HΦ tutorial

Full diagonalization method

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2018/8/22

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Calculation mode

1. Single node (from ver.1.0)
   Solver: LAPACK
2. **Multi** node (from ver.3.1)
   Solver: ScaLAPACK
3. **GPGPU** mode (from ver.3.1)
   Solver: MAGMA (**1 node** + multi GPU devices)

Priority：GPGPU mode > Multi node > Single node

HΦ preinstalled in sekirei → All modes can be used

How to compile (1)

1. Single node (from ver.1.0)
   no option

Example for GNU compiler

```
$ mkdir hphi.build && cd hphi.build
$ cmake -DCONFIG=gcc ../
$ make
```

How to compile (2)

2. Multi node (from ver.3.1)
   Add option **-DUSE_SCALAPCK=ON**

Example for GNU compiler

```
$ mkdir hphi.build && cd hphi.build
$ cmake -DCONFIG=gcc -DUSE_SCALAPACK = ON ../
$ make
```

How to compile (3)

3. GPGPU mode (from ver.3.1)

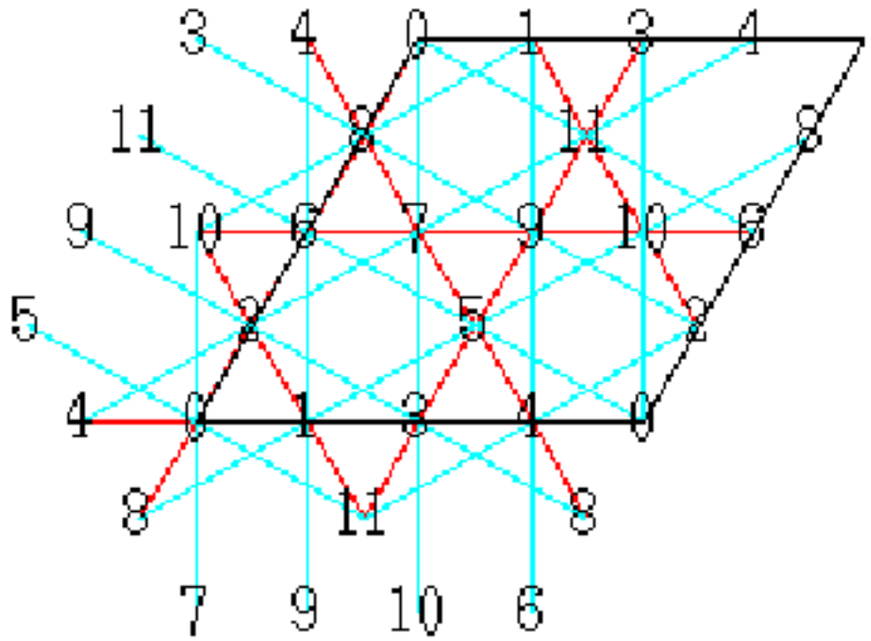
Edit sekirei_acc.cmake file
to compile HΦ with MAGMA on you own PC, cluster etc.

Example for sekirei

```
$ mkdir hphi_acc.build && cd hphi_acc.build
$ cmake -DCONFIG=sekirei_acc ../
$ make
```

Tutorial (1)

Spin system



Lattice

```
L = 2
W = 2
model = "SpinGC"
lattice = "Kagome"
method = "FullDiag"
J = 1.0
```

Input file for standard model (stan.in)

Hilbert space: 2^{12}=4096

Tutorial (2)

1. Single node (from ver.1.0)

   (1) Calculation

```
$ HPhi -s stan.in
```

Ref. Check consuming time (output/CalcTimer)

```
All                                          [0000]    144.94083
  sz                                         [1000]      0.00288
  diagonalcalc                               [2000]      0.00262
  CalcByFullDiag                             [5000]    144.86798
    MakeHam                                  [5100]      0.13374
    LapackDiag                               [5200]    138.16219
    CalcPhys                                 [5300]      6.56411
      calc flctuation in expec_energy_flct   [5301]      0.11938
      mltply in expec_energy_flct            [5302]      0.66882
    Output                                   [5400]      0.00758
    OutputHam                                [5500]      0.00000
```

Tutorial (3)

2. Multy node (from ver.3.1)

(1) Make input files for expert mode

```
$ HPhi -sdry stan.in
```

(2) Edit calcmod.def file

Add 「Scalapack 1」 (0: not use ScaLAPACK)

```
CalcType    2
CalcModel    4
ReStart    0
CalcSpec    0
CalcEigenVec    0
InitialVecType    0
InputEigenVec    0
OutputEigenVec    0
NGPU 0
Scalapack 1
```

(3) Start calculation

```
$ HPhi -e namelist.def
```

Tutorial (4)

3. GPGPU node (from ver.3.1)

(1) Make input files for expert mode

```
$ HPhi -sdry stan.in
```

(2) Edit calcmod.def file

Add NGPU (number of GPU devices used for calculation)

```
CalcType    2
CalcModel    4
ReStart    0
CalcSpec    0
CalcEigenVec    0
InitialVecType    0
InputEigenVec    0
OutputEigenVec    0
NGPU 2
```

Default number of NGPU is **2**.

(3) Start calculation

```
$ HPhi -e namelist.def
```

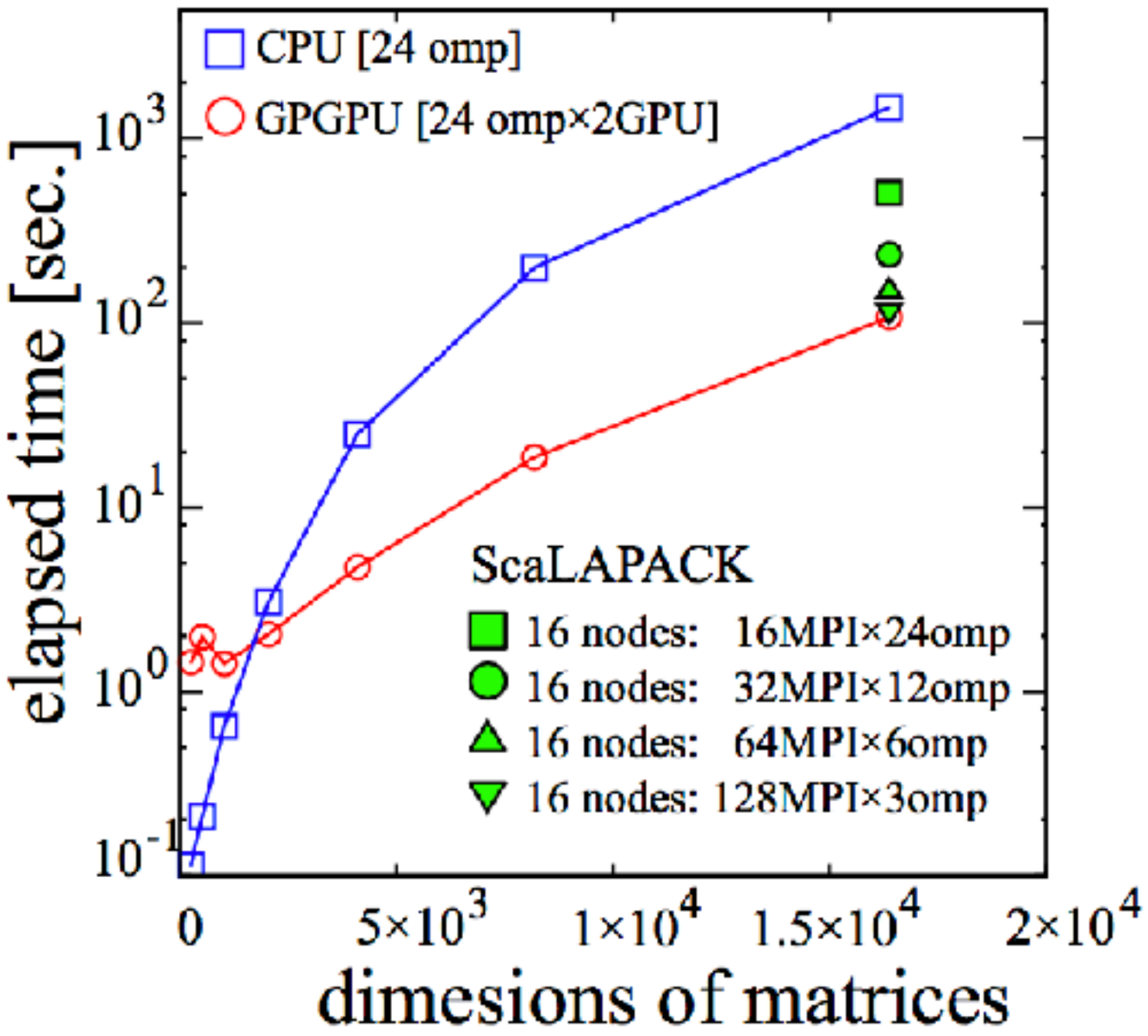
Tutorial (5)

Consuming time for full diagonlization in sekirei

Queue i9acc

1. LAPACK (1node: 1mpi, 24omp)
   138.16219 [s]
2. ScaLAPACK (1node: 24mpi, 1omp)
   17.00050 [s]
3. GPGPU (1node: 2GPU)
   5.35803 [s]

Benchmark result in sekirei



1 node
- CPU: Intel Xeon 2.5 GHz (12cores) ×2
- GPU: Nvidia Tesla K40 ×2

Ref. “Implementation of GPGPU computing in full diagonalization for HΦ” , T. Misawa and K. Yoshimi, Activity report 2017 in ISSP, http://www.issp.u-tokyo.ac.jp/supercom/activity-reports/2017