A parallel eigensolver using contour integration for generalized eigenvalue problems in molecular simulation

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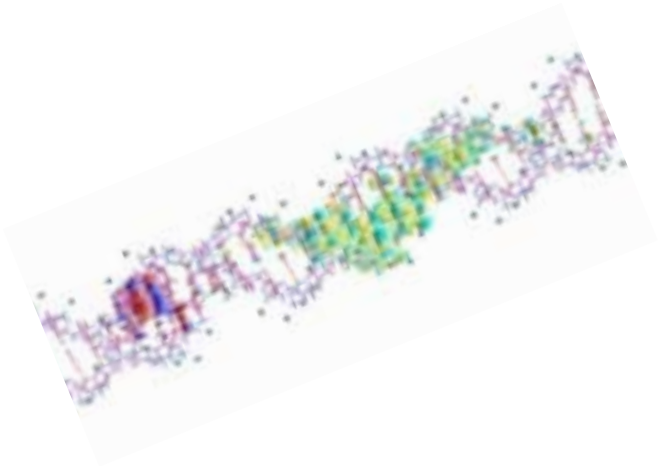
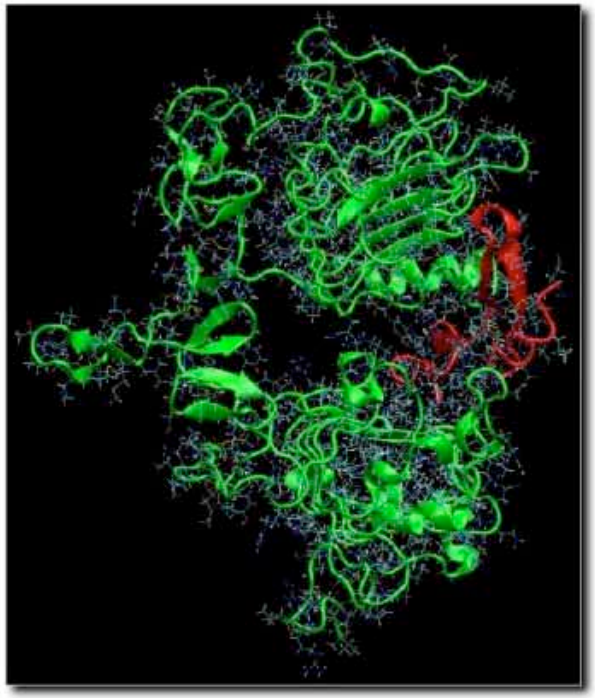


Molecular Orbital Computation

Design of Anticancer Drugs



EGFR
(Epidermal Growth Factor Receptor)

Schrödinger Equation

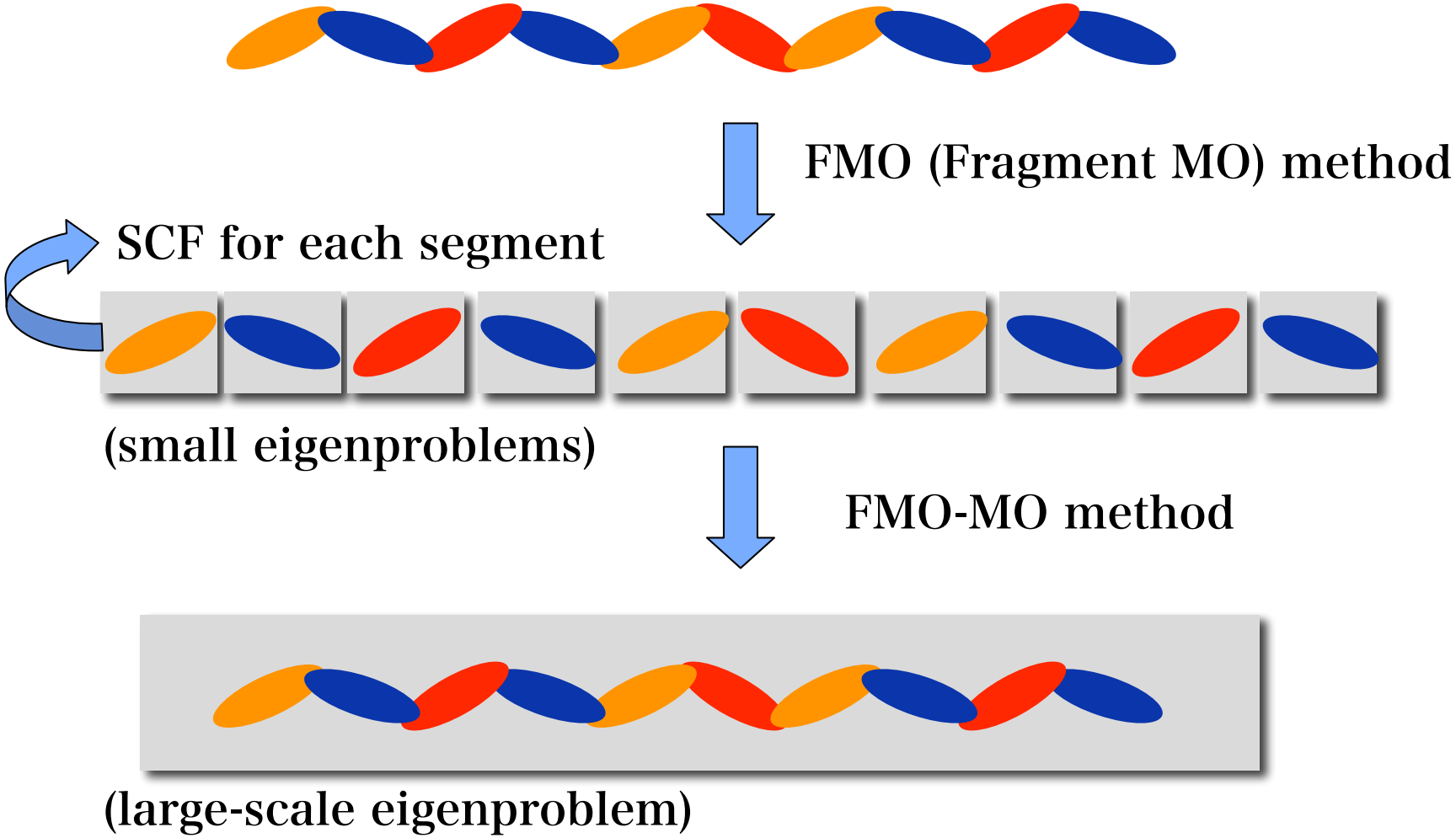
$$H\Psi = E\Psi$$

↓ Hartree-Fock approximation

Generalized Eigenvalue Problems

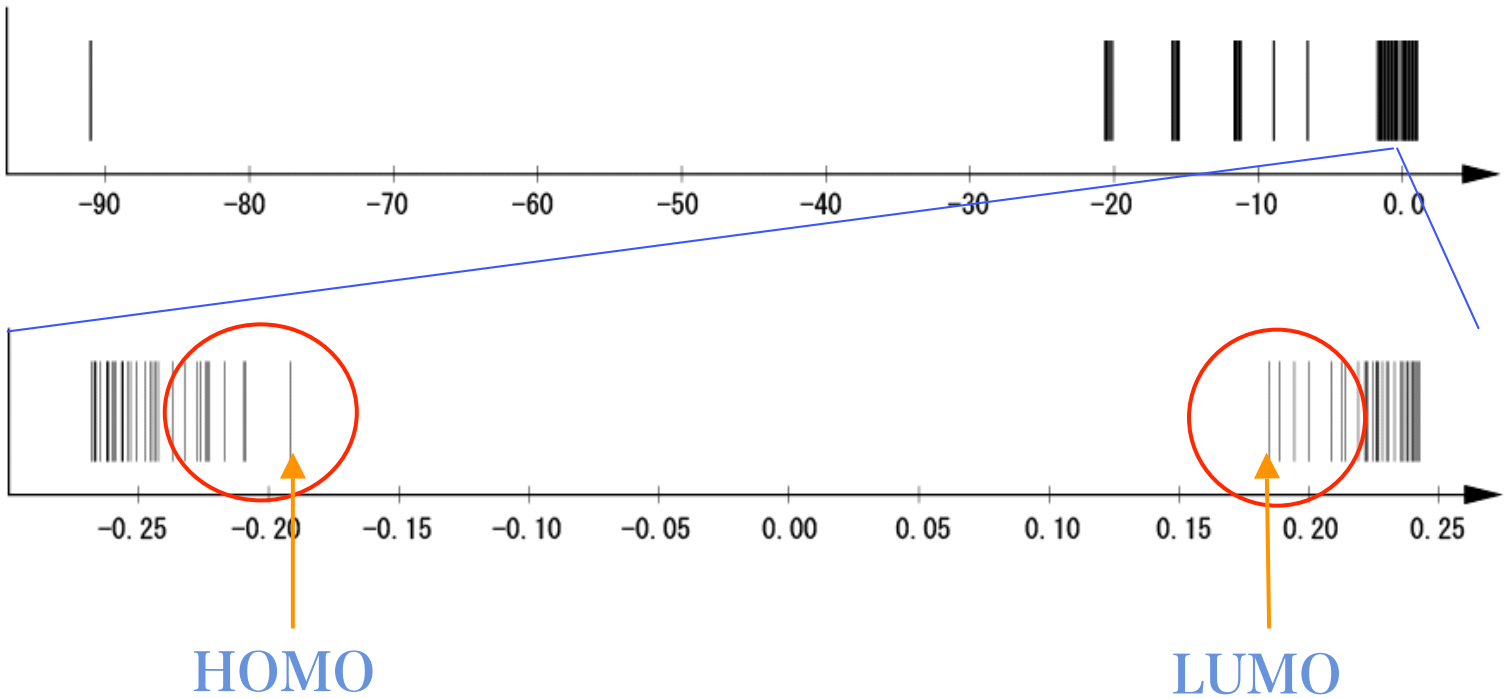
Matrix Generation

A large molecule is separated to small segments.



Required Orbitals

Energy state:



Eigenvectors related to chemical activities:

→ Interior eigenvalue problems

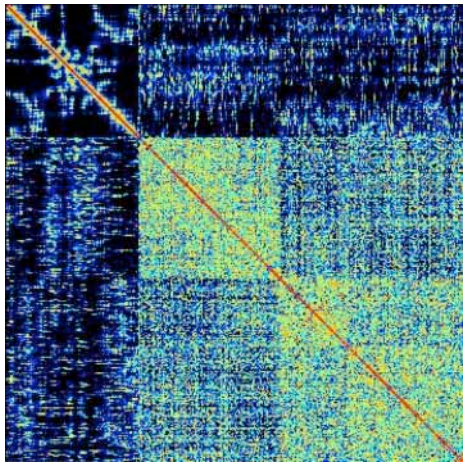
Matrix Properties

- The size of matrix: 2K ~ 200K
  The number of nonzero elements: 1M ~ 400M

  - relatively large number of nonzero elements

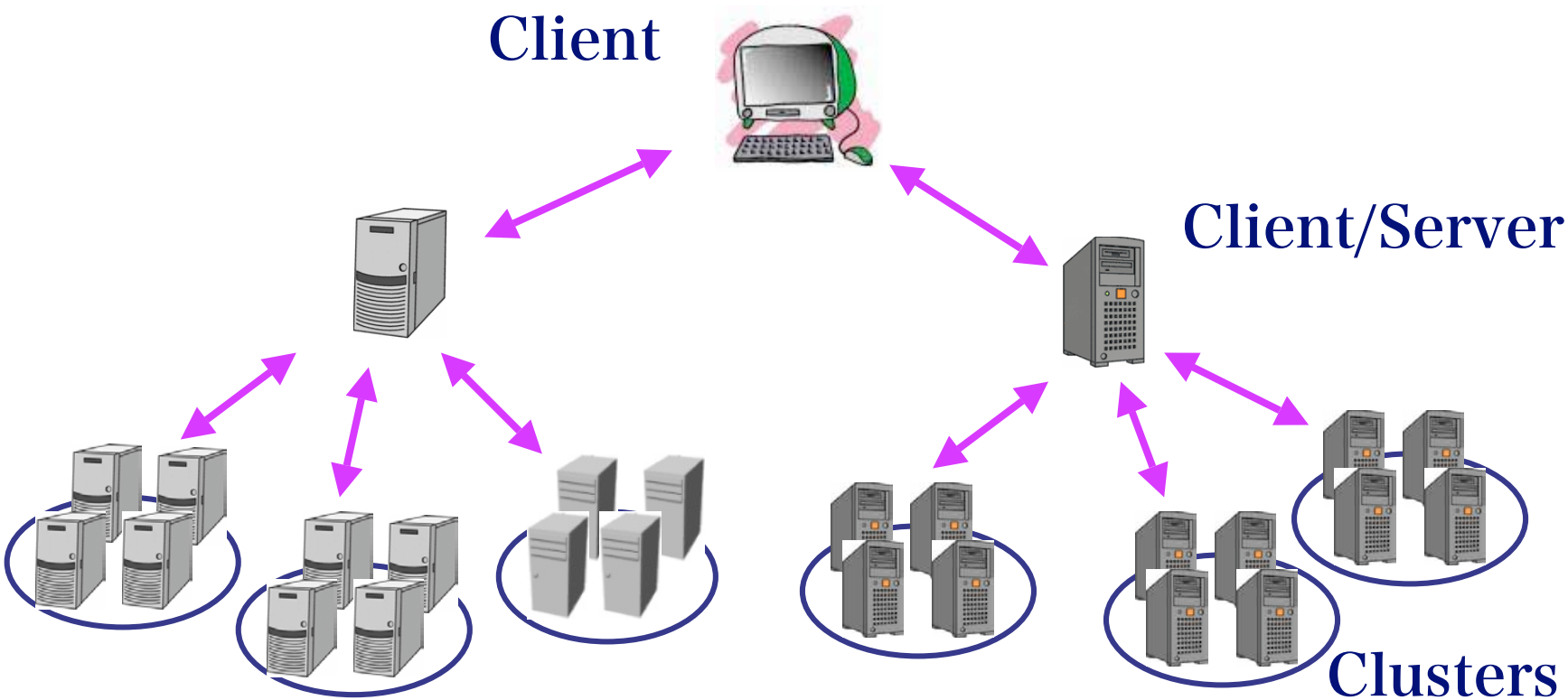
  - unstructured sparsity pattern

Fock matrix of
Lysozyme + H2O



Computing Environment

FMO-MO method is suitable for GRID computing.



Highly parallelized eigensolver is required.

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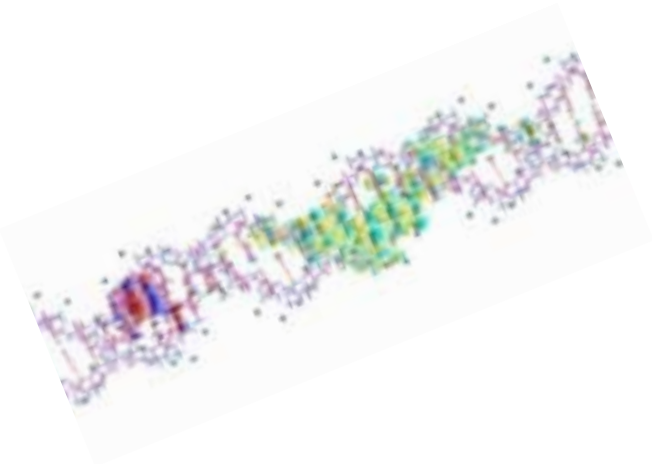


Generalized Eigenvalue Problem

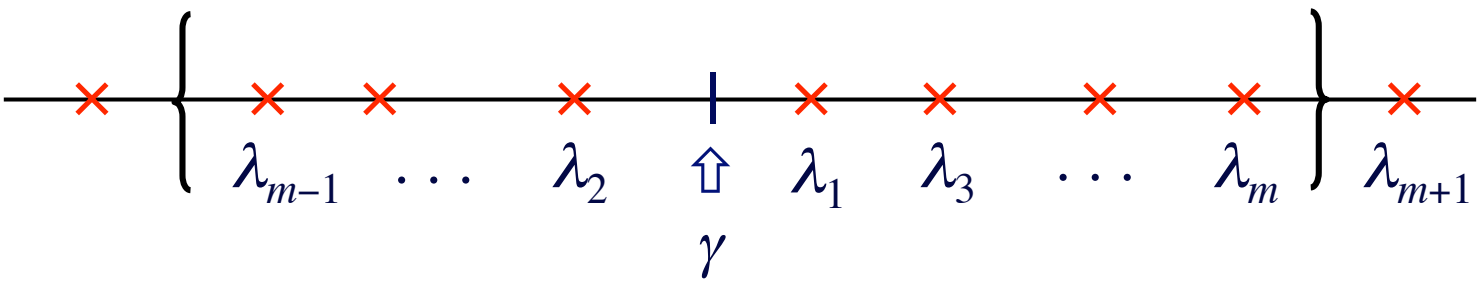
The generalized eigenvalue problem:

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

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

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

We find eigenpairs in a given interval:



Rayleigh-Ritz Procedure

Algorithm:

Inner Loop

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 $\boldsymbol{p}_j \leftarrow Q\boldsymbol{w}_j$, $j = 1, \ldots, m$.

Outer Loop

(A_Q, B_Q) : Projected pencil

θ_j : Ritz value

$\boldsymbol{p}_j$: Ritz vector

Contour Integral of Resolvent

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

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

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

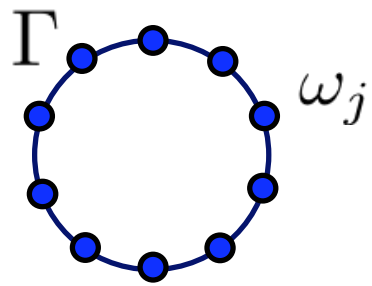
where $\Gamma \in \mathbb{C}$ is a Jordan curve that includes $\lambda_1, \ldots, \lambda_m$.

$$\boxed{\mathrm{span}(\boldsymbol{s}_0, \ldots, \boldsymbol{s}_{m-1}) = \mathrm{span}(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m)}$$

[S and Tadano (2007)]

Approximation for Contour Integral

Γ : Circle with center γ and radius ρ



Equidistributed points on the circle:

$$\omega_j = \gamma + \rho e^{\frac{2\pi \mathrm{i}}{N}(j+1/2)}, \quad j = 0, 1, \ldots, N-1$$

$\boldsymbol{s}_k$ are approximated by the N-point trapezoidal rule:

$$\boldsymbol{s}_k \approx \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} \boldsymbol{y}_j, \quad k = 0, \ldots, m-1$$

where

$$\boxed{\boldsymbol{y}_j = (\omega_j B - A)^{-1} \boldsymbol{v}, \quad j = 0, \ldots, N-1}$$

Contour Integral Rayleigh-Ritz Method

Algorithm of CIRR (Contour Integral Rayleigh-Ritz) method:

1. Set $\tau_j \leftarrow \exp(2\pi \mathrm{i}(j+1/2)/N)$, $j = 0, \ldots, N-1$.
2. Set $\omega_j \leftarrow \gamma + \rho\,\tau_j$, $j = 0, \ldots, N-1$.
3. Solve $(\omega_j B - A)\boldsymbol{y}_j = \boldsymbol{v}$ for $\boldsymbol{y}_j$, $j = 0, \ldots, N-1$.
4. Set $\hat{\boldsymbol{s}}_k \leftarrow \sum_{j=0}^{N-1} \tau_j^{k+1} \boldsymbol{y}_j$, $k = 0, \ldots, M-1$.
5. Construct an orthonormal basis Q from $\{\hat{\boldsymbol{s}}_0, \ldots, \hat{\boldsymbol{s}}_{M-1}\}$.
6. Form $A_Q = Q^{\mathrm{T}}(A - \gamma B)Q$ and $B_Q = Q^{\mathrm{T}} B Q$.
7. Compute the eigenpairs $(\theta_j, \boldsymbol{x}_j)$ $(1 \le j \le M)$ of (A_Q, B_Q).
8. Set $\hat{\lambda}_j \leftarrow \theta_j + \gamma$, $j = 1, \ldots, M$.
9. Set $\hat{\boldsymbol{u}}_j \leftarrow Q\boldsymbol{x}_j$, $j = 1, \ldots, M$.

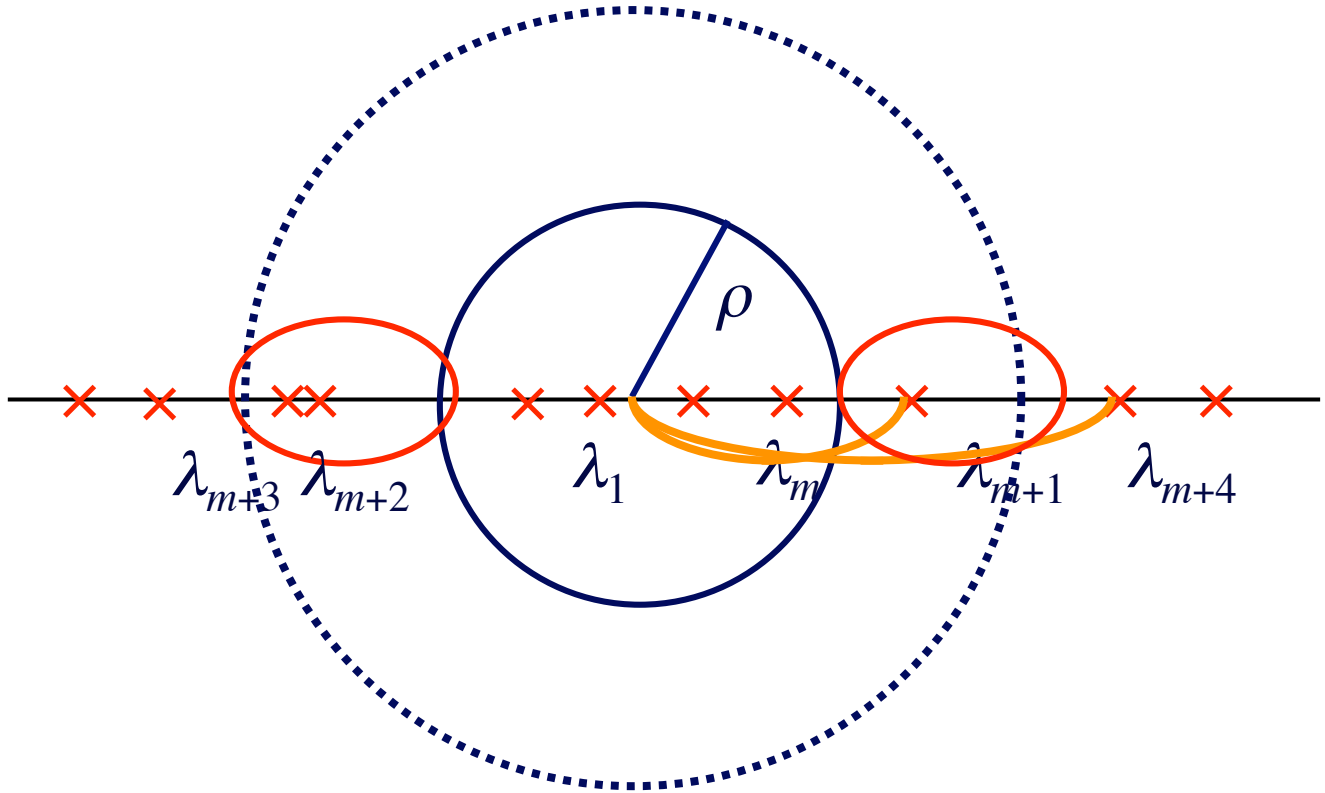
Construct a subspace

Rayleigh-Ritz procedure

Influence of Quadrature Error

Let $$\eta := \min_{j>m} \frac{\lambda_j - \gamma}{\rho} \qquad \eta \to \min_{j>m'} \frac{\lambda_j - \gamma}{\rho}, \quad m' > m$$

Then $$|\hat{\lambda}_j - \lambda_j| = O(\eta^{-N}), \quad 1 \le j \le m$$



Block Method

Block variant is also obtained by using a matrix

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

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

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

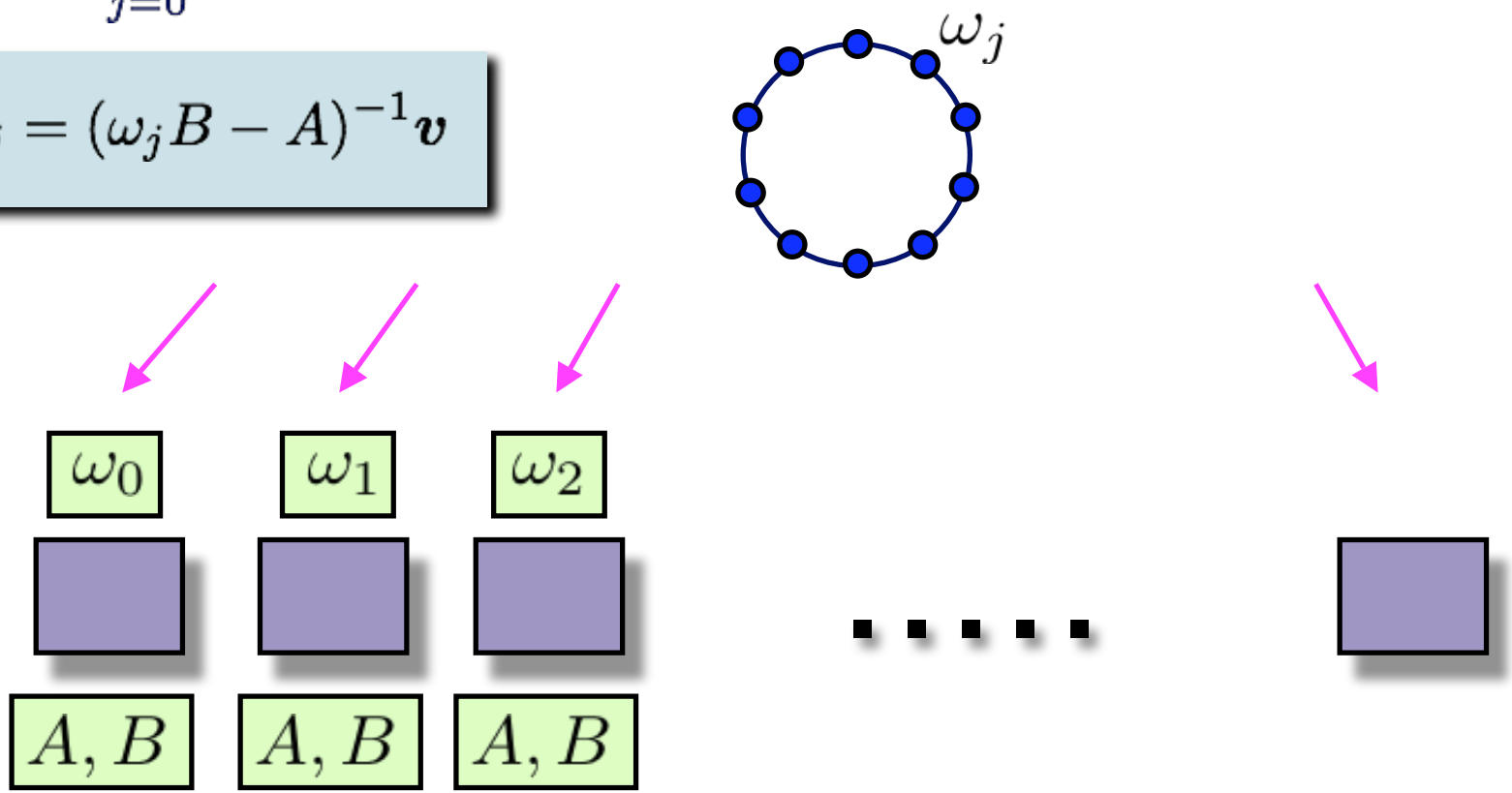
$$\Downarrow$$

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

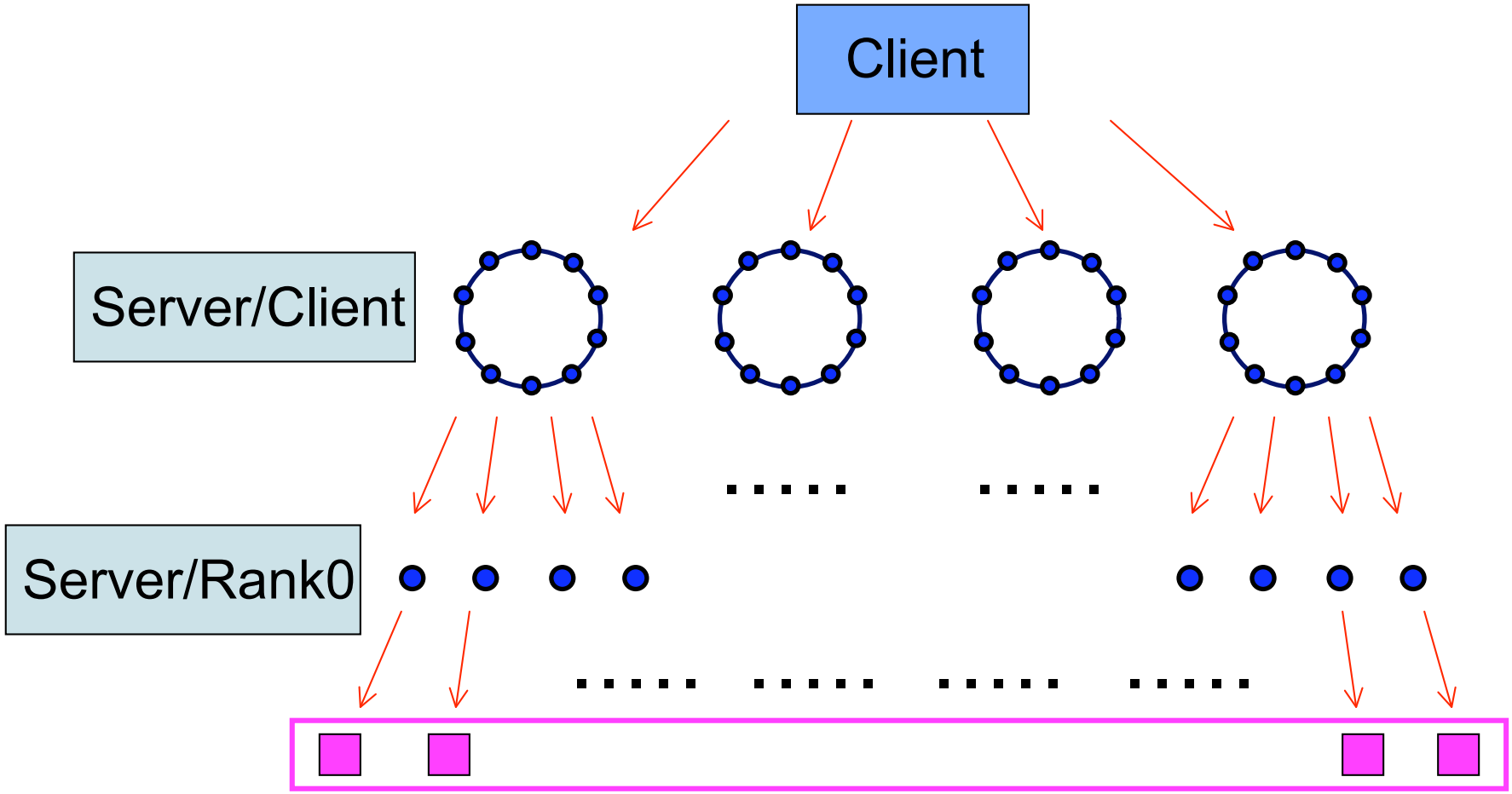
Parallel Implementation

$$\boldsymbol{s}_k \approx \frac{1}{N} \sum_{j=0}^{N-1} (\omega_j - \gamma)^{k+1} \boldsymbol{y}_j$$

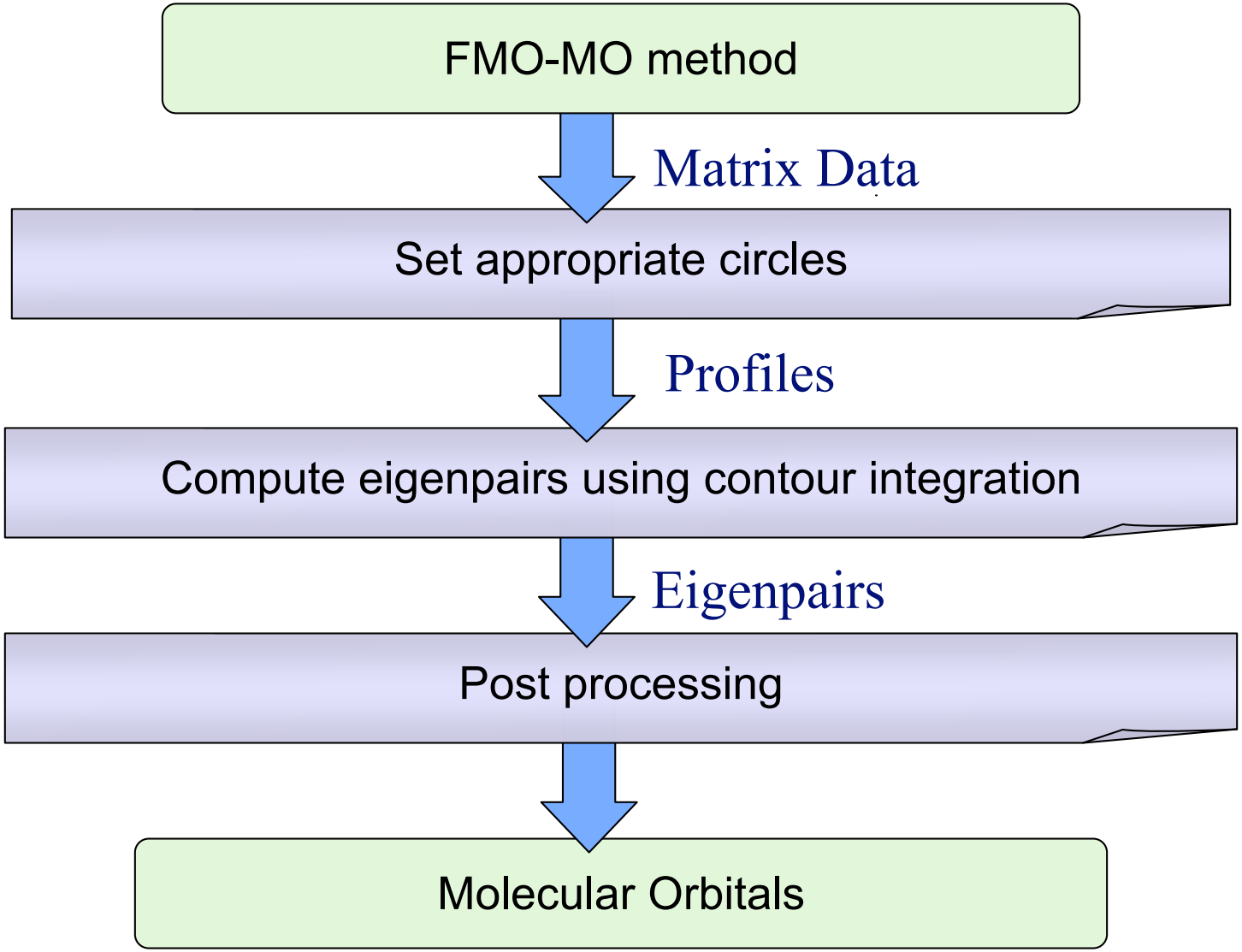
$$\boldsymbol{y}_j = (\omega_j B - A)^{-1} \boldsymbol{v}$$



Parallel Implementation



Flow of the Eigensolver



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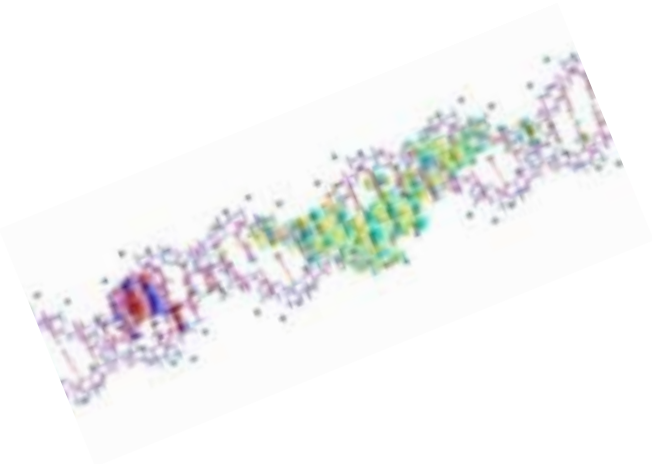
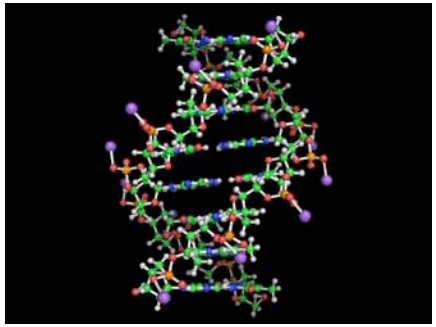


Numerical Example (1)

- Test problem:
  - Model of 8 DNA base pairs
  - Matrix size: 1,980 × 1,980
  - nnz: 728,080

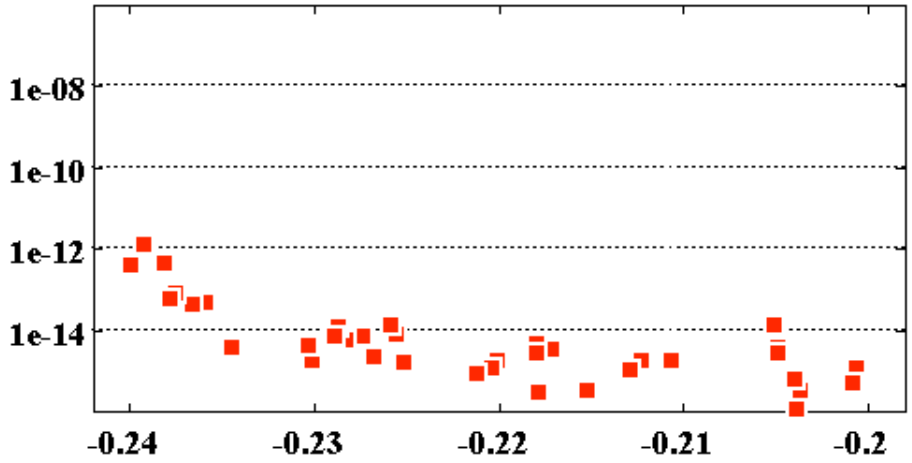


- Test Environment:
  - OS: MacOSX 10.5
  - CPU: Core 2 Duo 2.2GHz (2GB memory)
  - Software: MATLAB 7.5
  - Solver: UMFPACK (sparse direct solver)

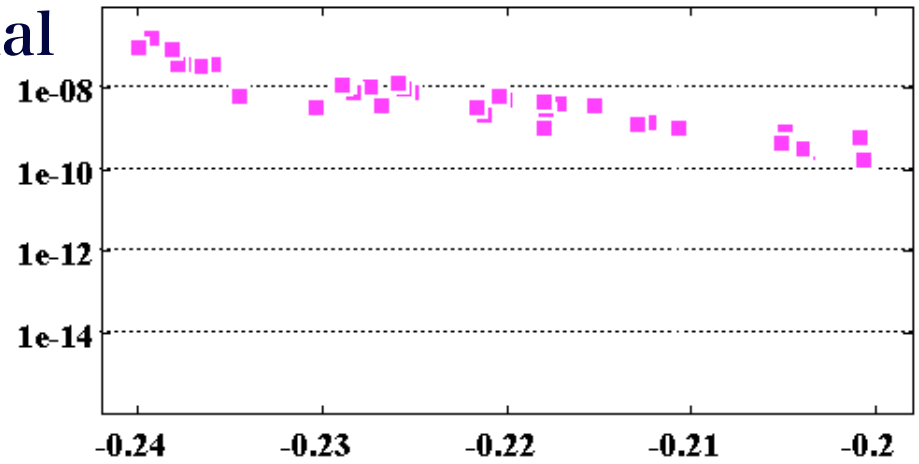
Numerical Example (1)

L= 12, N = 16, center = -0.22, radius = 0.02, 38 eigs

error



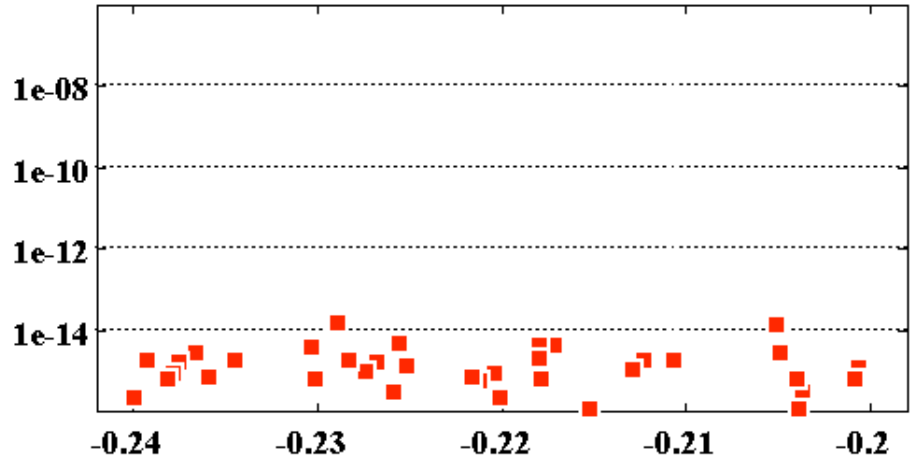
residual



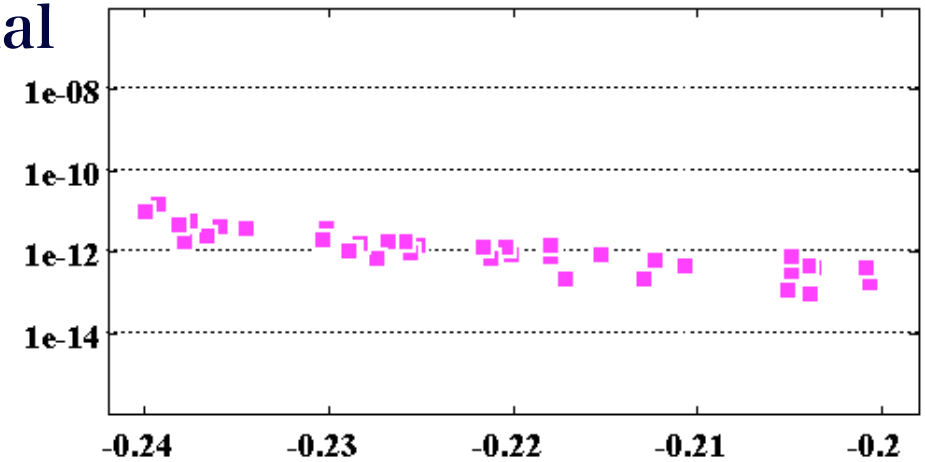
Numerical Example (1)

L = 16, N = 24, center = -0.22, radius = 0.02, 38 eigs

error



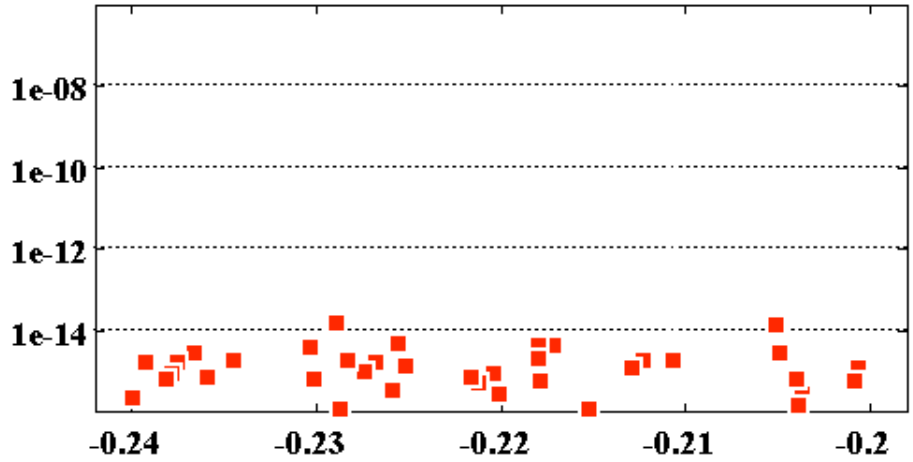
residual



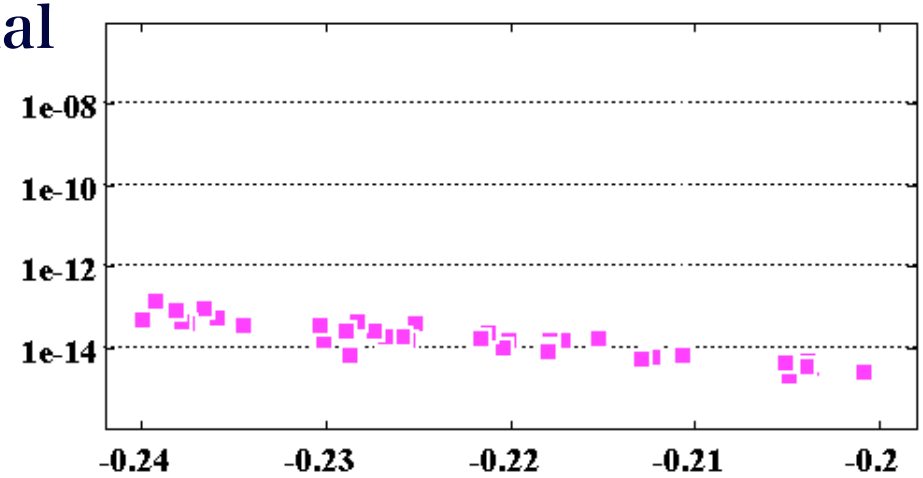
Numerical Example (1)

L = 20, N = 24, center = -0.22, radius = 0.02, 38 eigs

error

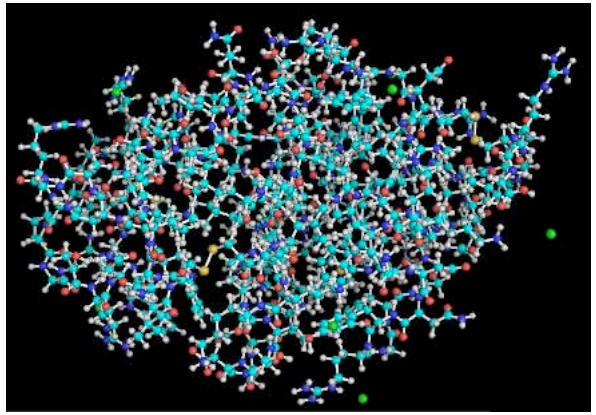


residual



Numerical Example (2)

- Test Problem:
  - Lysozime + H2O
  - Basis function: STO-3G
  - Size: 20,758 × 20,758
  - nnz: 20,064,444

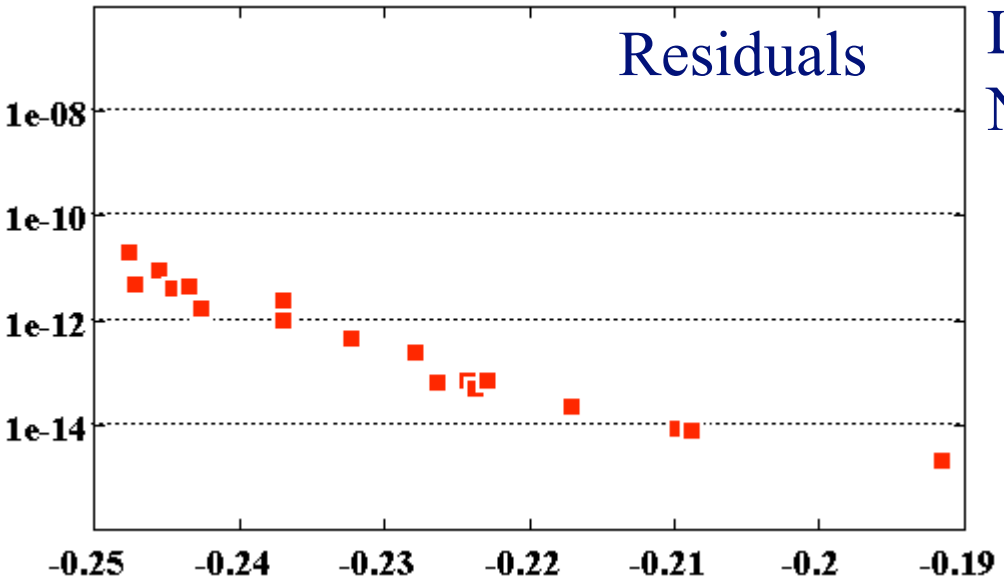


- Test Environment:
  - OS: MacOSX 10.5
  - CPU: Core 2 Duo 2.2GHz (2GB memory)
  - Compiler: icc 10.1, ifort 10.1
    Solver: COCG method [van der Vorst and Melissen (1990)]
  - Preconditioner: Complete Factorization for Approximate Matrix [Okada, S and Teranishi (2007)]
  - Sparse Direct Solver for Preconditioner: PARDISO

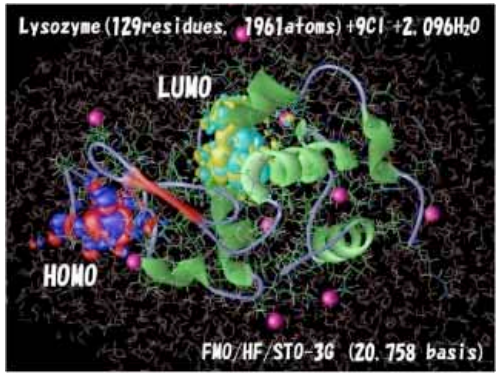
Numerical Example (2)

Center: -0.22 Radius: 0.03 18 eigs

Wall-clock time: 233.2 sec



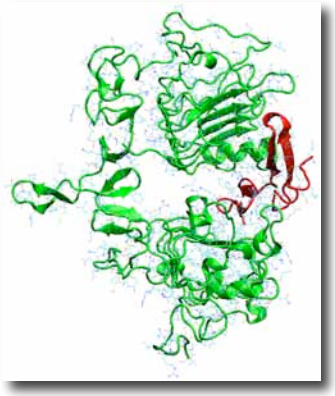
L = 12
N = 24



ARPACK+PARDISO: 316.1 sec, 20 eigs, max(res) = 6.6e-6
(Xeon 3.2GHz 2MB Memory)

Numerical Example (3)

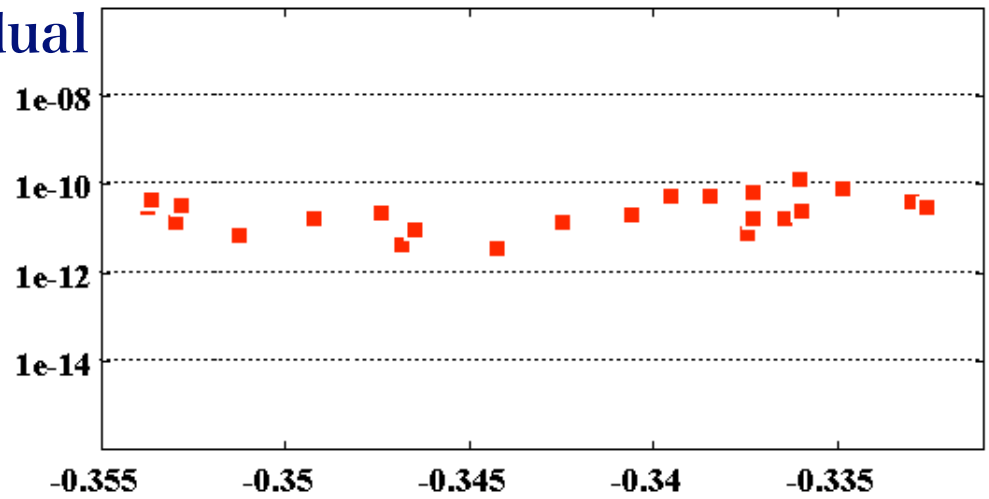
- Test Problems:
  - EGF (Epidermal Growth Factor)
  - Basis function: 6-31G
  - Size: 43,612 × 43,612
  - nnz: 73,175,935



- Test Environment:
  - OS: MacOSX 10.5
  - CPU: Core 2 Duo 2.2GHz (2GB memory)
  - Compiler: icc 10.1, ifort 10.1, MKL 10.0
  - 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 (3)

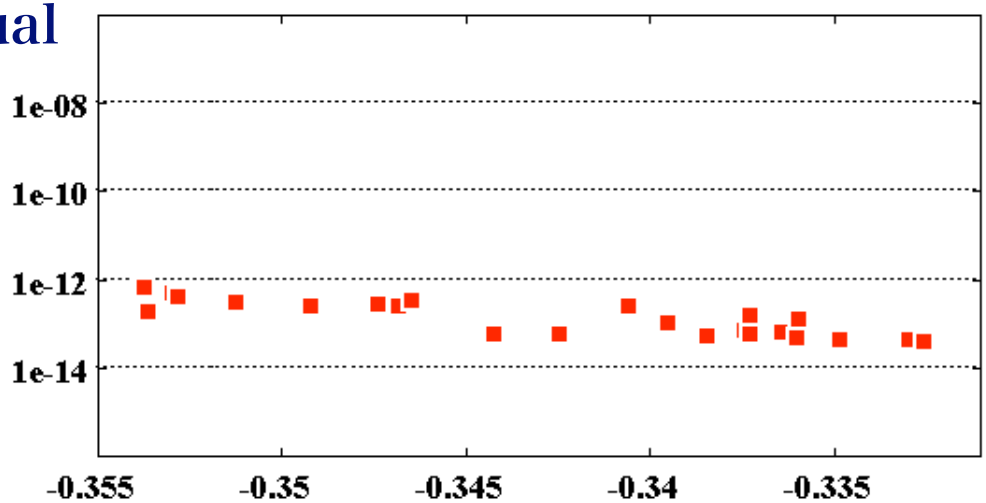
Residual



L = 8
N = 24

1583.1 sec

Residual



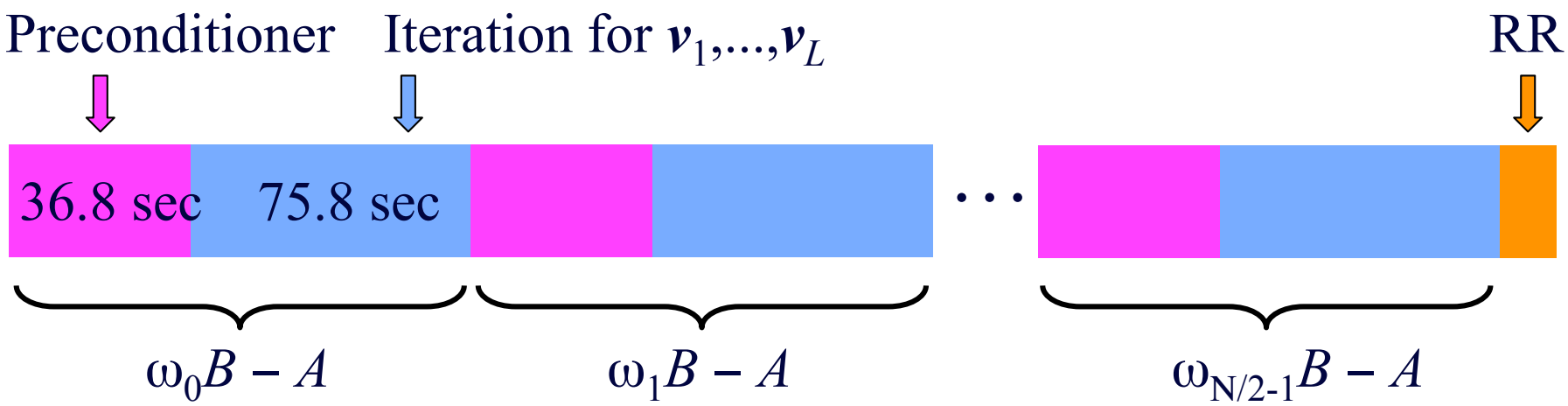
L = 12
N = 24

2017.7 sec

Numerical Example (3)

Timing result (serial case):

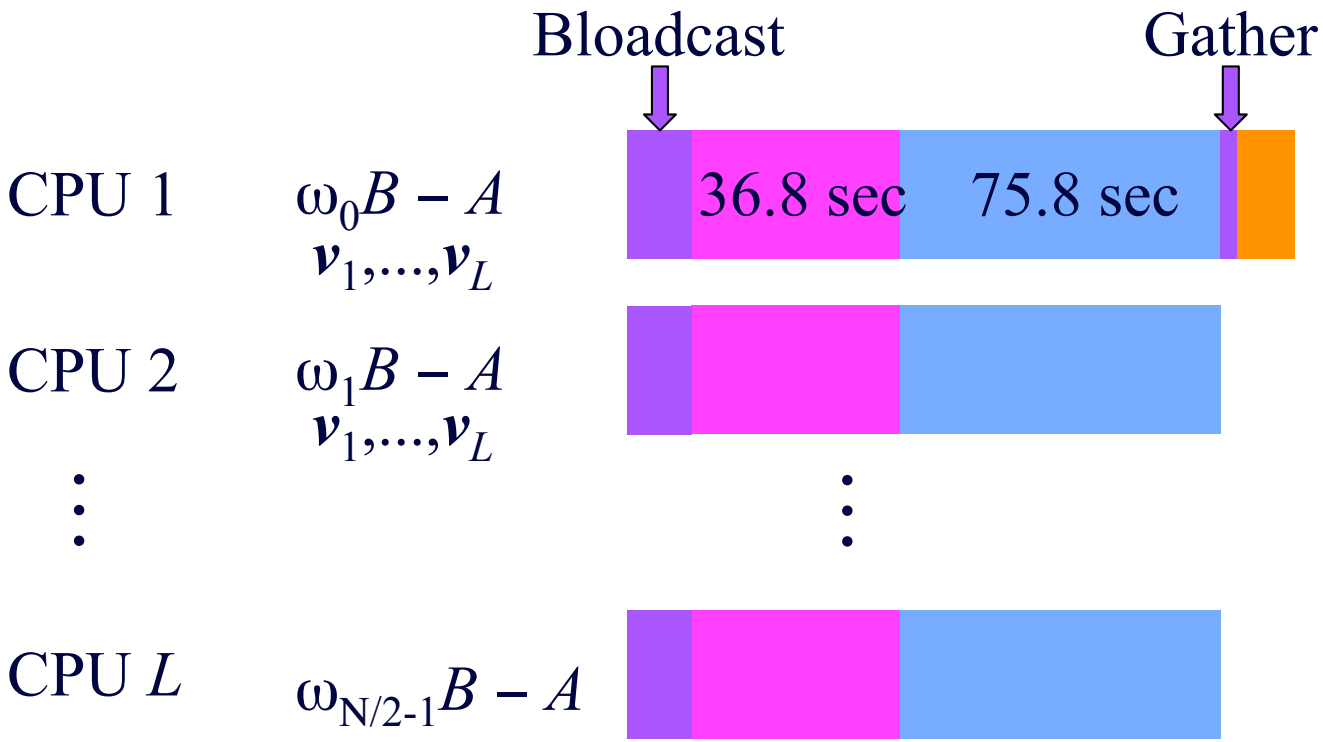
L = 12 N = 24 2017.7 sec



Numerical Example (3)

Timing result estimation (parallel case 1):

L = 12 N = 24



Numerical Example (3)

Timing result estimation (prallel case 2):

L = 12 N = 24

CPU 1 $\omega_0 B - A$

$\boldsymbol{v}_1$

CPU 2 $\omega_0 B - A$

$\boldsymbol{v}_L$

⋮ ⋮

CPU L*(N/2) $\omega_{N/2-1} B - A$

$\boldsymbol{v}_L$

Summary

- A Rayleigh-Ritz type method using the contour integral was proposed.
- This method finds limited number of eigenpairs in a given interval.
  - Efficient for molecular orbital computation.
  - Easy to implement for distributed computing.
- Find good preconditioner.
- Application for other problems.
  (Not only for SPD case)