Setup for gauss

2019/10/9

About gauss

1. Information of gauss can be seen in the terminal when you log in to gauss.

```
# System

  * Login node : gauss
  * Computational nodes : gauss01 - gauss13
    * 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/

# Scheduled Maintainance

  * None
```

13 nodes
28 cores/node

2. Sample script (/home/public/sample.sh)

```
#!/bin/sh
#PBS -l nodes=2:ppn=7
#PBS -n
#
ulimit -m `expr 60000000 / ${PBS_NUM_PPN}`
ulimit -v `expr 60000000 / ${PBS_NUM_PPN}`
source ~/.bashrc
#
export OMP_NUM_THREADS=4
#
cd $PBS_O_WORKDIR
#
mpiexec -hostfile $PBS_NODEFILE /home/public/bin/openmx GaAs.dat -nt $OMP_NUM_THREADS
```

use 2 nodes and 7cores /node

use 4 threads for OpenMP

Submit a job

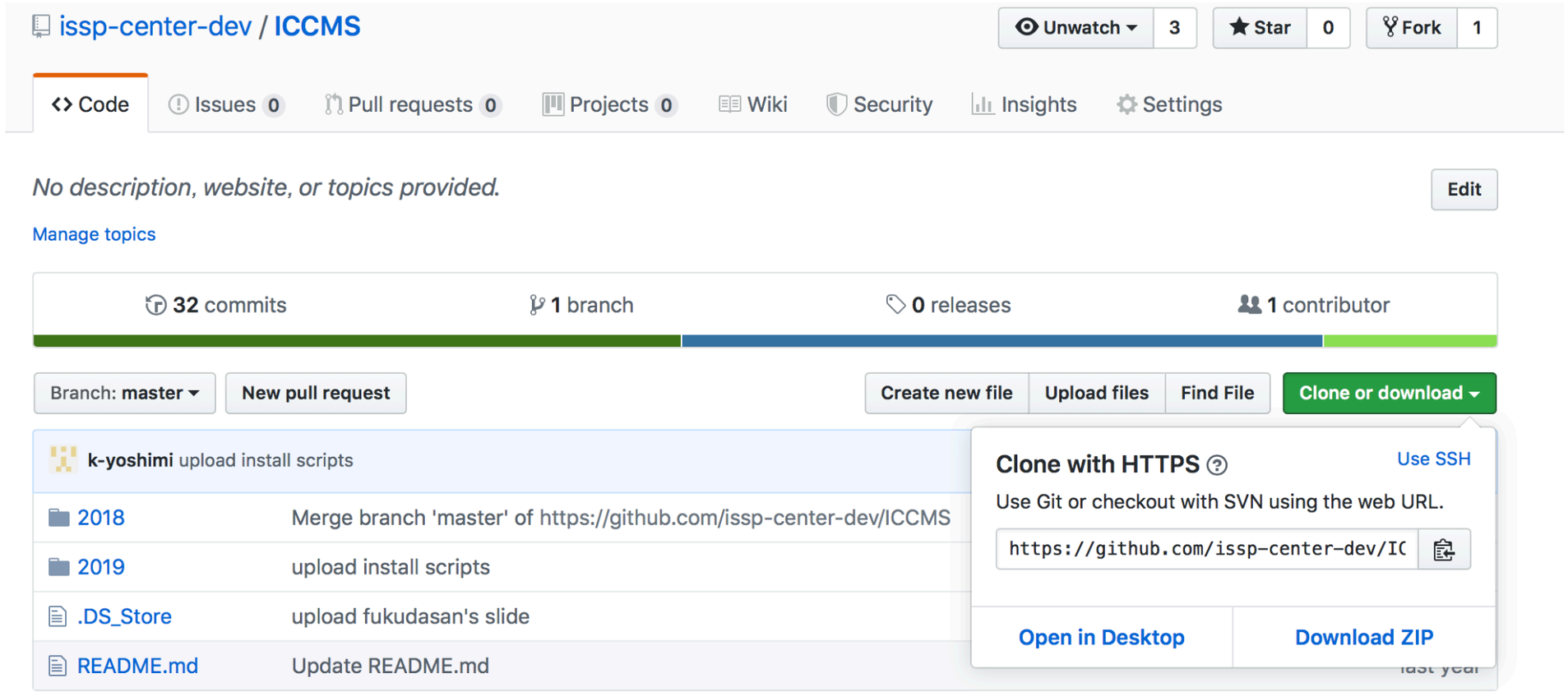
$ qsub /home/public/sample.sh

If you do not know how to use job scheduler, ask Fukuda-sann (organizer).

Installation of COMBO and HΦ(1)

1. Copy URL of Github repository for ICCMS

   - https://github.com/issp-center-dev/ICCMS



Click 「Clone or download」 and copy URL

Installation of COMBO and HΦ(2)

2. Git clone in terminal(Below https is the URL you copied).

- $ git clone https://github.com/issp-center-dev/ICCMS.git

```
[guest20@gauss ~]$ git clone https://github.com/issp-center-dev/ICCMS.git
Initialized empty Git repository in /home/guest20/ICCMS/.git/
remote: Enumerating objects: 16, done.
remote: Counting objects: 100% (16/16), done.
remote: Compressing objects: 100% (14/14), done.
remote: Total 195 (delta 0), reused 16 (delta 0), pack-reused 179
Receiving objects: 100% (195/195), 104.99 MiB | 23.78 MiB/s, done.
Resolving deltas: 100% (37/37), done.
```

3. Make and change to tutorial directory and copy scripts.

- $mkdir tutorial & cd tutorial

- $cp ~/ICCMS/2019/2019-10-08/script/* .

Installation of COMBO and HΦ(3)

4. Install COMBO

- $ sh install_combo.sh
- $ python
  - import combo

Check

```
[guest20@gauss ~]$ python
Python 2.7.15 (default, Sep 23 2019, 01:06:26)
[GCC Intel(R) C++ gcc 5.10 mode] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import combo
>>> exit()
```

5. Install HPhi

- $ sh install_HPhi.sh
- $ cd HPhi.build && make test

Check all tests are passed.

```
48/49 Test #48: te_spin_chain_interall ..............   Passed    0.70 sec
      Start 49: te_kondo_chain_interall
49/49 Test #49: te_kondo_chain_interall .............   Passed    0.71 sec

100% tests passed, 0 tests failed out of 49

Total Test time (real) =  40.93 sec
```

About HΦ, see http://www.pasums.issp.u-tokyo.ac.jp/hphi/

About HΦ (1)

From MateriApps

HΦ

Openness:3 ★★★　Document quality:2 ★★☆

An exact diagonalization package for a wide range of quantum lattice models (e.g. multi-orbital Hubbard model, Heisenberg model, Kondo lattice model). HΦ also supports the massively parallel computations. The Lanczos algorithm for obtaining the ground state and thermal pure quantum state method for finite-temperature calculations are implemented. In addition, dynamical Green's functions can be calculated using Kω, which is a library of the shifted Krylov subspace method. It is possible to perform simulations for real-time evolution from ver. 3.0.

Supported by
Project for Advancement of Software Usability in Materials Science
(http://www.issp.u-tokyo.ac.jp/supercom/softwaredev)

About HΦ (2)

Target substance/model	Hubbard model, Heisenberg model, Kondo lattice model, Kitaev model, Kitaev-Heisenberg model, multi-orbital Hubbard model
Physical quantities that can be computed	specific heat, susceptibility, ground state energy, free energy, structure factors
Methodology	Lanczos algorithm, thermal pure quantum state, full diagonalization

For details, see
http://www.pasums.issp.u-tokyo.ac.jp/hphi/en/

Lecture slides :
http://www.pasums.issp.u-tokyo.ac.jp/hphi/en/doc/presentation