

Hands-on practice

《How to connect a PC cluster which is used during this innovation camp》

login_name: guest**

host_name: gauss.issp.u-tokyo.ac.jp

login_name is announced when you sent a PUBLIC ssh-key.

If you didn't receive your *login_name*, please contact us.

Linux or mac:

```
ssh -l login_name -i identity_file host_name
```

or

```
ssh -i identity_file login_name@host_name
```

(example: `ssh -i private_key.ppk guest99@gauss.issp.u-tokyo.ac.jp`)

Windows:

You can use Cygwin, Windows Subsystem for Linux or some terminals (such as Putty, Tera Term, Poderosa, and so on).

System

- * Login node : gauss
- * Computational nodes : gauss01 - gauss13 (13 nodes)
 - * CPU : Xeon E5-2680v4, 28 cores/node
 - * RAM : 64 GB/node
 - * Do not login directly the computational nodes.
Use the queuing system.
- * Sample of batch job script : /home/public/sample.sh

Programs

- * Binary : /home/public/bin/
- * Source : /home/public/program/

samples for the practice

/home/lctr/iccms2/

These samples also have been uploaded in
[https://github.com/issp-center-dev/ICCMS/
tree/master/2018/2018-10-02/fukuda](https://github.com/issp-center-dev/ICCMS/tree/master/2018/2018-10-02/fukuda)

```
|-- MateriApps_review_template.zip
|-- practice
|   |-- doc_how_to_use_each_program_code.zip
|   |-- eigenkernel
|       |-- Makefile
|       |-- Makefile.inc
|       |-- run.sh
|-- k-ep
|   |-- Makefile.inc
|   |-- run.sh
|-- komega
```

EigenKernel

(https://github.com/eigenkernel/eigenkernel/tree/eigenkernel_dev)

- generalized eigenvalue problems

$$A\vec{y}_k = \lambda_k B\vec{y}_k$$

$A, B : M \times M$ real-symmetric matrices
(B is positive definite.)

$\{\lambda_k\}$: Eigenvalues

$\{\vec{y}_k\}$: Eigenvectors

input

$$AY = BY\Lambda$$

output

$$\Lambda \equiv \text{diag}(\lambda_1, \lambda_2, \dots)$$

$$Y \equiv (\vec{y}_1, \vec{y}_2, \dots)$$

- standard eigenvalue problem

$$A'Z = Z\Lambda$$

$$B = U^T U$$

$$A' \equiv U^{-T} A U^{-1} : \text{real symmetric}$$

$$Y = U^{-1} Z$$

```
./eigenkernel_app -s general_scalapack A.mtx B.mtx
```

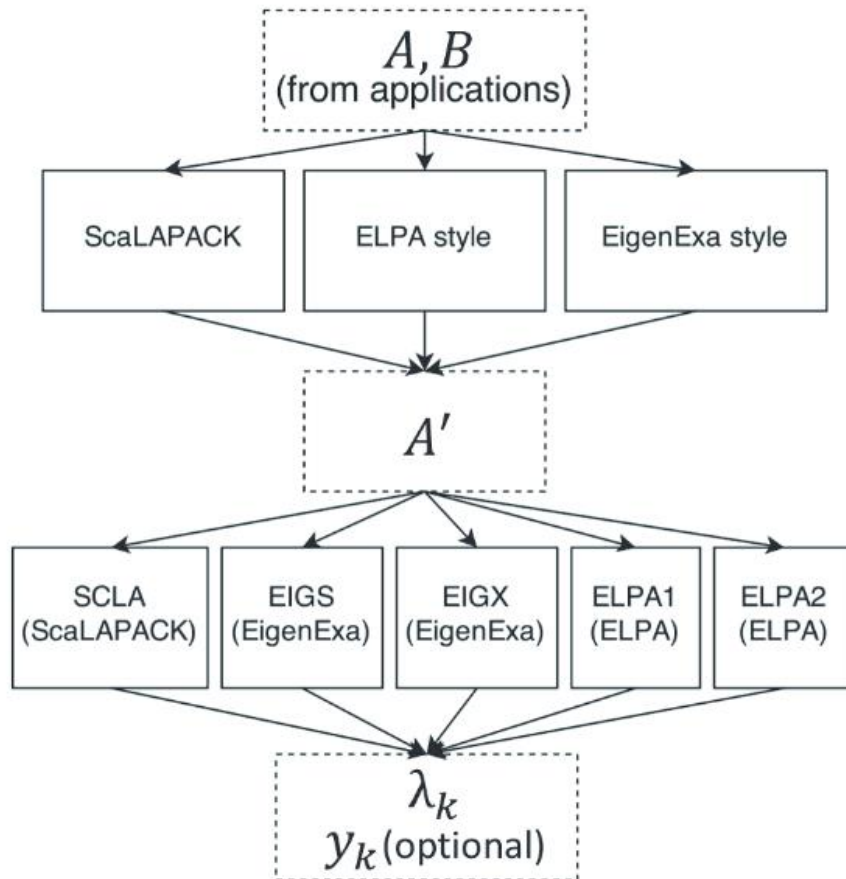


Fig. 3 Workflow of the hybrid GEP solver.

sample code : `src/main.f90`

k-ep

(Solution of the k -th eigenvalue problem)

(<https://github.com/lee-djl/k-ep>)

We assume that the eigenvalue problem-specific target index k satisfies $1 \ll k \ll n$ such that λ_k is not at either end of $[\lambda_1, \lambda_n]$.

A diagram showing the equation $A\vec{y}_k = \lambda_k B\vec{y}_k$. Above the equation, the word "input" is written in red. Below the equation, the word "output" is written in red. Red lines connect "input" to both \vec{y}_k terms and "output" to both \vec{y}_k terms.

$$A\vec{y}_k = \lambda_k B\vec{y}_k$$

$A, B : n \times n$ large sparse Hermitian matrices
(B is positive definite.)

$\lambda_k : k$ -th Eigenvalue $\lambda_1 \leq \cdots \lambda_k \leq \cdots \lambda_n$

$\vec{y}_k : k$ -th Eigenvector

If you want to calculate 2343rd eigenvalue and eigenvector,

```
./example.out A.mtx B.mtx 2343 > output.txt
```

sample code : `example/example.f90`

$K\omega$

(<https://github.com/issp-center-dev/Komega/releases>)

$K\omega$ is a library to solve the shifted linear equation within the Krylov subspace.

$$G_{ij}(z) = \langle i | (z\hat{I} - \hat{H})^{-1} | j \rangle \equiv \varphi_i^* \cdot (z\hat{I} - \hat{H})^{-1} \varphi_j$$

output

input

For example,

$$\hat{H} = \sum_i \begin{pmatrix} \hat{S}_{ix} & \hat{S}_{iy} & \hat{S}_{iz} \end{pmatrix} \begin{pmatrix} J_x & D_z & 0 \\ -D_z & J_y & 0 \\ 0 & 0 & J_z \end{pmatrix} \begin{pmatrix} \hat{S}_{i+1x} \\ \hat{S}_{i+1y} \\ \hat{S}_{i+1z} \end{pmatrix}$$

- $(\hat{H}, z) = (\text{complex}, \text{complex})$: Shifted Bi-Conjugate Gradient(BiCG) method [1]
- $(\hat{H}, z) = (\text{real}, \text{complex})$: Shifted Conjugate Orthogonal Conjugate Gradient(COCG) method [2]
- $(\hat{H}, z) = (\text{complex}, \text{real})$: Shifted Conjugate Gradient(CG) method (using complex vector)
- $(\hat{H}, z) = (\text{real}, \text{real})$: Shifted Conjugate Gradient(CG) method (using real vector)

Hands-on practice

Presentation:

Please review for an app in MateriApps (<https://ma.issp.u-tokyo.ac.jp/en/>).

The screenshot shows the MateriApps website. At the top, it says "now 232 Apps" and "Inquiry / Application Request". The logo "MateriApps" is prominently displayed with the tagline "A Portal Site of Materials Science Simulation". There are links for "JP / EN" and a search bar with a "Search" button and a "Detailed search" link. Below the header, there is a navigation bar with links: "News / Hands-on / Event", "List of Apps", "Search Apps", "Keywords", "Research Showcase", and "Concierge". The main content area has a dark blue banner with the text "Try the app without installing 「MateriApps LIVE」" and a "MORE" button. Below this is a green section titled "Search by category" with nine buttons arranged in a 3x3 grid: "Electronic structure (solid state physics)", "Electronic structure (quantum chemistry)", "Molecular dynamics", "Visualization/modeling", "Strong correlation/effective models", "Data analysis/supplementary tool", "Continuum models", "Database", and "Integrated Environment".

now 232 Apps
Inquiry / Application Request

JP / EN

MateriApps
A Portal Site of Materials Science Simulation

What's MateriApps? Call for reviews

Search

Detailed search

News / Hands-on / Event List of Apps Search Apps Keywords Research Showcase Concierge

Try the app without installing 「MateriApps LIVE」 MORE

Search by category

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- Continuum models
- Database
- Integrated Environment