) \\ (K_{22}^\sigma, M_{22}) \end{bmatrix} \leftarrow (\hat{K}_{33}^\sigma, \hat{M}_{33})$$

- Subspace projection onto span$\{S_m\}$

$$K_m^\sigma = S_m^T \tilde{K}^\sigma S_m = \begin{bmatrix} k_{11}^\sigma & k_{22}^\sigma \\ k_{22}^\sigma & \hat{k}_{33}^\sigma \end{bmatrix}, \quad M_m = S_m^T \tilde{M} S_m = \begin{bmatrix} m_{11} & \hat{m}_{13} \\ m_{22} & \hat{m}_{23} \\ \hat{m}_{31} & \hat{m}_{32} & \hat{m}_{33} \end{bmatrix}$$
Eigenvalue calculation

- Projected (smaller) eigenvalue problem:
  \[ K_m^\sigma \Phi = M_m \Phi \Theta^\sigma, \]

- “Global” eigenpairs:
  \[ \Theta^\sigma = \text{diag}(\theta^\sigma) = \text{diag}(\Theta_l^\sigma, \Theta_n^\sigma, \Theta_r^\sigma) \]
  \[ \Phi = (\phi) = [ \Phi_l \Phi_n \Phi_r ] \]

- Retained modes: \( \Phi_n \) (determined by “global cutoff values”)
- Truncated modes: \( \Phi_t = [ \Phi_l \Phi_r ] \)

- Ritz pairs \( (\Theta_n^\sigma + \sigma, L^{-1} S_m \Phi_n) \approx (\lambda, q)’s \text{ of } (K, M) \)

- Why does it work, ... [Yang et al], [Voss et al], ...
AS algorithm for eigenvalue computation

0. Substructure partition, if necessary
1. Block elimination and congruence transformation
2. Mode selection/computation for sub-structures and separators
3. Subspace assembling
4. Projection calculation
5. Projected eigenvalue problem
• Major operations:
  1. Congruence transformations and projection
  2. projected eigenvalue problem

• Cost
  1. flops: more than a single sparse Cholesky factorization
  2. storage: Block Cholesky factors + projected matrices + ... 

But no triangular solvers, no (re)-orthogonalization ... vs. SIL

• ASEIG package [ACM TOMS ’08]
  1. interleaves steps 1-4 computations
  2. recomputes some of intermediate matrix blocks instead of storing

  50% of memory saving trade with 15% recomputes time
Case study: accelerator cavity design (SLAC)

- EMC simulation for accelerator design

- Challenges:
  1. Small eigenvalues (tightly clustered) out of a large-eigenvalue dominated eigenspectrum: many small nonzero eigenvalues desired
  2. Large null space in the stiffness matrix $K$
  3. Requires high accuracy for eigenpairs
Case study: accelerator cavity design (SLAC)

Performance results:

- A 6-cell DDS realistic structure, $N = 65,740$
- 4-level AS, $n_{\text{proj}} \approx 3K$

- SIL (shift-Invert Lanczos) requires multiple shifts (factorizations)
Frequency response calculation on $[\omega_{\text{min}}, \omega_{\text{max}}]$ I.3

- $H(\omega)$-projection onto $\text{span}\{L^{-1}S_m\}$:

$$H_m(\omega) = l_m^T (\gamma_1 K_m^\sigma + \gamma_2 M_m)^{-1} b_m = l^T p_m(\omega)$$

- **Frequency response equation**

$$\left(\gamma_1 K_m^\sigma + \gamma_2 M_m\right) p_m(\omega) = b_m$$

- Recall: global modes $\Phi = (\phi) = [\Phi_l \Phi_n \Phi_r]$ of $(K_m^\sigma, M_m)$

- Partition

$$p_m(\omega) = p_n(\omega) + p_t(\omega)$$

and

$$p_n(\omega) \in \text{span}\{\Phi_n\}, \quad p_t(\omega) \in \text{span}\{[\Phi_l \Phi_r]\}$$
• Phase 1: compute $p_n(\omega)$ directly

$$p_n(\omega) = \Phi_n (\gamma_1 \Theta_n + \gamma_2 I)^{-1} \Phi_n^T b_m.$$ 

• Phase 2: compute $p_t(\omega)$ iteratively

– iterative refinement

$$p_t^\ell(\omega) = p_t^{\ell-1}(\omega) + \Delta p_t^\ell(\omega),$$

– Initial $p_t^0(\omega)$ given by an extrapolation from the previous frequency point $\omega'$

– Gerlerkin projection approximation for solving

$$G_m(\omega) \Delta p_t^\ell(\omega) = r_m^{\ell-1}(\omega)$$

– Frequency sweeping iteration (FSI)

$$p_t^\ell(\omega) = p_t^{\ell-1}(\omega) + \frac{1}{\gamma_1} \left[ (K_m^{-1} - \Phi_n (\Theta_n)^{-1} \Phi_n^T) r_m^{\ell-1}(\omega) \right] \approx \Delta p_t^\ell(\omega)$$

• ... [Bennighof and Kaplan] ... [Ko and B.]
What local eigenmodes to retain?

- Convergence analysis of FSI \( \implies \) cutoff values for the modes \( \Phi_n \) to be retained

- Truncated modal residuals

\[
\Phi_t^T r_m^\ell(\omega) = -\frac{\gamma_2}{\gamma_1} \Theta^\sigma \Phi_t^T r_m^{\ell-1}(\omega).
\]

- Contraction for the truncated mode \( \Phi_t = (\phi_k) \):

\[
\left| \frac{\phi_k^T r_m^\ell(\omega)}{\phi_k^T r_m^{\ell-1}(\omega)} \right| \leq \frac{d_{\text{max}}}{|\theta^\sigma_k|} \leq \xi < 1,
\]

where

\[
d_{\text{max}} = \max\{d(\omega_k, \sigma), 1 \leq k \leq n_f\}, \quad d(\omega, \sigma) = \left| -\frac{\gamma_2}{\gamma_1} \right|
\]

- Global cutoff values (to determine retained modes \( \Phi_n \)) of \( (K^\sigma_m, M_m) \):

\[
\lambda_{\text{min}}^\sigma = -\frac{d_{\text{max}}}{\xi} \quad \text{and} \quad \lambda_{\text{max}}^\sigma = \frac{d_{\text{max}}}{\xi}.
\]

i.e., retained eigenpairs of the original matrix pair \((K, M)\) within

\[
[\lambda_{\text{min}}, \lambda_{\text{max}}] = \left[ \sigma - \frac{d_{\text{max}}}{\xi}, \sigma + \frac{d_{\text{max}}}{\xi} \right]
\]
• Initial steps: $\sigma$, ... cutoff values

• Compute $K_{m}^{\sigma}$, $M_{m}$, $b_{m}$, $l_{m}$

• Compute the retained eigenpairs $(\Theta_{n}^{\sigma}, \Phi_{n})$ of $(K_{m}^{\sigma}, M_{m})$

• FSI:
  
  – calculate $p_{n}(\omega_{k})$ by retained modes $\Phi_{n}$
  – set the initial response $p_{t}^{0}(\omega_{k})$
  – $\ell$–loop for the frequency point $\omega_{k}$
    
    * update residual $r_{m}^{\ell-1}(\omega_{k})$
    * calculate the correction $\Delta p_{t}^{\ell}(\omega_{k})$
    * test for convergence ...
    * compute $p_{t}^{\ell}(\omega_{k})$

  – $p_{m}(\omega_{k}) = p_{n}(\omega_{k}) + p_{t}^{\ell}(\omega_{k})$

  – $H_{m}(\omega_{k}) = l_{m}^{T}p_{m}(\omega_{k})$
Case study: checkerboard filter

- FE simulation of a prototype checkerboard MEMS resonator for a high-frequency bandpass filter for, e.g., the surface acoustic wave devices

The SEM picture of a fabricated device and FE models courtesy of David Bindel, Sunil Behave, Roger Howe.
- $N = 15258$, $[f_{\text{min}}, f_{\text{max}}] = [230, 250]\text{MHz}$,
**Performance**

<table>
<thead>
<tr>
<th>checkerboard filter $N = 15258$</th>
<th>Direct Solution</th>
<th>SIL</th>
<th>ASFRA$^0$</th>
<th>ASFRA</th>
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<tbody>
<tr>
<td>$m$ (AS subspace)</td>
<td>–</td>
<td>–</td>
<td>1635</td>
<td>307</td>
</tr>
<tr>
<td>$n$ (retained modes)</td>
<td>–</td>
<td>242</td>
<td>231</td>
<td>37</td>
</tr>
<tr>
<td>Total FS iter</td>
<td>–</td>
<td>–</td>
<td>96</td>
<td>145</td>
</tr>
<tr>
<td>Elapsed time (sec.)</td>
<td>1612.6</td>
<td>86.23</td>
<td>208.15</td>
<td>26.72</td>
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</table>
1. **ASEIG + ASFRA** package
   
   General purpose, memory efficient, application tunable, ...

2. Better understanding of AS accuracy and applicability

3. Performance evaluation
   
   Tuning parameters: number of AS levels, local and global cutoff values, stopping criteria, ...

4. To some extent, **ASEIG + ASFRA** generalizes the underlying algorithms, functionality and applicability of commercial viable AMLS of Bennighof *et al.*
Part II

Nonlinear Rayleigh-Ritz ITerative (NRRIT) technique for solving nonlinear eigenvalue problems

joint work with

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Simens

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# SciDAC ESS Team

## Advanced Computations Department

### Accelerator Modeling
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- Z. Li, C. Ng, A. Candel

### Computational Mathematics
- L. Lee, L. Ge, V. Akcelik
- C. Sheng, H. Jiang, E. Prudencio

### Computing Technologies
- N. Folwell, A. Guetz, G. Schussman, R. Uplenchwar

### ISICs – TSTT, TOPS, PERC; SAPP- Stanford, LBNL, UCD

<table>
<thead>
<tr>
<th>LBNL</th>
<th>LLNL</th>
<th>SNL</th>
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<tr>
<td>E. Ng, W. Gao, P. Husbands, X. Li, C. Yang</td>
<td>L. Diachin, D. Brown, K. Chand, B. Henshaw, D. Quinlan</td>
<td>P. Knupp, T. Tautges, K. Devine</td>
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<th>CMU</th>
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<tr>
<td>O. Ghattas</td>
<td>D. Keyes</td>
<td>B. Liao, Z. Bai, K. Ma, H. Yu</td>
<td>G. Golub</td>
<td>M. Shephard, A. Bauer, E. Seol</td>
</tr>
</tbody>
</table>
The ILC is a proposed new electron-positron collider that would allow physicists to answer compelling questions on identity of dark matter to the existence of extra dimensions. In the ILC's design, two facing linear accelerators, each 20 kilometers long, accelerate electrons and positrons to TeV energy using superconducting accelerating cavities.

The Global Design Effort will establish the design of the ILC, focusing the efforts of hundreds of accelerator scientists and particle physicists in North America, Europe and Asia.
Various ILC Cavities

- BCD

Low-Loss

- ICHIRO

SST

STF1
Outline of Part II

1. NEP
2. Initial approximations and ordering
3. NEP methods
4. NRRIT (Nonlinear Arnoldi Method)
5. Numerical experiments
6. Ongoing work
• NEP

\[ T(\lambda)x = 0 \]

where

\[ T(\lambda) = K - \lambda M + E(\lambda), \]

• Origin: Nedelec-type FE discretization of the frequency domain Maxwell’s equation with waveguide BCs [ISH95, KFG+06, Lee05a, Lee05b]

• \( K^T = K \geq 0, M^T = M > 0, W_j^T = W_j \)

• Multiple waveguide modes,

\[ E(\lambda) = i \sum_{j=1}^{p} \sqrt{(\lambda - \sigma_j^2)} \ W_j, \]

\( \sigma_j \) are given nonnegative scalars (cutoff values), \( i = \sqrt{-1} \).

• Future: coupling of multiple waveguide modes, where

\[ E(\lambda) = i \sum_{j=1}^{p} \sqrt{(\lambda - \sigma_j^2)} \ W_j^{TE} + i \sum_{j=1}^{p} \frac{\lambda}{\sqrt{(\lambda - \sigma_j^2)}} \ W_j^{TM} \]
Eigenvalues of interest

• Let $\kappa = \sqrt{\lambda}$,

\[
\text{resonant frequency} \quad = \quad f(\kappa) = \frac{c}{2\pi} \cdot \text{Re}(\kappa),
\]

\[
\text{external } Q_e\text{-value} \quad = \quad Q_e(\kappa) = \frac{1}{2} \cdot \frac{\text{Re}(\kappa)}{\text{Im}(\kappa)}.
\]

• The external $Q_e$-values measure the electromagnetic coupling between the cavity and waveguide and characterize the energy loss.

• Computational task: find eigenvalues $\lambda$ satisfying

\[
\begin{aligned}
\kappa &= \sqrt{\lambda} \text{ is close to the shift value } \sigma_0 = \frac{2\pi}{c} f_0 \text{ and } \\
\lambda &\in \mathcal{D} = \{\lambda \mid \lambda = \kappa^2, \text{Re}(\kappa) > \sigma_0, \text{Im}(\kappa) > 0 \text{ and } Q_e(\kappa) > \hat{Q}_e > 1\},
\end{aligned}
\]

where $f_0$ and $\hat{Q}_e$ are prescribed.
Region for the desired eigenvalues

- ○: “exact” eigenvalues;
- ×: initial approximations

- Real part of square root of eigenvalues
- Imaginary part of square root of eigenvalues

- Region of interest
- $Q_e = 10$
- Shift point

II.1
Initial approximations and ordering

• Linearization via the first order truncation:

\[ T(\lambda) \approx T(\lambda_0) + (\lambda - \lambda_0)T'(\lambda_0) \]

\[ \equiv \hat{K}(\lambda_0) - \lambda \hat{M}(\lambda_0), \]

• Initial approximations:

selected eigenpairs \((\theta_{\ell}, v_{\ell})\) of \((\hat{K}(\sigma_0^2), \hat{M}(\sigma_0^2))\)

• Ordering: selected eigenpairs \((\theta_{\ell}, v_{\ell})\) of

\[ |\theta_{1/2}^{1/2} - \sigma_0| \leq |\theta_{2/2}^{1/2} - \sigma_0| \leq \cdots \leq |\theta_{n/2}^{1/2} - \sigma_0|. \]

• Example:

\[ T(\lambda)x = [K - \lambda M + i\sqrt{(\lambda - \sigma_1^2)} W_1] x = 0 \iff \text{QEP} \]
Initial approximations and ordering

### Region of interest

- \( Q_e = 10 \)
- \( \sigma \): shift point

- \( \circ \): “exact” eigenvalues
- \( \times \): initial approximations
NEP methods for $T(\lambda)x = 0$

- **Newton’s methods:**
  - Inverse Iteration (IIT), Residual Inverse Iteration (RIIT)
  - Nonlinear Rayleigh Quotient Iteration (NRQI)
  - Safeguarded Newton method

- **Linearization Methods:**
  - Picard iteration, Self-Consistent Iteration (SCI)
  - Successive Linear Approximation Method (SLAM)

- **“Nonlinear” Subspace Projection Methods** ← this talk
  - Nonlinear Arnoldi method
  - Nonlinear Rayleigh-Ritz Iterative (NRRIT)

**Must-read papers:**


NRRIT framework:

1. Select a *proper* projection subspace $\mathcal{V}$.
2. Compute a *proper* pair $(\theta, z)$ satisfying the Galerkin condition:
   \[ T(\theta)z \perp \mathcal{V} \quad \text{for} \quad z \in \mathcal{V}. \]
3. Expand or restart the projection subspace $\mathcal{V}$

Origin: Nonlinear Arnoldi method [Betcke and Voss,’04], [Voss,’04]
1. Compute an orthonormal basis $Q$ of the properly selected subspace $\mathcal{V}$ (and initial approximations $(\theta^\ell, v^\ell)$)

2. Compute an eigenpair $(\theta, g)$ with initials $(\theta^\ell, Q^T v^\ell)$ of the reduced NEP

$$T_Q(\theta)g = 0,$$

where

$$T_Q(\theta) = Q^H T(\theta) Q$$

3. Compute Ritz pairs $(\theta, Qg)$ of the original NEP

4. Expand or restart $Q$ as necessary
NRRIT in practice

Key issues:

1. what’s a proper initial projection subspace $\mathcal{V}$?
2. what’s the order to compute the desired eigenvalues (proper ordering of the initial approximations)?
3. how to expand or restart $Q$ when necessary?
Main features of our implementation of NRRIT

1. Proper initial approximations \((\theta^\ell, v^\ell)\):

\[
K - \lambda M \text{ vs. } \tilde{K}(\sigma_0^2) - \lambda\tilde{M}(\sigma_0^2)
\]

2. Ordering \((\theta^\ell, v^\ell)\) by

\[
|\theta_1^{1/2} - \sigma_0| \leq |\theta_2^{1/2} - \sigma_0| \leq \cdots \leq |\theta_n^{1/2} - \sigma_0|.
\]

3. Preserving real symmetry with the projection matrix

\[
Q = \text{orth}([\text{Re}(V) \ \text{Im}(V)]),
\]

4. Structure-preserved reduced NEP

\[
T_Q(\theta)y = 0,
\]

where

\[
T_Q(\theta) = Q^T T(\theta)Q = K_Q - \theta M_Q + i \sum_{j=1}^{p} (\theta - \sigma_j^2)^{1/2} W_{Q,j}
\]

with

\[
K_Q = Q^H K Q, \ M_Q = Q^T M Q \text{ and } W_{Q,j} = Q^T W_j Q.
\]
5. Subspace expansion: with the current Ritz pair \((\sigma, z)\),

\[ v := v - QQ^T v, \quad v = T^{-1}(\sigma_0^2)T(\theta)z \]

and

\[ Q := \begin{bmatrix} Q & \text{Re}(v) & \text{Im}(v) \end{bmatrix} \]

6. Restarting and purging:

(a) restart with \( Q \) by replacing \( v^\ell \leftarrow z \)

(b) purge all vectors \( v \) induced by the initial \((\theta^\ell, v^\ell)\) leading to the failure of convergence

7. Reference:

Example 1: the NEP with one cutoff values, $N = 10102$

$$T(\lambda)x = [K - \lambda M + i\sqrt{(\lambda - \sigma^2_1)}W_1+]x = 0,$$

Equivalent Quadratic Eigenvalue Problem:

$$(\nu^2 M + \nu W + \overline{K})x = 0$$

where $\nu = (\lambda - \sigma^2_1)^{1/2}$, $W = iW_1$ and $\overline{K} = \sigma^2_1 M - K$.

$$\lambda_1$$
SOAR (1.9474685976542845+E02, 4.6015939351662103E-01)
NRRIT (1.9474685976743996+E02, 4.6015939593544449E-01)

$$\lambda_2$$
SOAR ...... 
NRRIT ......
**Numerical experiments**

II.5

Example 2: the NEP with two cutoff values

\[ T(\lambda)x = \left[ K - \lambda M + i\sqrt{\lambda - \sigma_1^2}W_1 + i\sqrt{\lambda - \sigma_2^2}W_2 \right] x = 0, \]

\[ N = 9956, \; \text{nnz}(K) = \text{nnz}(M) = 148318. \; \text{nnz}(W_1) = 57, \; \text{nnz}(W_2) = 293. \]
Example 2: CPU in second:

<table>
<thead>
<tr>
<th>$\epsilon$</th>
<th>IIT</th>
<th></th>
<th>SLAM</th>
<th></th>
<th>NRRIT</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-8}$</td>
<td>15</td>
<td>71.98</td>
<td>12</td>
<td>79.48</td>
<td>46</td>
<td>22.95</td>
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<tr>
<td>$10^{-10}$</td>
<td>18</td>
<td>85.92</td>
<td>16</td>
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<td>22</td>
<td>104.47</td>
<td>20</td>
<td>115.33</td>
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<td>$10^{-14}$</td>
<td>24</td>
<td>113.97</td>
<td>21</td>
<td>120.22</td>
<td>114</td>
<td>57.59</td>
</tr>
</tbody>
</table>

IIT = Inverse ITeration
SLAM = Successive Linear Approximation Method
Convergence threshold:

$$\frac{\| T(\theta) Q g^\ell \|}{\| T(\theta) \| \| Q g^\ell \|} \leq \epsilon \quad \text{for } \ell = 1, 2, \ldots, 10$$
Ongoing work II.6

- Understanding of NRRIT: subspace expansion, restarting, convergence analysis
- Accuracy of computed eigenvalues (external $Q_e$-values)
- Verification: how to enumerate eigenvalues and detect missing ones?
- Recent work of Huang and Su on NEP arising from fiber optic design [Kaufman ’06]:
  \[
  [A + s(\lambda)uu^T]x = \lambda x
  \]
- Large-scale NEP (cut-off values $p = 8 \sim 24$, DOFs $= 10^6 \sim 10^7$)
- SLAC’s Omega3P package for next-generation accelerator design (DOE SciDAC)