An Inner/Outer Loop Free Parallel Method for Interior Eigenvalue Problems

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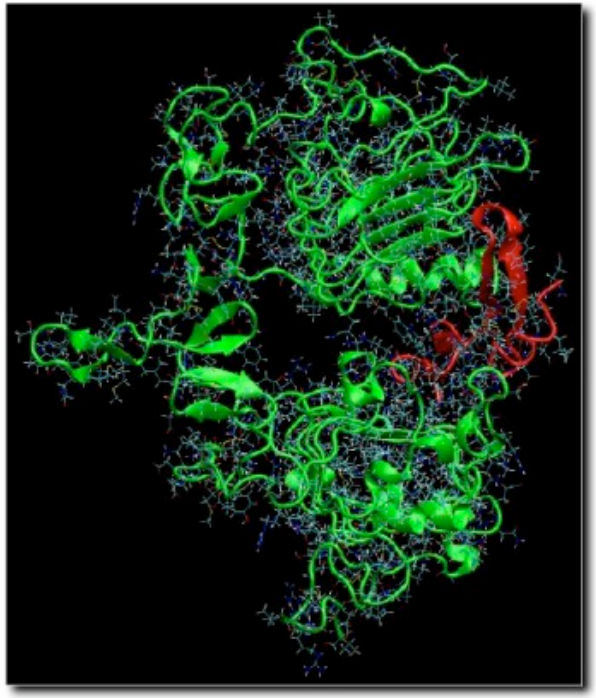
  - Background
  - Target problem & matrix
- A Parallel Eigenvalue Solver
  - An algorithm using contour integration
  - Numerical properties
  - Parallel implementation
- Numerical Examples
- Conclusions

Molecular Orbital Computation

Design of Anticancer Drugs



EGFR
(Epidermal Growth Factor Receptor)

Schrödinger Equation

$$H\Psi = E\Psi$$

Hartree-Fock approximation

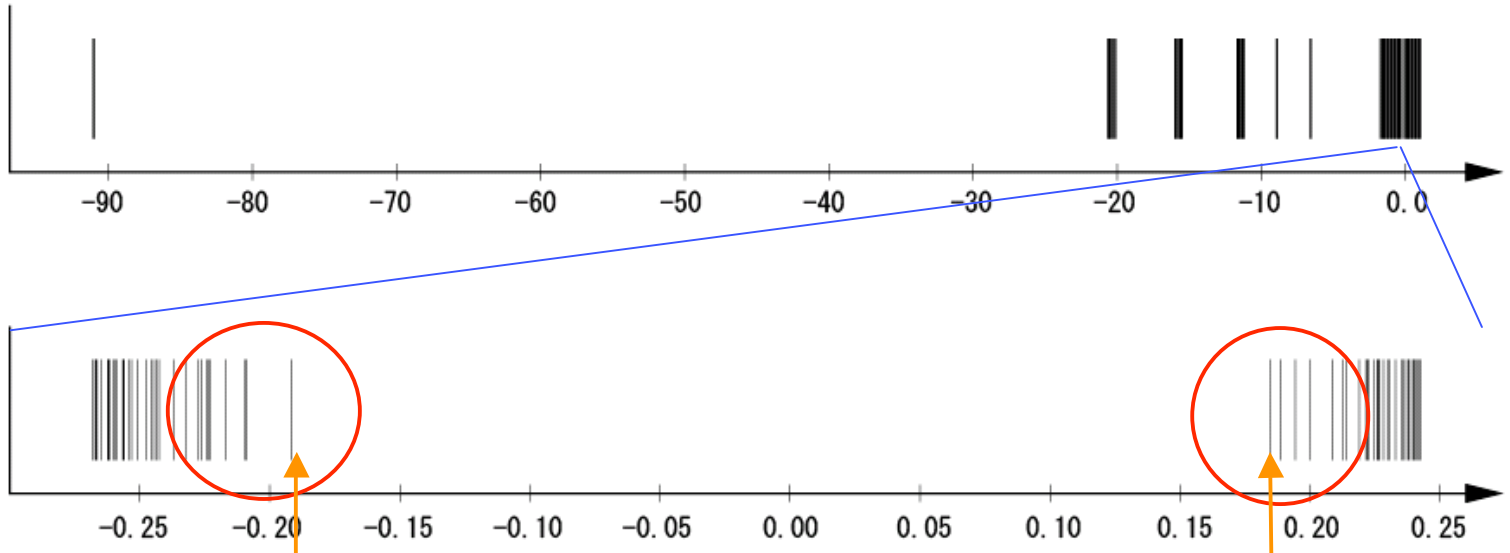
Generalized Eigenvalue Problems

$$A\,\boldsymbol{x} = \lambda\, B\,\boldsymbol{x}$$

(A, B are real symmetric, B is positive definite)

Interior Eigenvalue Problems

Energy state:



HOMO
(Highest Occupied MO)

LUMO
(Lowest Unoccupied MO)

Eigenpairs related to chemical activities:

→ Interior eigenvalue problems

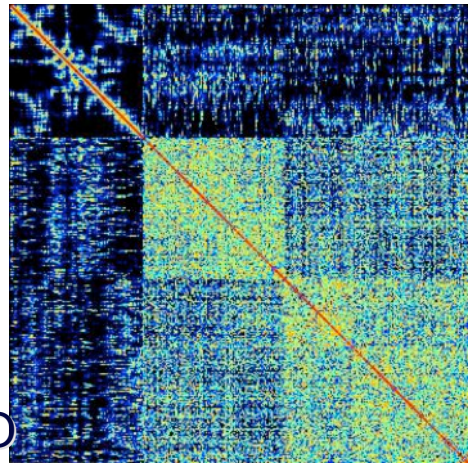
Target Matrix

- The size of matrix:
  50,000 ～ 5,000,000

- The number of nonzero elements:
  200,000,000 ～ 20,000,000,000(est.)

  - relatively large number of nonzero elements

⇒ Semi-sparse matrix



Fock matrix of
Lysozyme + H2O

A Parallel Eigenvalue Solver using Contour Integral

Generalized Eigenvalue Problem

The generalized eigenvalue problem:

$$A\boldsymbol{x} = \lambda B\boldsymbol{x},$$

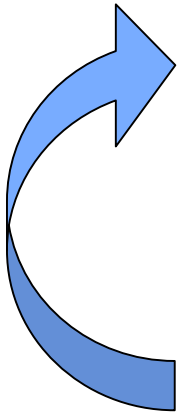
where $A, B \in \mathbb{R}^{n\times n}$ symmetric, and *B* is positive definite.

$(\lambda_j, \boldsymbol{x}_j)$: Eigenpair of the matrix pencil (A, B).

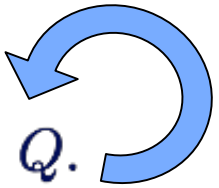
We find eigenpairs in a given interval $[\gamma - \rho, \gamma + \rho]$.

Rayleigh-Ritz Procedure

Algorithm:



1. Construct an orthonormal basis Q.
2. Form $A_Q = Q^{\mathrm{T}} A Q$ and $B_Q = Q^{\mathrm{T}} B Q$.
3. Compute the eigenpairs $(\theta_j, \boldsymbol{w}_j)$ $(1 \le j \le m)$ of (A_Q, B_Q).
4. Set $\boldsymbol{p}_j \leftarrow Q\boldsymbol{w}_j$, $j = 1, \ldots, m$.



Inner Loop

Outer Loop

(A_Q, B_Q) : Projected pencil

θ_j : Ritz value

$\boldsymbol{p}_j$: Ritz vector

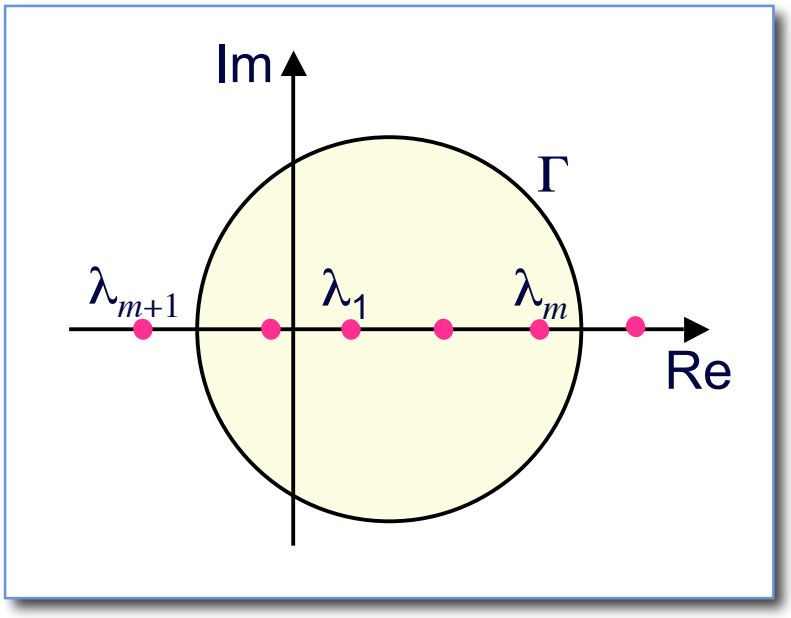
Construction of Subspace

To **avoid inner/outer loops**, we use a contour integral in construction of a subspace.

For a nonzero vector $\boldsymbol{v}$, let

$$\boldsymbol{s}_k = \frac{1}{2\pi \mathrm{i}} \int_\Gamma z^k (zB - A)^{-1} B\boldsymbol{v}\, \mathrm{d}z,$$

where $\Gamma \in \mathbb{C}$ is a Jordan curve that includes $\lambda_1, \ldots, \lambda_m$.



Construction of Subspace

Since

$$(zB - A)^{-1}B\boldsymbol{v} = \sum_{j=1}^{n} \frac{\alpha_j \boldsymbol{x}_j}{z - \lambda_j},$$

where $\alpha_j = \boldsymbol{x}_j^T \boldsymbol{v}$, we have

$$\boldsymbol{s}_k = \frac{1}{2\pi \mathrm{i}} \int_\Gamma z^k (zB - A)^{-1} B\boldsymbol{v}\, \mathrm{d}z = \sum_{j=1}^{m} \alpha_j \lambda_j^k \boldsymbol{x}_j$$

If $\lambda_1, \ldots, \lambda_m$ are simple, then

$$\operatorname{span}\{\boldsymbol{s}_0, \ldots, \boldsymbol{s}_{m-1}\} = \operatorname{span}\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}$$

Construction of Subspace

Block variant is also obtained by using an $n \times L$ matrix

$$V = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_L]$$

instead of a vector $\boldsymbol{v}$.

$$\boldsymbol{s}_k = \frac{1}{2\pi \mathrm{i}} \int_\Gamma z^k (zB - A)^{-1} B \boldsymbol{v} \, \mathrm{d}z$$

$$\Rightarrow \quad S_k = \frac{1}{2\pi \mathrm{i}} \int_\Gamma z^k (zB - A)^{-1} B V \, \mathrm{d}z$$

If the maximum multiplicity of $\lambda_1, \ldots, \lambda_m$ is less than or equal to L, then

$$\mathrm{span}\,\{S_0, \ldots, S_{\tilde{m}-1}\} = \mathrm{span}\,\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}$$

Construction of Subspace

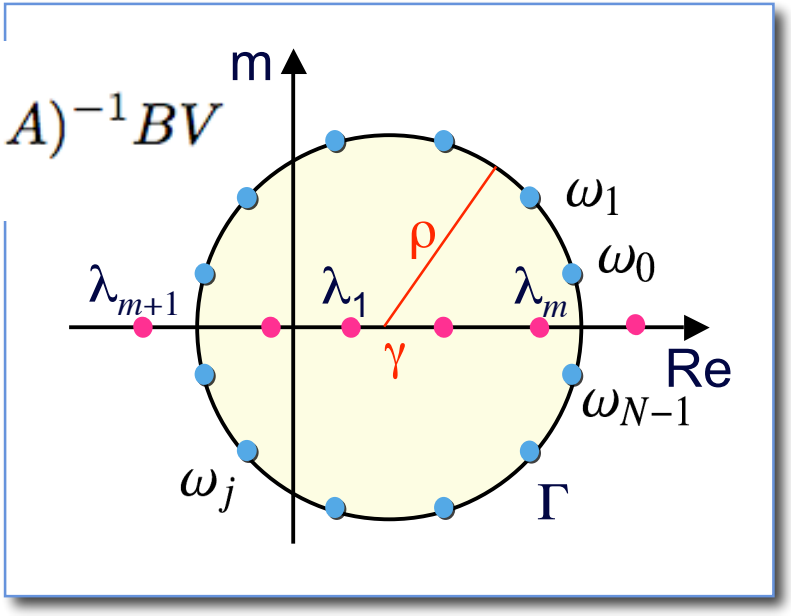
Let Γ be a circle with center γ and radius ρ, then the integration

$$S_k = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} z^k (zB - A)^{-1} BV \, \mathrm{d}z$$

is approximated by *N*-point trapezoidal rule:

$$\hat{S}_k = \frac{1}{N} \sum_{j=0}^{N-1} \left(\frac{\omega_j - \gamma}{\rho} \right)^{k+1} (\omega_j B - A)^{-1} BV$$

where $\omega_j = \gamma + \rho \mathrm{e}^{\frac{2\pi \mathrm{i}}{N}\left(j+\frac{1}{2}\right)}$.



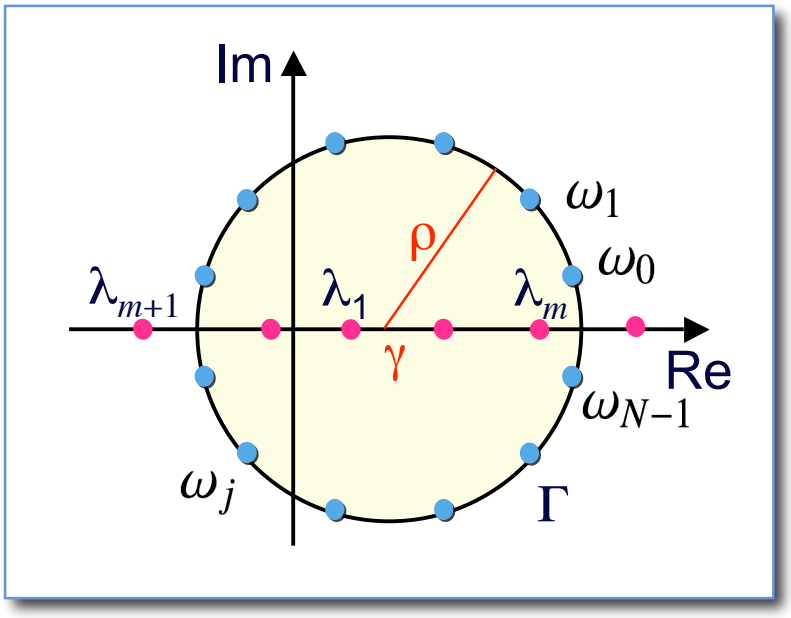
Construction of Subspace

When *A* and *B* are real, we only need *N*/2 points:

$$\hat{S}_k = \frac{2}{N} \sum_{j=0}^{N/2-1} \mathrm{Re}\left(\left(\frac{\omega_j - \gamma}{\rho} \right)^{k+1} Y_j \right),$$

where

$$(\omega_j B - A) Y_j = BV\,.$$



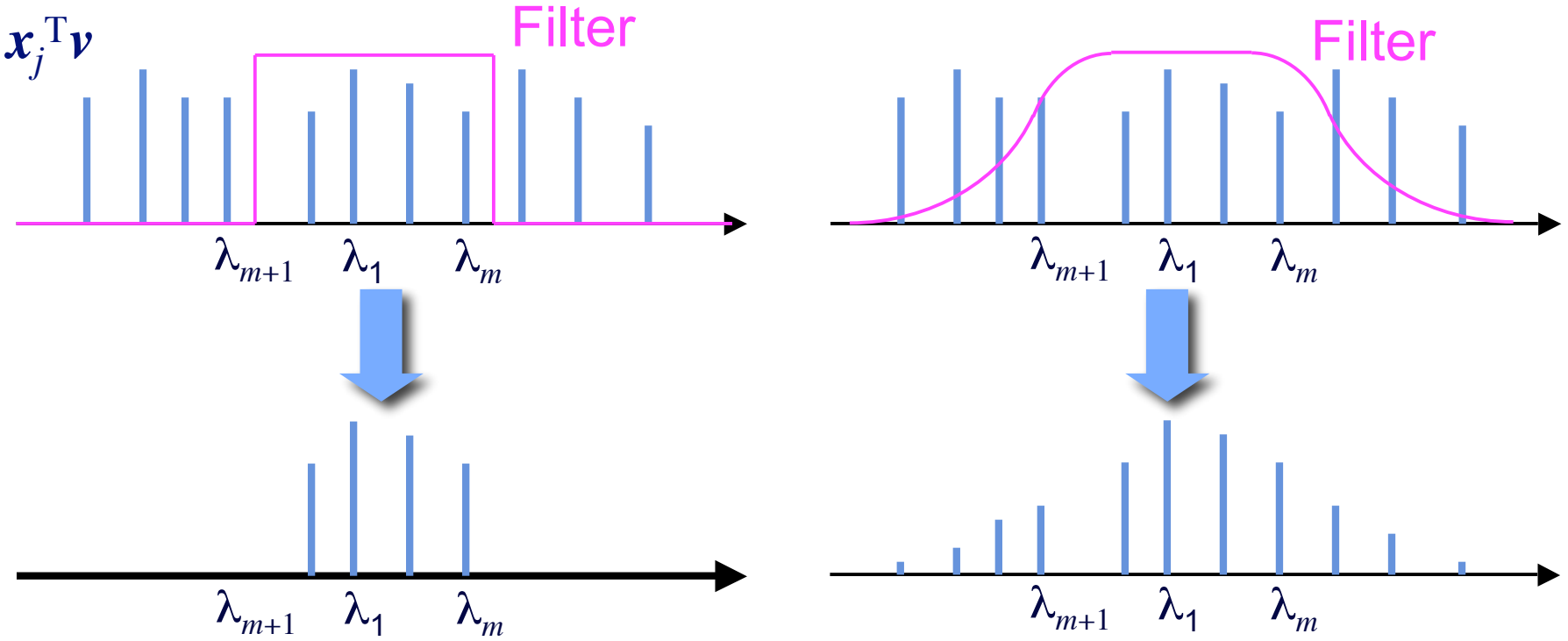
Filter Function

Contour integral:

$$\boldsymbol{s}_k = \frac{1}{2\pi \mathrm{i}} \int_\Gamma z^k (zB - A)^{-1} B\boldsymbol{v} \mathrm{d}z$$

Trapezoidal rule:

$$\hat{\boldsymbol{s}}_k = \frac{1}{N} \sum_{j=0}^{N-1} z^{k+1} (\omega_j B - A)^{-1} B\boldsymbol{v}$$



We set the size of the subspace by SVD of $\hat{S}=\{\hat{S}_0, \hat{S}_1, \ldots\}$.

Algorithm

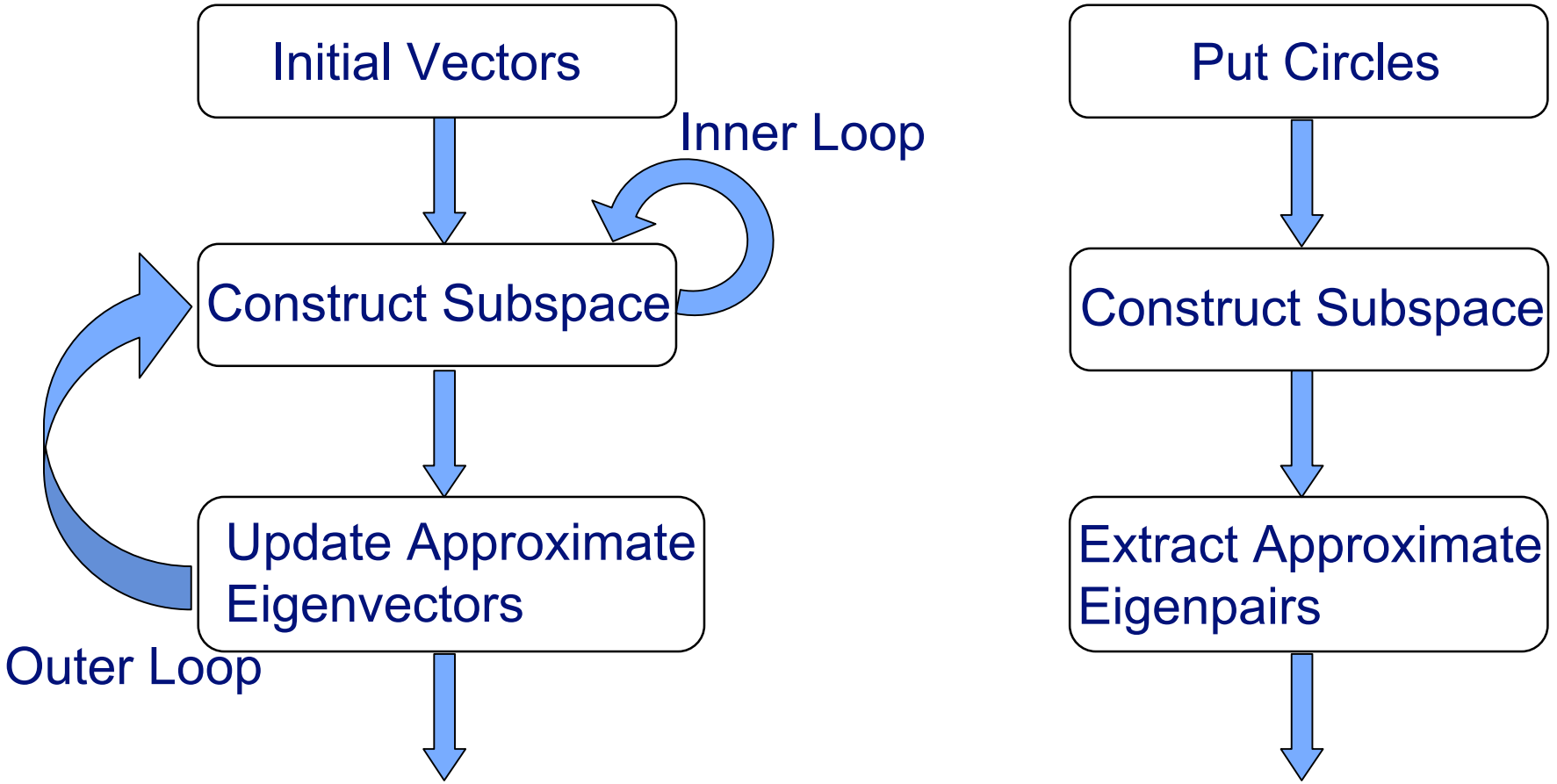
Construction of a subspace

1. Solve $(\omega_j B - A)Y_j = BV$ for Y_j, $j = 0, \ldots, N/2 - 1$
2. Compute $\hat{S}_k = \frac{2}{N} \sum_{j=0}^{N/2-1} \mathrm{Re}\left(\left(\frac{\omega_j - \gamma}{\rho} \right)^{k+1} Y_j \right)$, $k = 0, 1, \ldots, K - 1$
3. Set $\tilde{K}$ using the singular value decomposition of $\hat{S} = [\hat{S}_0, \ldots, \hat{S}_{K-1}]$

Rayleigh-Ritz procedure

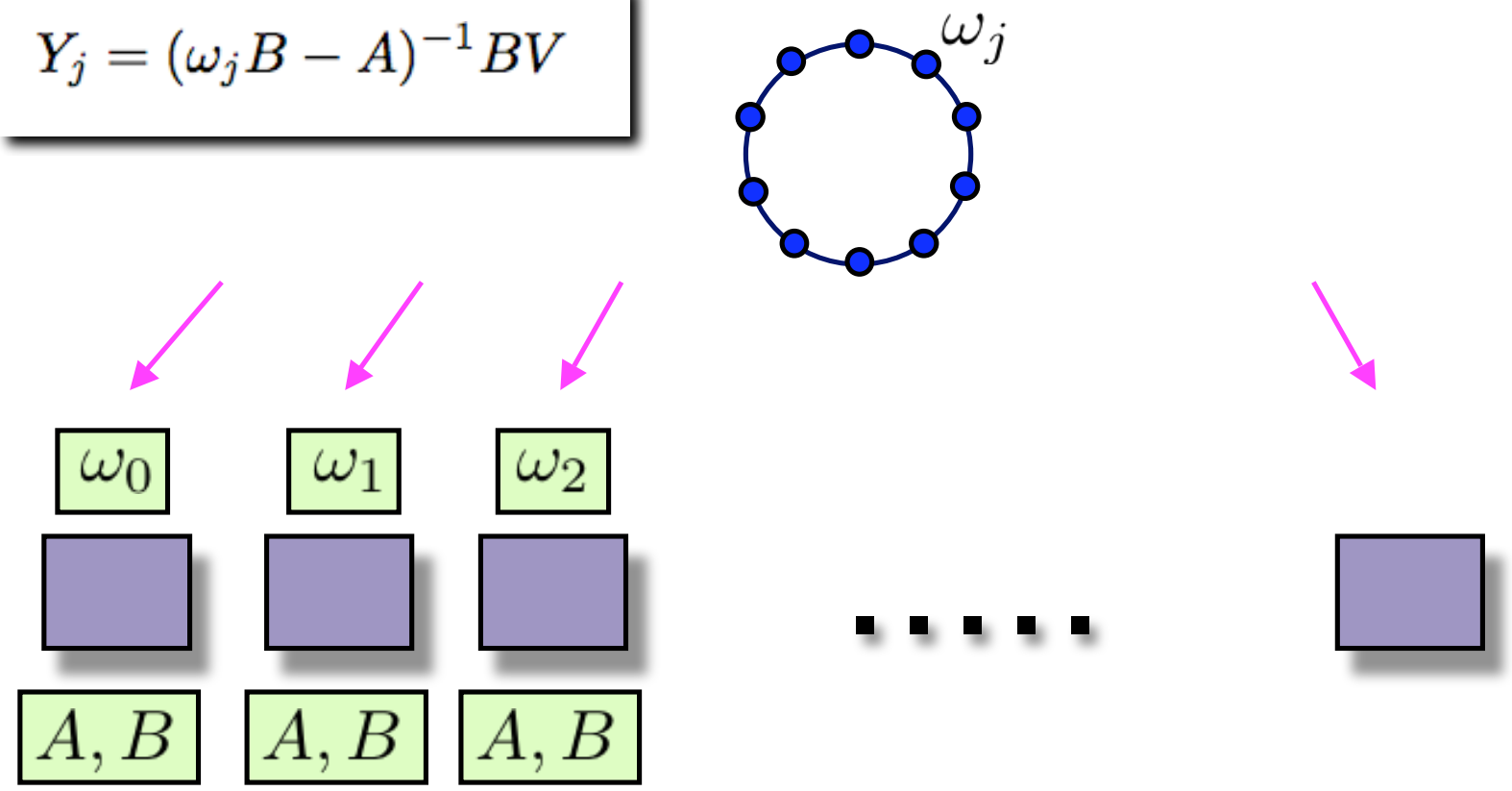
4. Construct an orthonormal basis Q from $\hat{S}(:, 1 : \tilde{K})$
5. Form $A_Q = Q^{\mathrm{T}} A Q$ and $B_Q = Q^{\mathrm{T}} B Q$
6. Compute the Ritz pairs $(\hat{\lambda}_j, \hat{\boldsymbol{x}}_j)$, $1 \leq j \leq \tilde{K}$ with the projected pencil (A_Q, B_Q)

Flow of the method



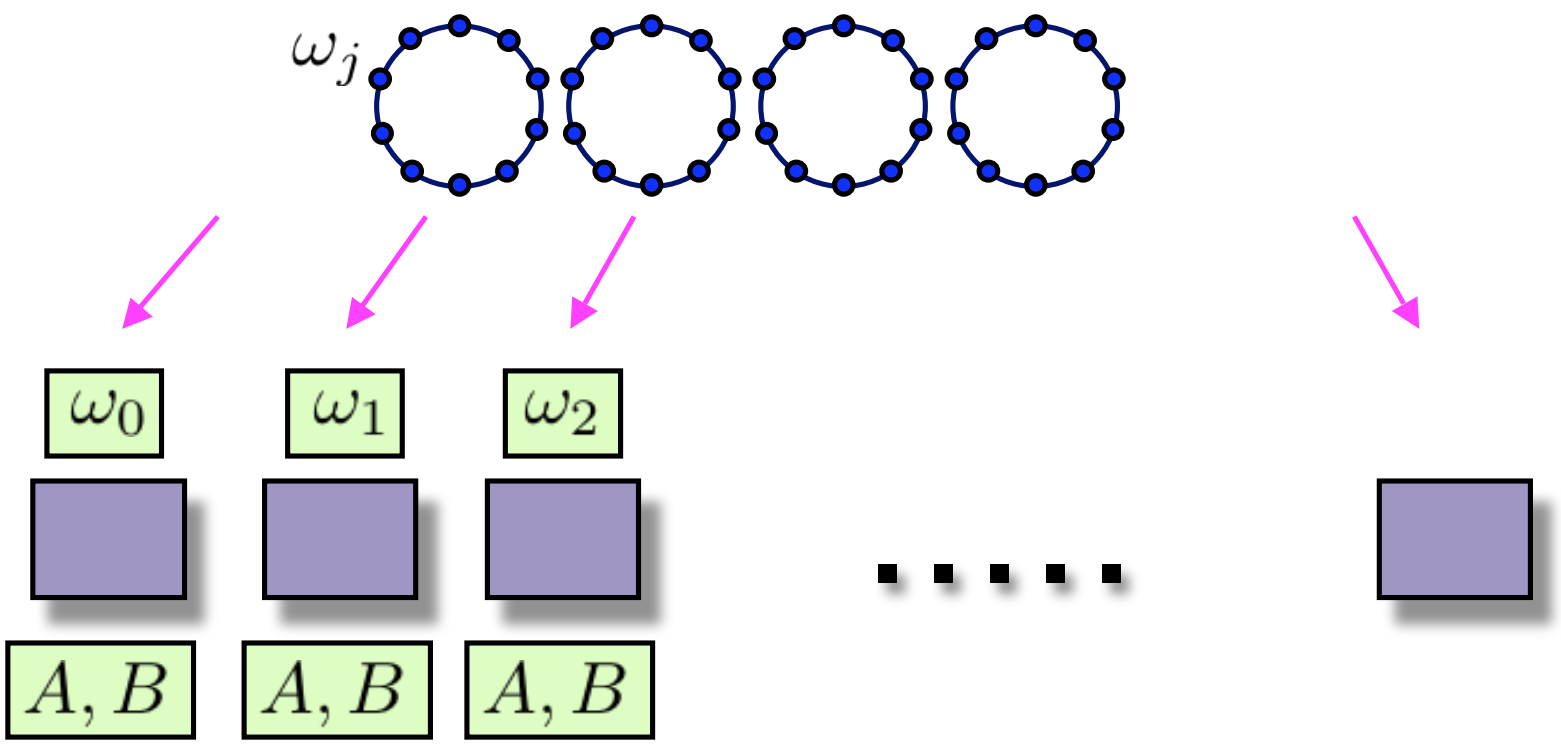
Parallel Implementation

$$Y_j = (\omega_j B - A)^{-1} BV$$



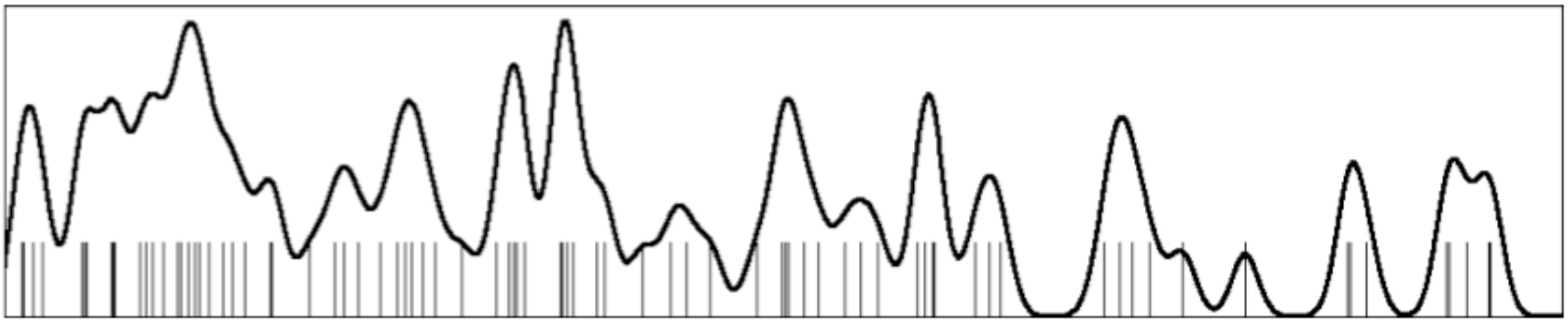
Parallel Implementation

$$Y_j = (\omega_j B - A)^{-1} BV$$



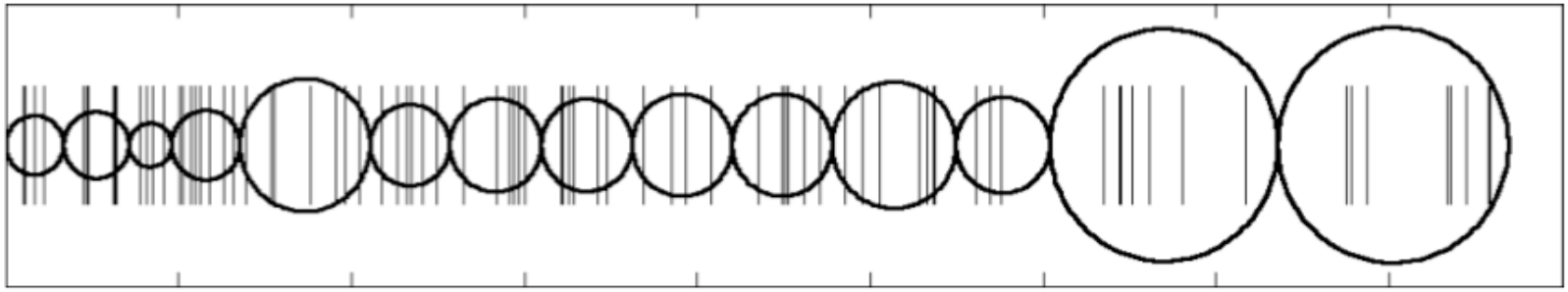
Estimation of Eigenvalue Distribution

Rough estimation of eigenvalue distribution:



Results by Algebraic Sub-structuring method

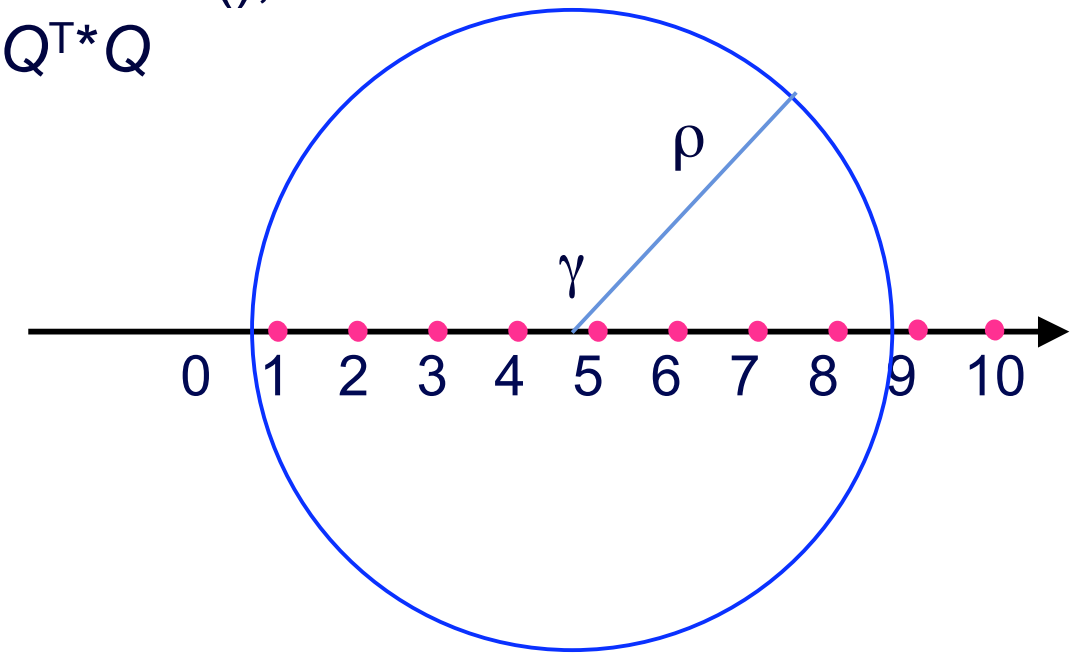
Put circles:



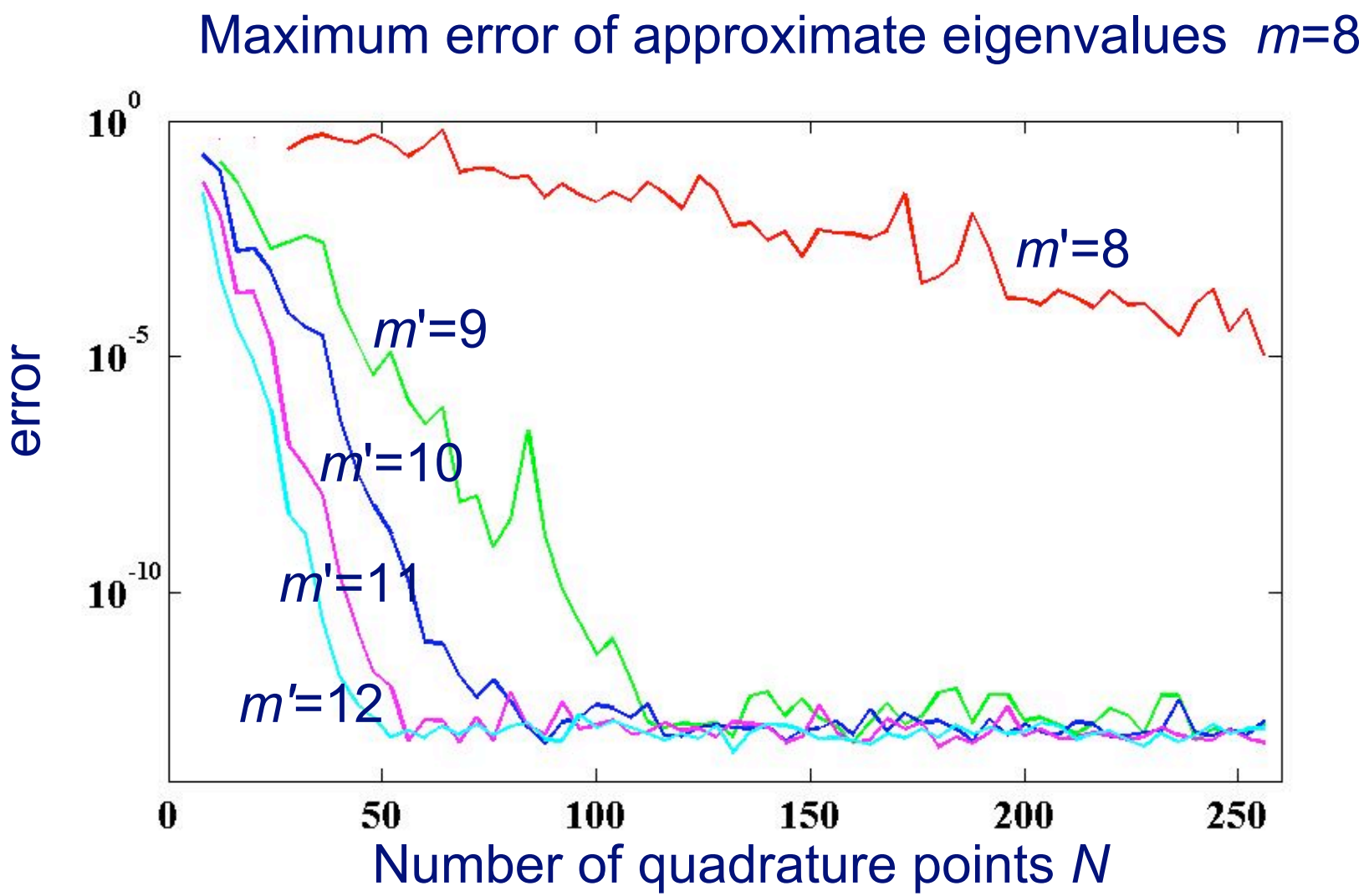
Numerical Examples

Size of a subspace

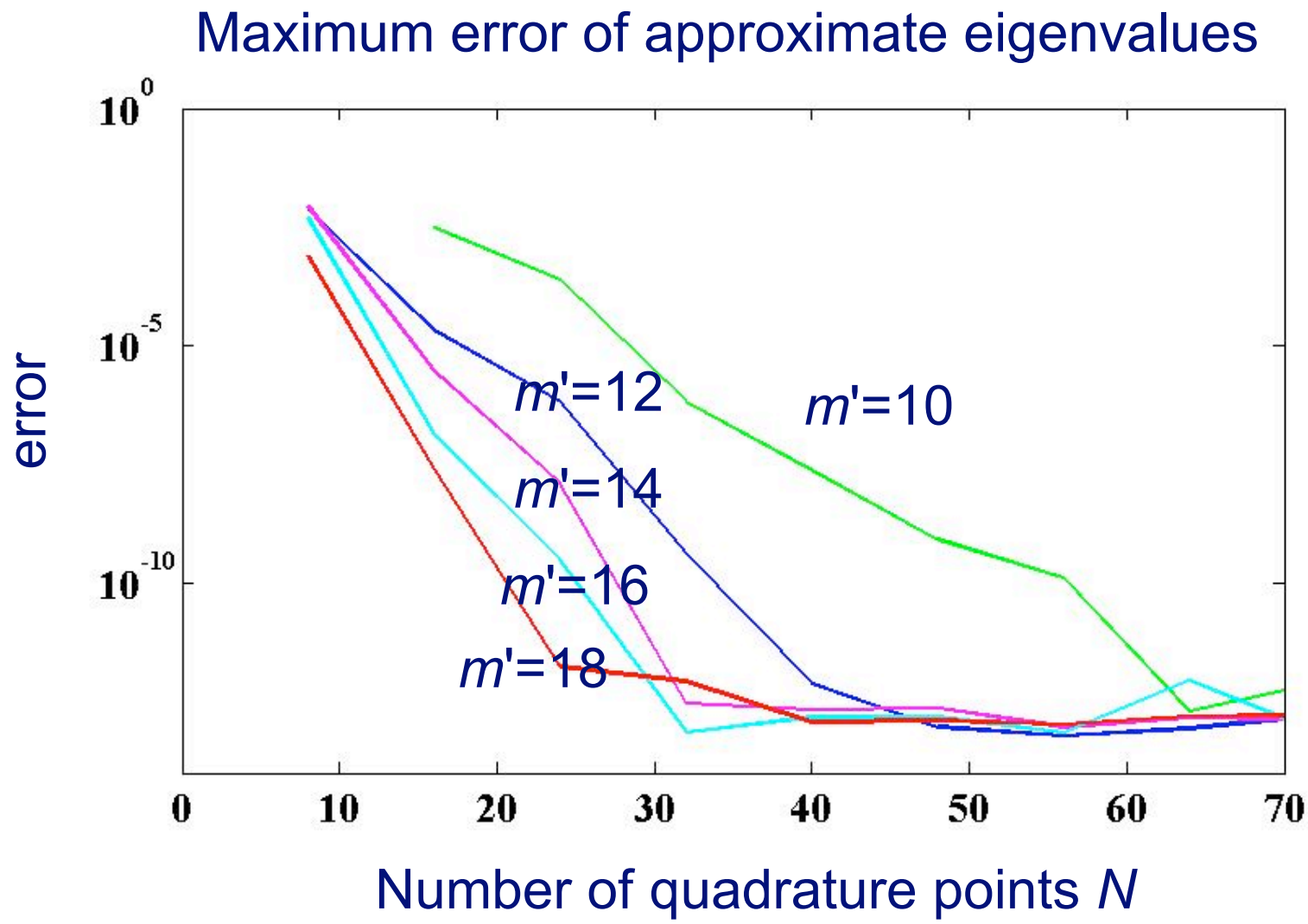
- Test problem:
  - $n = 20$
  - $D = \mathrm{diag}([1\ 2\ \ldots\ 20])$
  - $Q = \mathrm{QR}(C)$, $C(i,j) = \mathrm{Rand}()$, $A = Q^T * D * Q$, $B = Q^T * Q$
  - $\gamma = 4.8$, $\rho = 4.0$



Size of a subspace

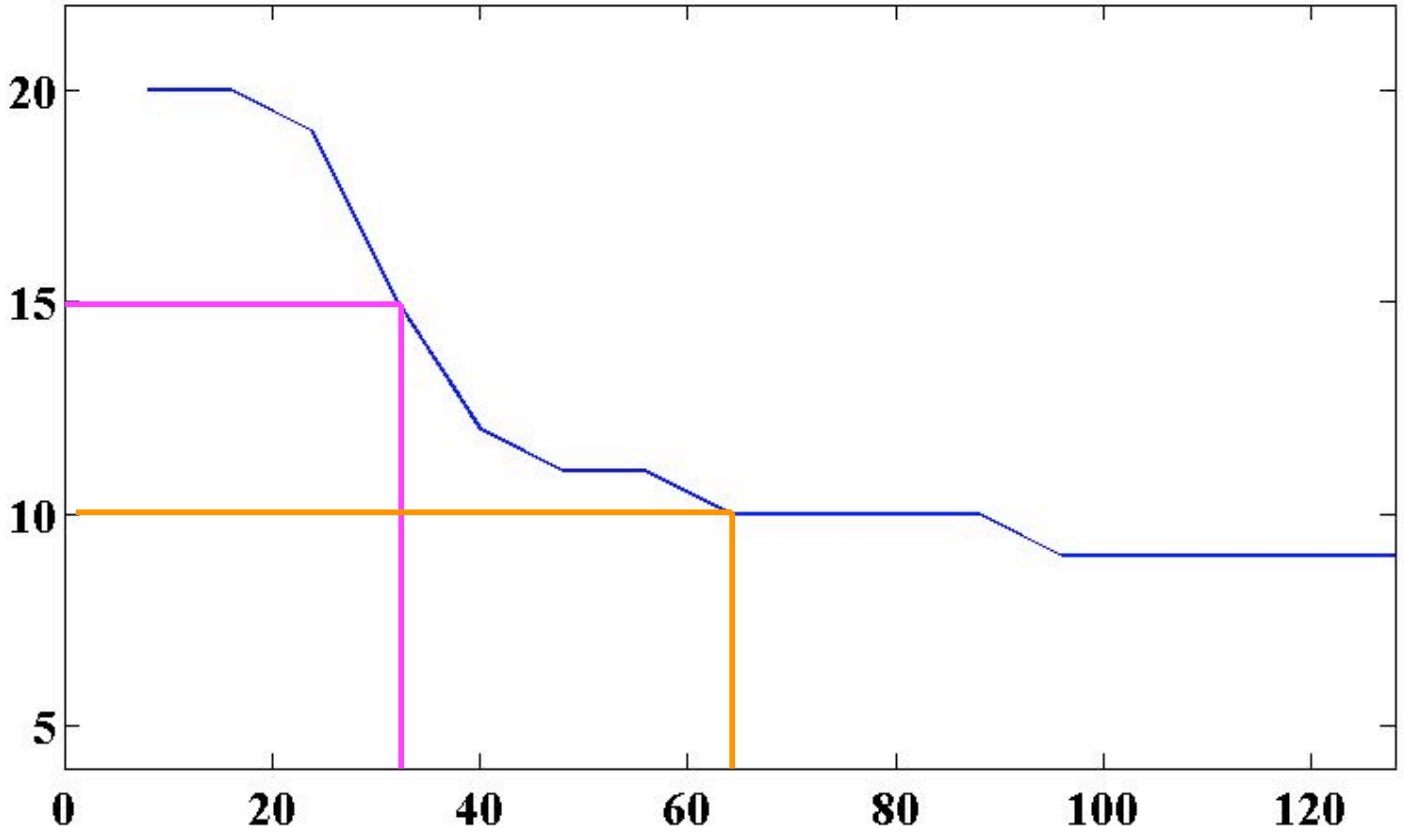


Size of a subspace



Size of a subspace

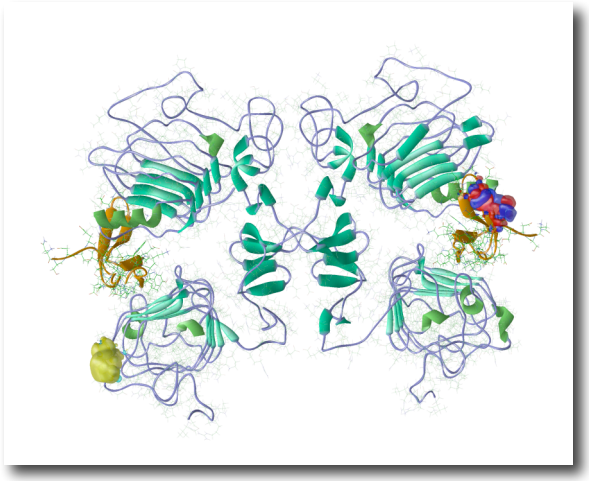
Number of singular values of $\hat{S}$ .s.t. $\sigma_k \geq 10^{-12} \times \max |a_{ij}|$



Number of quadrature points *N*

Numerical Example

- Test Problems:
  - EGFR (Epidermal Growth Factor Receptor) dimmer
  - Basis function: 6-31G
  - Size: 96,234 × 96,234
  - nnz: 456,807,648

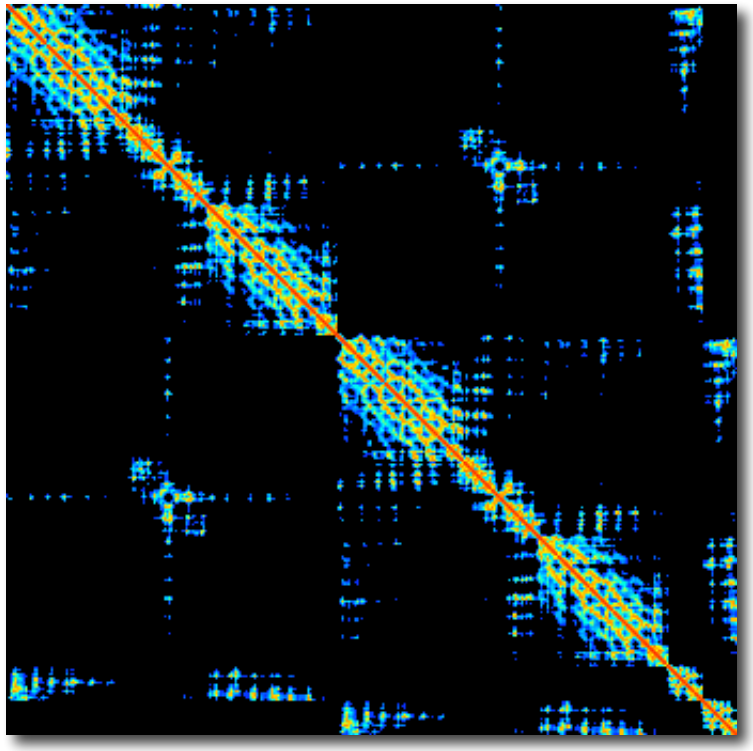


- Test Environment:

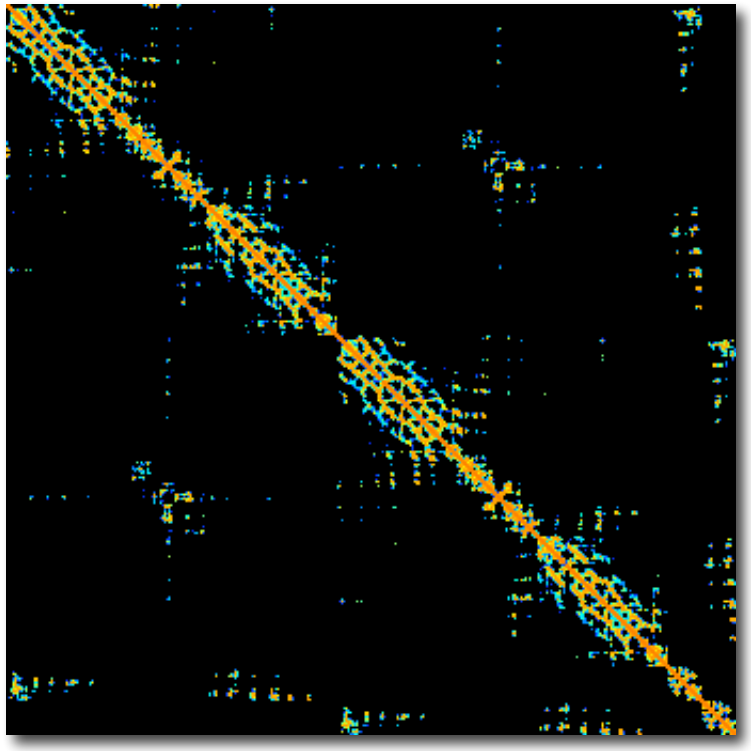
  AMD Opteron Processor Dual CPU x 128 nodes
  - Solver: COCG method [van der Vorst and Melissen (1990)]
  - Preconditioner: Complete Factorization for Approximate Matrix [Okada, S and Teranishi (2007)]
  - Sparse Direct Solver for Preconditioner: PARDISO

Numerical Example

Sparsity pattern of the matrix



A

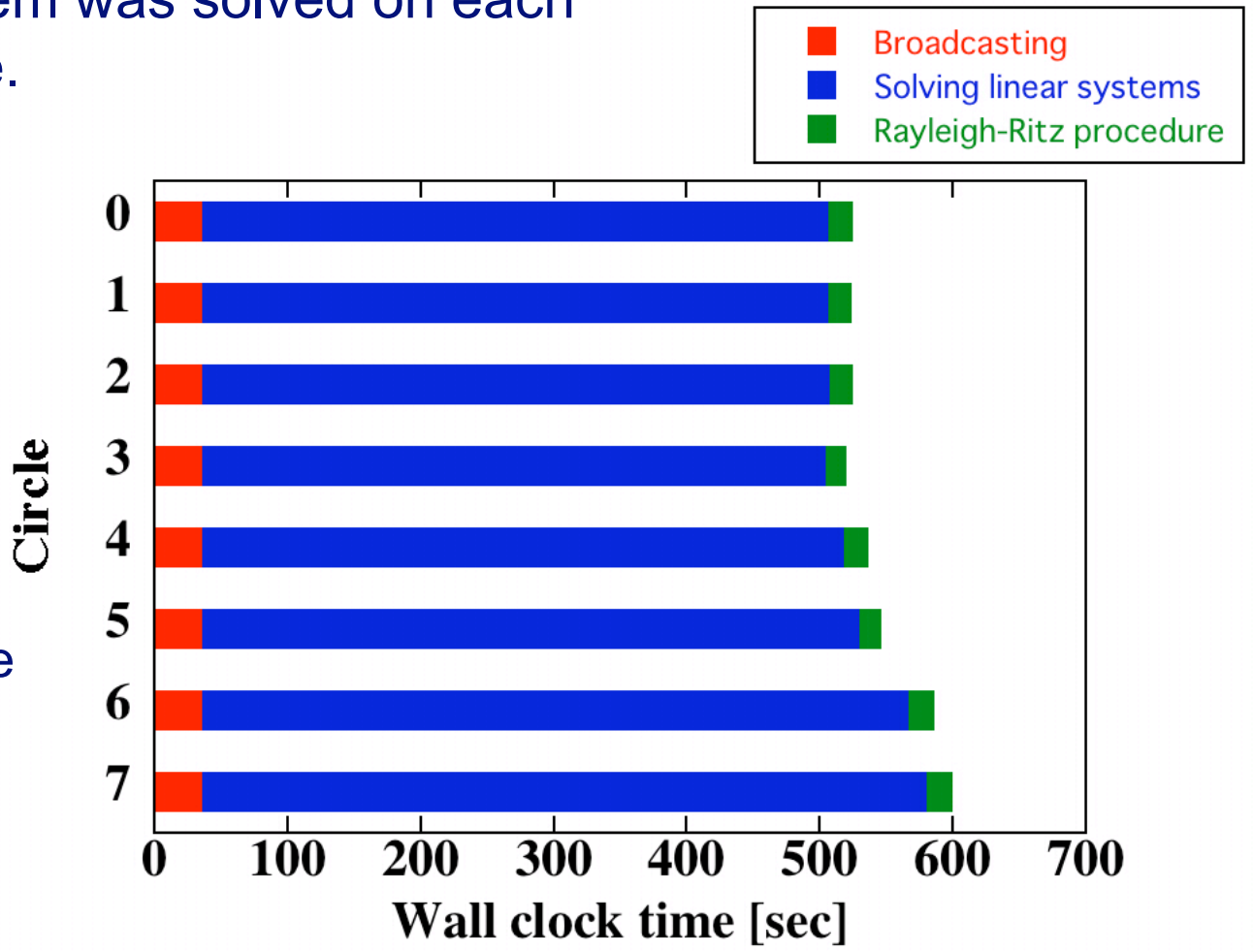


B

Timing Results with 256CPUs

- 32 CPUs for one circle, 8 Circles, Total 256 CPUs.
  One linear system was solved on each computing node.

$N = 32$
$L = 4$



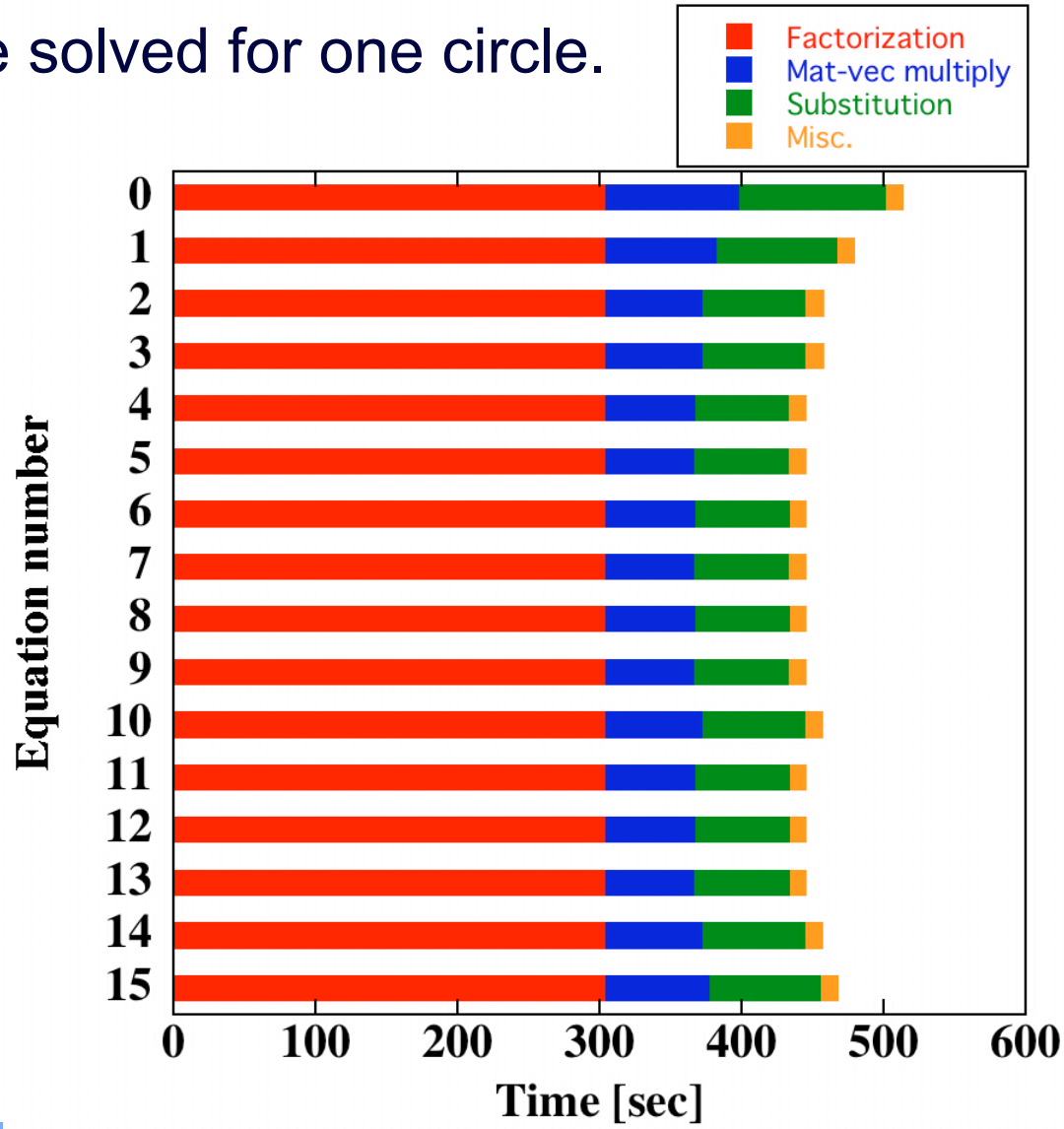
- 94 eigenpairs were obtained.
- Maximum residual was 3.4×10^{-10}.

Time in one circle

- 16 linear systems were solved for one circle.

Preconditioner
- Factorization

Iteration
- Forward/Backward Substitution
- Sparse Mat-Vec Multiply



Summary

- We consider an parallel eigenvalue solver for Molecular Orbital computations:
  - Interior eigenvalur problem
  - Semi-sparse matrix
- A subspace is constructed by a contour integral.
  - We can avoid inner/outer loops
- Systems of linear equations are solved for each quadrature node simultaneously.
  - Parallel implementation
- Future work
  - Find appropriate parameters
  - Estimation of eigenvalue distribution