

How to find and share information on software in computational materials science using MateriApps

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Outline

0. Self introduction
1. What's MateriApps
2. MateriApps Live! - an easy way to use software
3. Reviews on software packages
4. Short introduction to HΦ and Kω



2018.10.2 Innovation Camp

Self introduction

2004.4 - 2006.3 : Master (ISSP, Imada lab)

2006.4 - 2008.9 : Doctor (Dep. of Applied Physics, Imada lab)

2008.10 - 2009.1 : JST PD (Dep. of Applied Physics, Imada lab)

2009.1 - 2009.11 : CREST PD (Dep. of Applied Physics, Imada lab)

2009.11 - 2016.1 : Research Associate (Imada lab)

2016.2 - present : PCoMS PI (ISSP)

- **Unconventional quantum criticalities**

- Quantum criticality in metal-insulator transitions (MQCP)

- Quantum tricriticality (QTCP)

- **Development of numerical methods for SCES**

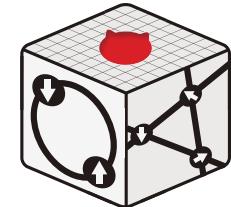
- Ab initio calculations for iron-based SCs, organic conductors

- Analysis of SC in the Hubbard models, interfaces of cuprates

- Exotic phases (CO triple-Q magnetic order) in the Kondo lattice model

- **Development of open-source softwares for SCES [HΦ, mVMC]**

- Finite-temperature effects on quantum spin liquids



MateriApps — a Portal Site for Materials Science Simulation

[Formal introduction]

- Aiming at the community formation through the promotion of application software



- Introducing **229 materials science applications and tools** (as of 2018.8)
- Finding applications
 - search tags: features, targets, calculation methods/algorithms
- Information of applications
 - brief introduction, link to official pages, information installation, usage, etc
- Information of hands-on sessions, software update, etc
- 10000+ pageviews / month, 2000+ unique visitors / month

Motivations for developing MA

Users



How to find software ?
How to use software ?
Information about hands-on?
(Which software is better?)

Developers



Ads on software require much costs ...
(making web page and holding hands-on)

MA for users: a portal sites for software and related useful info.

MA for developers: a site for advertise their software

MA aims to be tabelog (食べログ) in the community of CMS.

Tabelog - the site you can search *restaurant* through ranking
and reviews by users (口コミ)

Short history of MA

FY 2013-

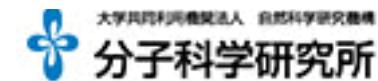
MA starts as a promotion project in CMSI

MA is operated by ISSP (物性研), IMR(金研), IMS(分子研)



Promote the computational materials science !

Main developers: N. Kawashima, S. Todo,
K. Yoshimi (he was working in industry), ...,
and many project researchers are involved in MA



FY 2015,2016: CMSI finishes and Post-K projects (CDMSI) starts but ...



sponsored by 元素戦略

No budget for the promotion in CDMSI!

FY 2015- : PCoMS starts and MA is taken over by PCoMS
MA is now operated by *only* ISSP



Operate MA by PCoMS in ISSP !



Main developers: T. Misawa, K.Ido,
Y. Motoyama,S. Todo, S. Kasamatsu,
T. Kato, K. Yoshikawa, N. Kawashima

Renovation of MateriApps on 2018.4

- New URL: <https://ma.issp.u-tokyo.ac.jp>

- New look & feel
- Improved word search
- New contents:

- 229 applications / tools in total
(including CrySPY, pymatgen, etc)
- Keywords
- "Concierge (アプリコンシェルジュ)"
- **Reviews of applications / tools**
- Ad. on SNS (twitter etc...)



Adding Apps, Reviews , Questions via concierge are welcome !

Applications on MateriApps

- Introducing **229 materials science applications and tools** (as of 2018.8)

DFT

AkaiKKR[☆]

OpenMX[☆]

xTAPP[☆]

ABINIT[☆]

... (42)

Quantum Chemistry

FMO[☆]

SMASH[☆]

GAMESS[☆]

DC[☆]... (20)

Molecular Dynamics

MODYLAS[☆]

Gromacs[☆]

ERmod[☆]

MDACP... (20)

Lattice Models

ALPS[☆]

DSQSS

BLOCK

DMRG++⁽²⁷⁾

Continuum Simulation

ANSYS Multiphysics

Octa ...

(13)

Materials Database (3)

Data Analysis

CLUPAN[☆]

phonopy[☆] (32)

Visualization

fu[☆]

TAPIOCA[☆] (28)

[☆] included in MateriApps LIVE!

MateriApps LIVE!



- Use in virtual machine or boot directly from USB stick (Debian Live Linux)

- run on Windows, Macintosh, etc
- just boot and get ready for materials science simulations without installation

• **Version 2.0 is released on Aug. 26 !**

• **Download from web site is a convenient way**

- Pre-installed applications and tools

- abinit, AkaiKKR, ALPS, CP2K, Feram ,ERmod, Gromacs, HΦ, LAMMPS, mVMC, Quantum Espresso, SMASH, xTAPP 等
 - ParaView, Tapioca, VESTA, VMD, XCrysDen...
 - GUI installer for GAMESS and VMD
- available from MateriApps LIVE! webpage
- distributed 3000+ copies since 2013.7



DSQSS,
OpenMX,

How to use MateriApps LIVE!

- Hands on MateriApps LIVE!
 - MateriApps LIVE! Hands on
 - HΦ, mVMC, xTAPP, ALPS, DCore..
 - Coming Hands on: xTAPP 10/19 , DDMRG 11/14 [You can attend !]
- Lectures in university (tokyo-tech, tokyo science univ.)
 - Numerical Physics
 - Numerical Experiments (UNIX + C , LaTeX、 version control system [git or svn])
- Non-experts (experimentalists, researchers in industry or in computations science) can easily try to use applications [No compile !]
- Troubles in hands on are very rare !(VirtualBox OVA ver.)、 Within 15 minutes you can finish setup
- Easy for trouble shooting and user supports because the environment is completely the same !

How to find software I

The screenshot shows the MateriApps website interface. At the top left, there's a green button for 'Inquiry / Application Request' and a link to 'now 231 Apps'. Language options 'JP / EN' are also at the top. The main header features the 'MateriApps' logo with a green swoosh and the subtitle 'A Portal Site of Materials Science Simulation'. A red box highlights the search bar area, which includes links for 'What's MateriApps?' and 'Call for reviews', and a search input field with a magnifying glass icon. Below the search bar are navigation links: 'News / Hands-on / Event', 'List of Apps', 'Search Apps', 'Keywords', 'Research Showcase', and 'Concierge'. A banner below these links says 'Try the app without installing 「MateriApps LIVE」' and has a 'MORE' button. The main content area is titled 'Category' and features a grid of nine rounded rectangular buttons representing different software categories:

- Electronic structure (solid state physics)
- Electronic structure (quantum chemistry)
- Molecular dynamics
- Visualization/modeling
- Strong correlation/effective models
- Data analysis/supplementary tool
- Continuum models
- Database
- Integrated Environment

Using search form → enter keywords (name of software, name of method, ...)

How to find software II

The screenshot shows the MateriApps website interface. At the top left, there is a green button labeled "Inquiry / Application Request". To its right, the text "now 231 Apps" is displayed above a language selection bar with "JP / EN". The central logo features the word "MateriApps" in a stylized font with a green swoosh, and below it, the text "A Portal Site of Materials Science Simulation". On the far right, there are links for "What's MateriApps?", "Call for reviews", a search bar, and a "Detailed search" link. Below the header, a navigation bar includes links for "News / Hands-on / Event", "List of Apps", "Search Apps", "Keywords", "Research Showcase", and "Concierge". A banner below the navigation bar says "Try the app without installing 「MateriApps LIVE」" and has a "MORE" button. The main content area is titled "Category" and contains a red-bordered box labeled "Search by category". Inside this box are nine categories listed in rounded rectangles: "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".

Select category → You can find list of applications
in the selected category

How to find software III

The screenshot shows the MateriApps website interface. At the top left, there is a green banner with the text "now 231 Apps" and a button for "Inquiry / Application Request". Next to it are language links "JP / EN". The central logo is "MateriApps" with the subtitle "A Portal Site of Materials Science Simulation". To the right, there are links for "What's MateriApps?", "Call for reviews", a search bar, and a "Detailed search" link. Below the header, there are navigation links: "News / Hands-on / Event", "List of Apps", "Search Apps" (which is highlighted with a red box), "Keywords", "Research Showcase", and "Concierge". A banner below these links says "Try the app without installing 「MateriApps LIVE」" and has a "MORE" button. The main content area is titled "Search by category" and lists several categories in rounded boxes: "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 231 Apps

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

- Electronic structure (solid state physics)
- Electronic structure (quantum chemistry)
- Molecular dynamics
- Visualization/modeling
- Strong correlation/effective models
- Data analysis/supplementary tool
- Continuum models
- Database
- Integrated Environment

How to find software ∞

Most convenient way = ググる (using google)

Dr. S.K. (developer of MA)

I have never used
search form in MA

1. Keyword + MateriApps in google
ex. Salmon MateriApps, Hubbard model MateriApps

2. Keywords + site:ma.issp.u-tokyo.ac.jp
ex. Salmon site:ma.issp.u-tokyo.ac.jp
Salmon site:ma.issp.u-tokyo.ac.jp/en

en = english

How to ask questions in MA

1. Inquiry

The screenshot shows the MateriApps homepage with a navigation bar at the top. In the center, there is a large form titled "Inquiry / application request". The form has two tabs: "Inquiry" (selected) and "Application request". Below the tabs are several input fields: "Name*" (required), "Affiliation", "E-mail Address*" (required), "E-mail address (confirmation)*", and "Inquiry contents*".

2. Apps concierge

The screenshot shows the MateriApps homepage with a "Concierge" section. The "Concierge" button is highlighted with a red box. Below it, there is a button labeled "Ask the App concierge" which is also highlighted with a red box. The "Concierge" section contains text explaining what an "application concierge" does and how to request one.

3. Question box in twitter

<https://twitter.com/materiapps>



How to add your apps

1. Apps request



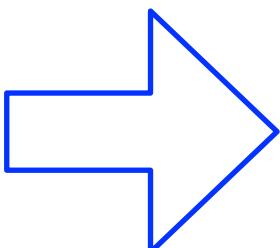
The screenshot shows the MateriApps homepage with a navigation bar at the top. Below it is a search bar and a main content area titled 'Inquiry / application request'. This section contains two tabs: 'Inquiry' (selected) and 'Application request'. The 'Application request' tab is highlighted with a green background. Below these tabs is a form with several input fields:

- Name*: [Text input]
- Affiliation: [Text input]
- E-mail Address*: [Text input]
- E-mail address (confirmation)*: [Text input]
- App: [Text input]
- APP URL: [Text input]
- very explanation*: [Text input]

2. e-mail to MA team

ma@cms-initiative.jp

We create web for your apps !



Elastic
Openness:3 *** Document quality:3 ***
Elastic is a set of python-routines for calculation of elastic properties of crystals (elastic constants, equation-of-state, sound velocities, etc.). It is implemented as a extension to the Atomic Simulation Environment ([ASE](#)) system. There is a script providing interface to the library not requiring knowledge of python or ASE system.

Information
Official site
<https://elastic.readthedocs.io/en/stable/>



DISCUS
Openness:3 *** Document quality:3 ***
An open source application to simulate crystal structures and to calculate and refine against diffraction pattern and the pair distribution function. A special emphasis placed is on the simulation of materials with disorder and the package provides many tools to create and distribute defects throughout the crystal. Another strong feature is the simulation of nanoparticles.

Information
Official site
<https://github.com/ghofrani/DisCuSCode>

Explanation of keywords in CMS

The screenshot shows the MateriApps website interface. At the top left, there is a green button for 'Inquiry / Application Request' and language links 'JP / EN'. The central logo is 'MateriApps' with the subtitle 'A Portal Site of Materials Science Simulation'. Top navigation includes 'What's MateriApps?', 'Call for reviews', a search bar, and a 'Detailed search' link. Below the header, a horizontal menu has 'Keywords' highlighted with a red box. Other menu items include 'News / Hands-on / Event', 'List of Apps', 'Search Apps', 'Research Showcase', and 'Concierge'. A large, semi-transparent watermark 'Keyword' is visible across the page. In the middle section, there is a navigation bar with letters A through U-Z and a search bar. The main content area features a section titled 'Atom-localized basis/Gaussian basis' with a detailed explanatory text.

now 232 Apps

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

Keywords

I will explain the terms that appear in computational material science.

A B-C D-E F-G H-L M N-O P-R S-T U-Z

Search

Atom-localized basis/Gaussian basis

Many calculation codes expand the wave function using functions localized around atoms. Usually, numerical solutions to the Kohn-Sham equation for the atom or atom-localized Gaussians are used. Since the wave function in molecules and solids usually resemble a linear combination of atomic wave functions, atom-localized basis sets can describe the wave function accurately using a much smaller number of basis functions compared to the plane wave basis set. However, since atom-localized basis functions are not orthogonal in general, the improvement with increasing basis size is not always monotonic. Moreover, atom-localized basis sets are usually unsuitable for describing systems where electrons exist at positions away from atoms (such as in electrides or floating electron states).

Writing “keywords” is welcome !

How to share information [Review, 口コミ]

検索結果
「アプリレビュー」での検索結果：21

アプリレビュー
RESPACKを用いたSrVO3のワニ工軌道の作製(物性研スパコンでの使用例)
使用方法: ここでは、RESPACKの物性研スパコンsystem Bへの使用方法について紹介します。RESPACKはsystem Bにプレインストールされているので、それを使いたいと思います。source /home… [続きを読む](#)

アプリレビュー
HPhiのMateriApps LIVE!での使用例
はじめに: ここでは、HPhiのMateriApps LIVE!での使用例について紹介します。MateriApps LIVE!とは様々な物性科学アプリがおさめられているLive Linux システムのことです。Mat… [続きを読む](#)

アプリレビュー
Quantum EspressoでSiのフォノンバンド図を作成する
MateriApps LIVE!にプレインストールされたQuantum Espressoで何か適当な物質のフォノンバンド図を描いてみようと思います。VirtualboxでMateriApps LIVE!2.0a1（α版）… [続きを読む](#)

You can share information about apps via Review !

- how to download, install, and use apps
- impression, comment on using apps
- etc...

Please write reviews in this camp !



Templates are available at
<https://github.com/issp-center-dev/ICCMS>

Writing “keywords” is also welcome !

Short introduction to HΦ



<https://github.com/issp-center-dev/HPhi>

History of HΦ

Around 2006: TM wrote the codes in C for the exact diagonalization (ED) for the Hubbard model based on **TITPACK ver.2** by Prof. Nishimori

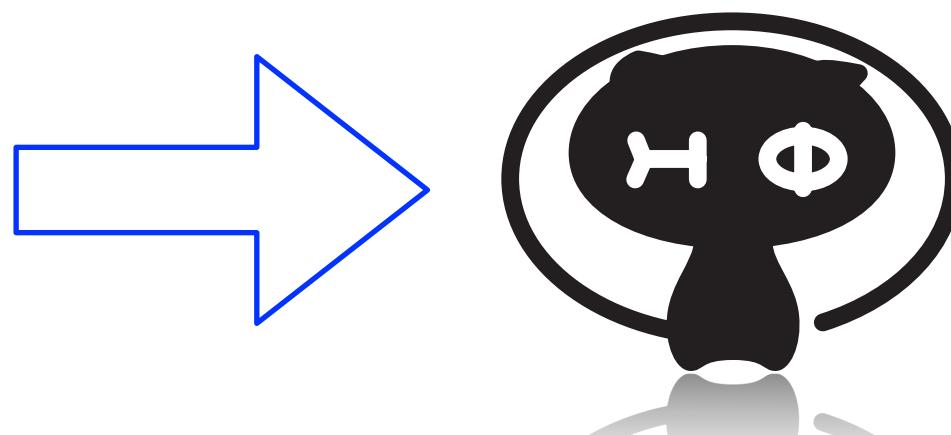
Around 2008: TM improved the interfaces of ED, which are compatible for variational MC codes by D. Tahara

2008-2015: TM had extended ED codes for calculating Kondo-lattice models, thermal pure quantum (TPQ) states and real-time evo., etc..

Problems:

Unsophisticated codes, Not support the MPI parallelization,
Unsophisticated user interfaces

2015-2017: “Project for advancement of software usability in materials science” by ISSP



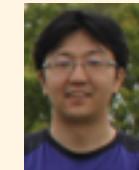
Project for *advancement of software usability* in materials science

ISSP Supercomputer (SC)

1995 1st SC → 2000 2nd SC → ⋯ → 2015 sekirei (System B)

Provide stable computing Environment

Occupancy rate > **95%**, over **500 articles** related to ISSP SC/year



K. Yoshimi



Enhance
the usability



Pre-install

Software in materials science



...

Develop 1-2 software per year
Release as Open source software
(mainly GNU Public License)
Public offering (December)

Faster and more powerful !

Developers of HΦ (2015-)

M. Kawamura



T. Misawa

K. Yoshimi

Y. Yamaji



S. Todo



K. Ido



N. Kawashima



Development of HΦ is supported by
*“Project for advancement of software
usability in materials science”* by ISSP



Summary of HΦ

What can we do by HΦ?

For Hubbard model, spin- S Heisenberg model,
Kondo-lattice model ...

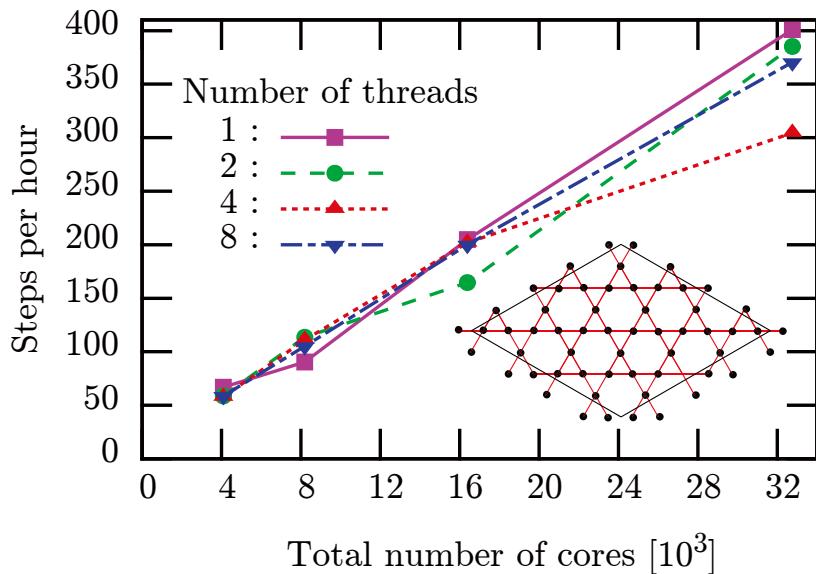
- Full diagonalization
- Ground state calculations by Lanczos method
- Finite-temperature calculations by thermal pure quantum (TPQ) states
- Low-energy states calculation by LOBCG method
- Dynamical properties [$S(q,\omega)$], real-time evo.

maximum system sizes@ ISSP system B (sekirei)

- spin 1/2: ~ 40 sites (S_z conserved)
- Hubbard model: ~ 20sites (# of particles & S_z conserved)

Parallelization of HΦ @ Kei[京]

Up to 32,768 cores on K computer



Measure calculation time of matrix-vector production.

Model

- **36 bits Heisenberg model**
- **Grand canonical calculation**
- **Hilbert space: $2^{36} \sim 6.87 \times 10^{10}$**

We obtain the almost linear scaling even if we use very large number of cores (more than 10^4 cores).
Parallelization efficiency $\sim 80\%$

We can efficiently investigate physical properties on Super computer by HΦ !

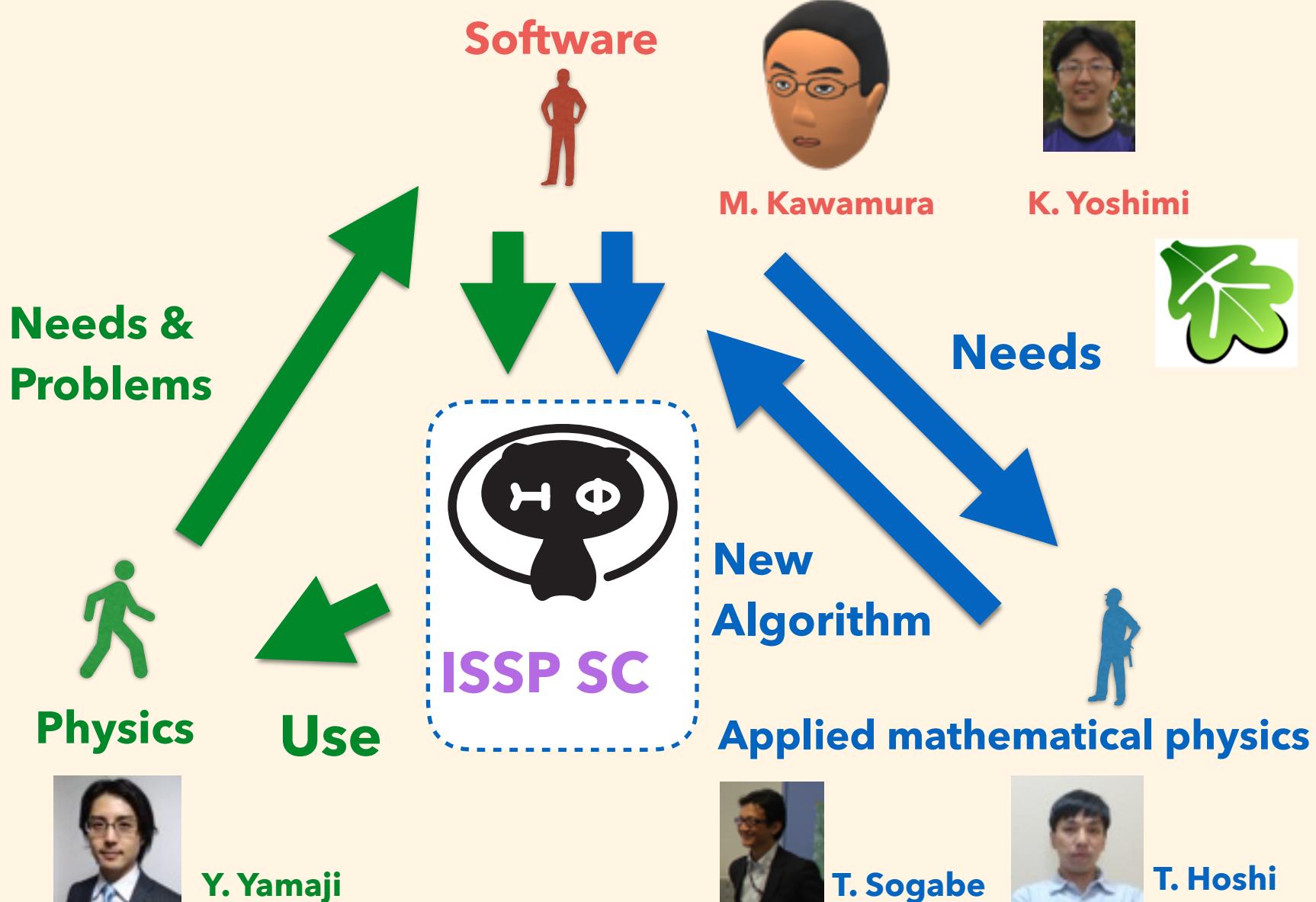
Collaboration with applied mathematics

What can we do by HΦ?

- Low-energy states calculation by LOBCG method
→ LOBCG method is introduced by Prof. Sogabe and Prof. Hoshi
- Dynamical properties [$S(q,\omega)$]
→ Shifted Krylov method is introduced by Prof. Sogabe and Prof. Hoshi



Example of collaboration through HΦ



Short introduction to K ω



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

What is $K\omega$ (1) ?

- Simulation: Calculate dynamical green's function



Linear response of ground state

$$G_{ij}(\omega) = \langle \Phi_0 | \hat{A}_i^\dagger (\omega - \hat{\mathcal{H}})^{-1} \hat{A}_j | \Phi_0 \rangle$$

$$G_{ij}(\omega) = \langle b_i | x_j(\omega) \rangle$$

$$\left\{ \begin{array}{l} |b_i\rangle = \hat{A}_i |\Phi_0\rangle \\ |x_j(\omega)\rangle = (\omega - \hat{H})^{-1} |b_j\rangle \end{array} \right.$$

$$(\omega - \hat{H}) |x_j(\omega)\rangle = |b_j\rangle$$

Solvable by BiCG method

- Shift invariance of Krylov subspace

Residual norm

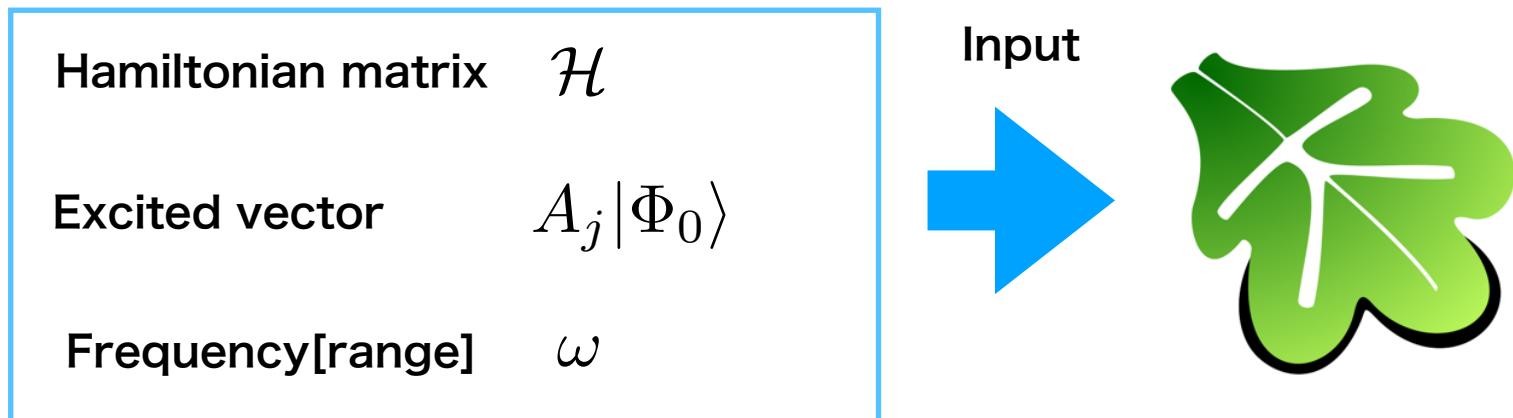
$$r_j(\omega) = |(\omega - \mathcal{H}) |x_j\rangle - |b_j\rangle|$$

$$|b\rangle, (\omega - \mathcal{H}) |b\rangle, (\omega - \mathcal{H})^2 |b\rangle, \dots, (\omega - \mathcal{H})^M |b\rangle$$

What is $K\omega$ (2) ?

- Simulation: Calculate dynamical green's function
Linear response of ground state

$$G_{ij}(\omega) = \langle \Phi_0 | \hat{A}_i^\dagger (\omega - \hat{\mathcal{H}})^{-1} \hat{A}_j | \Phi_0 \rangle$$



How to prepare Hamiltonian matrix and an excited vector ?

Two ways to use Kw

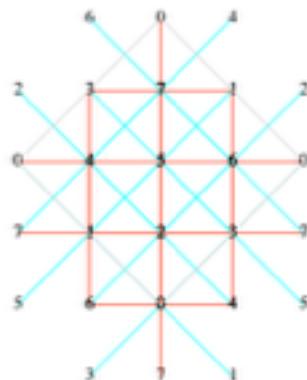
- As software (for beginner users)
 - Read a matrix (format: Matrix Market) and an excited vector
 - Make a matrix in Kw (Heisenberg model)
- As a library → $H\Phi$
 - Link Kw and insert functions to your codes.

Calculate dynamical Green's function by $\text{H}\Phi$ (1)

1st. step: Calculate an eigen state $|\Phi_0\rangle$

ex.) 2D Hubbard model (8 site) : samples/spectrum/stan1.in

```
a0W = 2
a0L = 2
a1W = -2
a1L = 2
model = "hubbard"
method = "CG"
lattice = "square"
t = 1.0
t' = 0.5
U = 4.0
2Sz = 0
nelec = 8
EigenvecIO = "out"
```



\$HPhi -s [stan1.in](#)



$\text{H}\Phi$

The ground state is obtained
in the output folder.

`zvo_eigenvec_0_rank_0.dat`

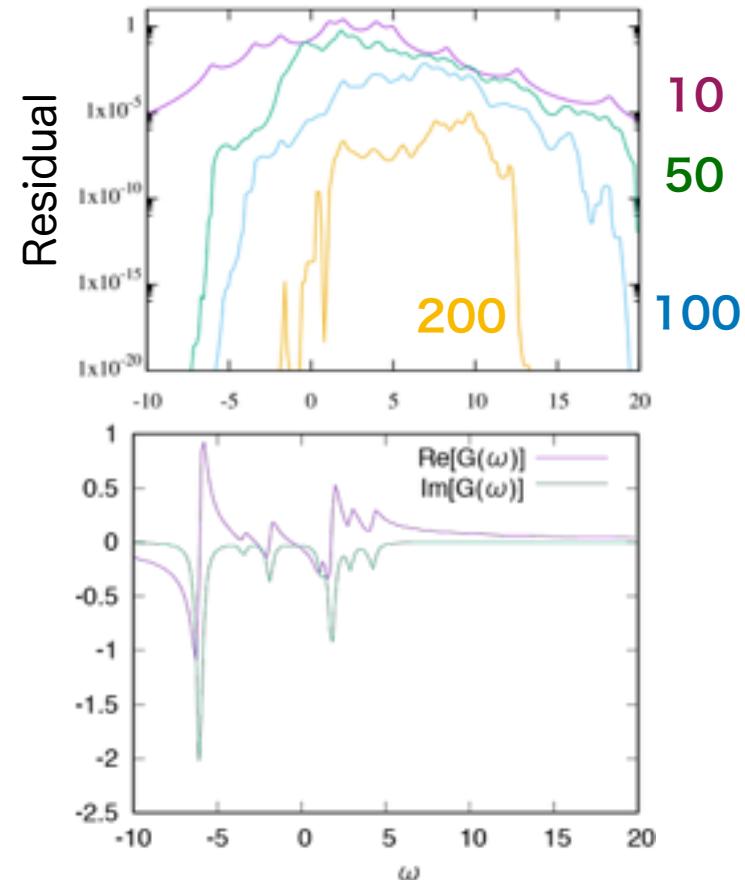
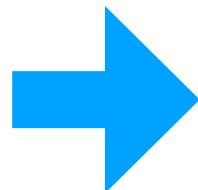
Calculate dynamical Green's function by $H\Phi$ (2)

2nd. step: Calculate spectrum by $K\omega$ (method = “CG”)

ex.) 2D Hubbard model (8 site) : samples/spectrum/stan2.in

Excited type : Spectrum Type

```
a0W=2
...
CalcSpec = "Normal"
SpectrumType = "SzSz"
SpectrumQW = 0.5
SpectrumQL = 0.5
OmegaMin = -10.0
OmegaMax = 20.0
OmegaIM = 0.2
```



\$HPhi -s [stan2.in](#)

Calculate dynamical Green's function by $\mathcal{H}\Phi$ (3)

$$G_{ij}(\omega) = \langle \Phi_0 | \hat{A}_i^\dagger (\omega - \hat{\mathcal{H}})^{-1} \hat{A}_j | \Phi_0 \rangle$$

Excited type $\hat{A}_j = \hat{A}_i$
1. SzSz $\langle S_z(q) S_z(-q) \rangle \rightarrow \hat{A}_j = S_z(-q)$

2. S+S- $\langle S_+(q) S_-(-q) \rangle \rightarrow \hat{A}_j = S_-(-q)$

3. Density $\langle n(q) n(-q) \rangle \rightarrow \hat{A}_j = n(-q)$

4. Up $\langle c_\uparrow^\dagger(q) c_\uparrow(-q) \rangle \rightarrow \hat{A}_j = c_\uparrow(-q)$

5. Down $\langle c_\downarrow^\dagger(q) c_\downarrow(-q) \rangle \rightarrow \hat{A}_j = c_\downarrow(-q)$

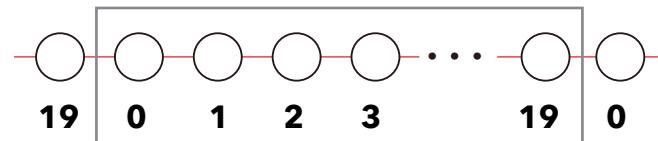
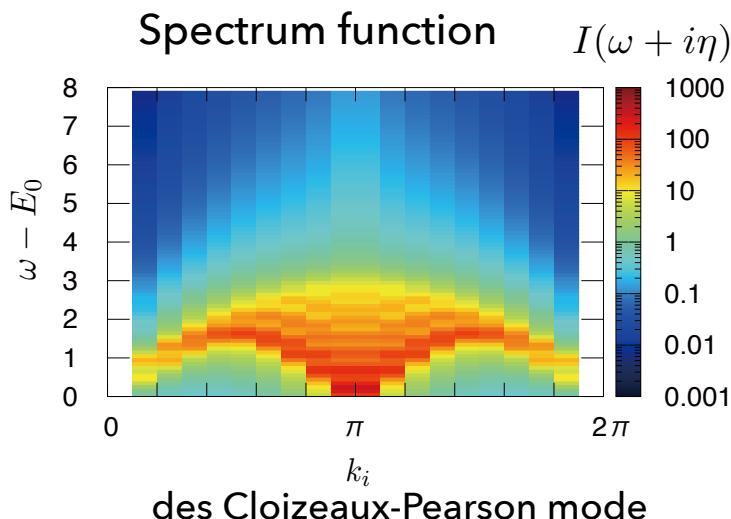
Calculation of spectrum

Ex. 20 bits one-dimensional Heisenberg model

$$\hat{\mathcal{H}} = J \sum_{i=0}^{19} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \quad (\mathbf{S}_{20} = \mathbf{S}_0)$$

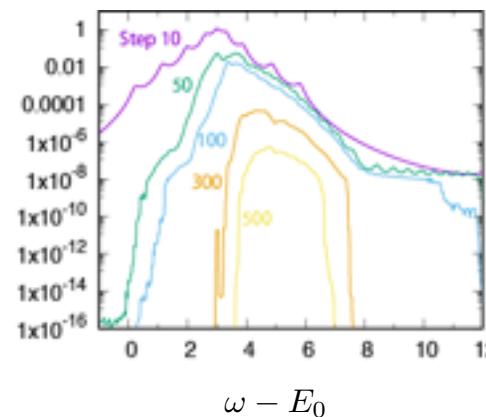
Spectrum function

$$I(\omega) = -\text{Im} \left[\langle \Phi_0 | \hat{S}(k_i)^\dagger (\omega - \hat{\mathcal{H}})^{-1} \hat{S}(k_i) | \Phi_0 \rangle \right]$$



$$\hat{S}(k_i) = \sum_{j=0}^{19} \hat{S}_j^z e^{ik_i r_j} \quad k_i = \frac{\pi}{20} i$$

Residual norm at $k_i = \pi$



Succeed to evaluate the convergence accuracy at each ω !

Summary

Overview of MateriApps

→ Add your apps in MA, *please write reviews*,
and questions are welcome !

Tabelog in CMS !

Overview of HΦ & Kω

→ You can perform shifted Krylov using Kω !

