Common code system for the lattice QCD simulations

Shinji MOTOKI (KEK, A04 team)

for

Bridge++ Code development Project

H.Matsufuru gives a talk instead, with a little update

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MEMBERS

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Also advised by H.Tadano, A.Imakura,
Seminars by M.Sato and A.Nakamura

Programmers, reviewers and users are wanted.
Any interested people are welcome anytime!

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SUPPORTED BY

Grant-in-Aid for Scientific Research on Innovative Areas
"Research on the Emergence of Hierarchical Structure of Matter by Bridging Particle, Nuclear and Astrophysics in Computational Science"
The A04 team
"Interdisciplinary algorithms and computer simulations"
http://bridge.kek.jp/A04/ (H. Matsufuru's talk)

HPCI Strategic Program Field 5
"The origin of matter and the universe"
http://www.jicfus.jp

- So far 60 meetings held every 1-2 weeks
- Advices given by experts in computer science and applied mathematics

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DEVELOPMENT POLICY

- Portability: running on various environment, from notebook PC to supercomputers
- High performance: fully making use of wide range of architecture, with state of the art techniques
- Easy to understand even for beginners
- Easy to extend to test new ideas

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WHY COMMON CODE?

- **Research environment may changes**

Collaboration members frequently come and go.
  – who maintains the code?
  – communication problem might occur.

Machine architecture may change.
  – have to rewrite a new code for updated machines?

- **Demands for "standard"**

Users should concentrate on their physics projects
Generated data can be shared by different groups.
Common language on the calculations is convenient.

- **Why not using existing codes?**

E.g. Chroma and CPS++ are widely used in the community.
We want a code completely under control of ourselves from foundation
  – Quick response to user's requests
  --Detailed documentation and consulting service
  – Accumulating experiences of the development is important. to keep technology

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PROFILE

Our aim:

well-organized portable code with a good performance, allowing beginners to carry out “professional simulations”

C++ language:

Design by the object oriented programming
Stick to the standard libraries for portability
Parallelized with MPI

Documentation

Doxygen is helpful: comments embedded in the code
Detailed manual in English/Japanese

Covering all basic calculations in Lattice QCD:

Gauge configuration generation + measurements
Commonly used lattice fermions
ILDG data format
Maximum flexibility in simulation parameters

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WHAT HAVE BEEN IMPLEMENTED

Ver.1.0 public release 24 July 2012

- **Gauge action:** Plquette, Rectangular
- **Fermion action:** Wilson, Clover, staggered, overlap, domain-wall
- **Link smearing:** APE or HYP x stout (+ projection)
- **Linear solvers:** CG,BiCGStab, GMRES, etc. + shift solver(CG)
- **Eigen solvers:** Implicitly restarted Lanczos (for Hermitan matrix)
- **HMC:** multi-time step, Hasenbusch, Omelyan integrator, Rational HMC
- **Gauge fixing:** (Coulomb, Landau)
- Schrodinger functional boundaries, isospin chemical potential
- meson/baryon correlators (Dirac/chiral spinor representations)
- Wilson loop, Polyakv loop, etc.
- **ILDG format is supported in configuration data I/O**
- **Now in progress:** multi-thread (openMP or pthread ?), GPU (OpenCL)

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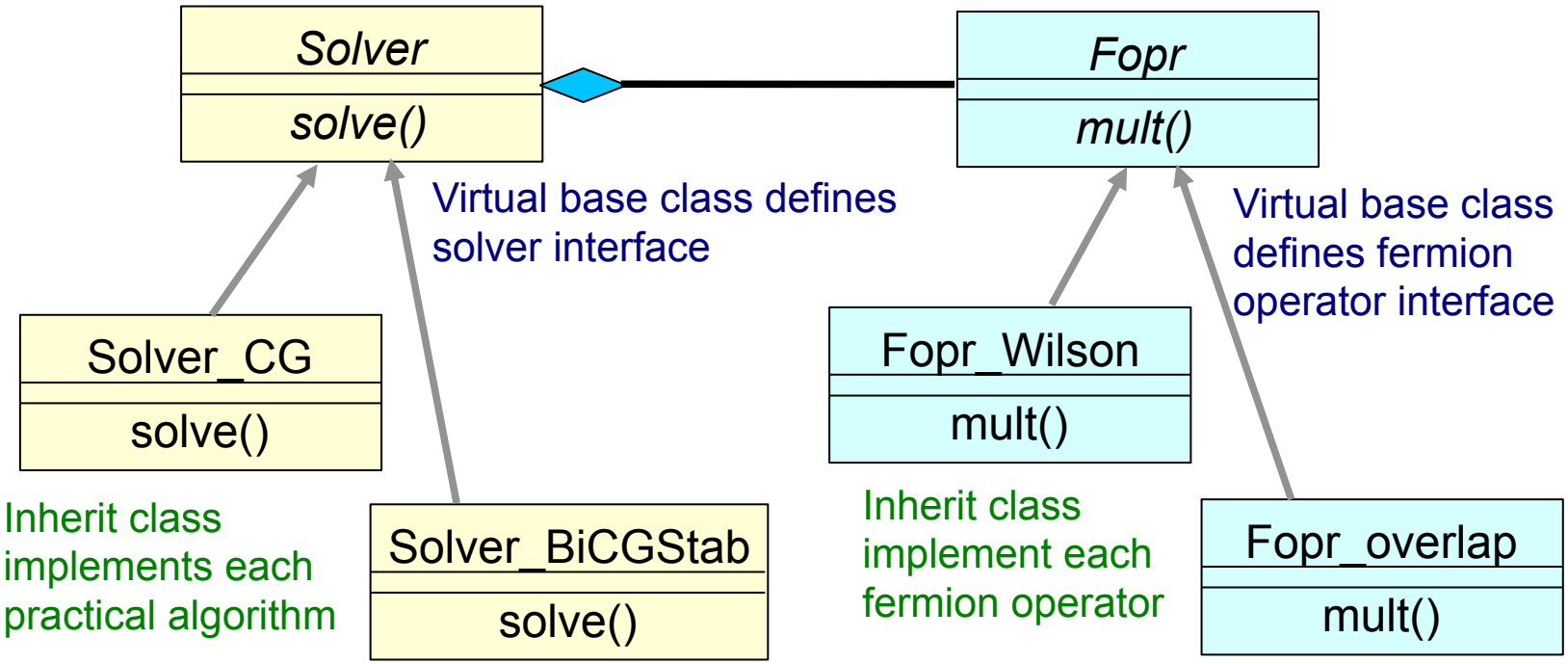
DESIGN

- Example: solver and fermion operator

Class diagram: relation between classes

Solver does not distinguish which fermion operators:
Fopr (base class) defines interface (virtual method)



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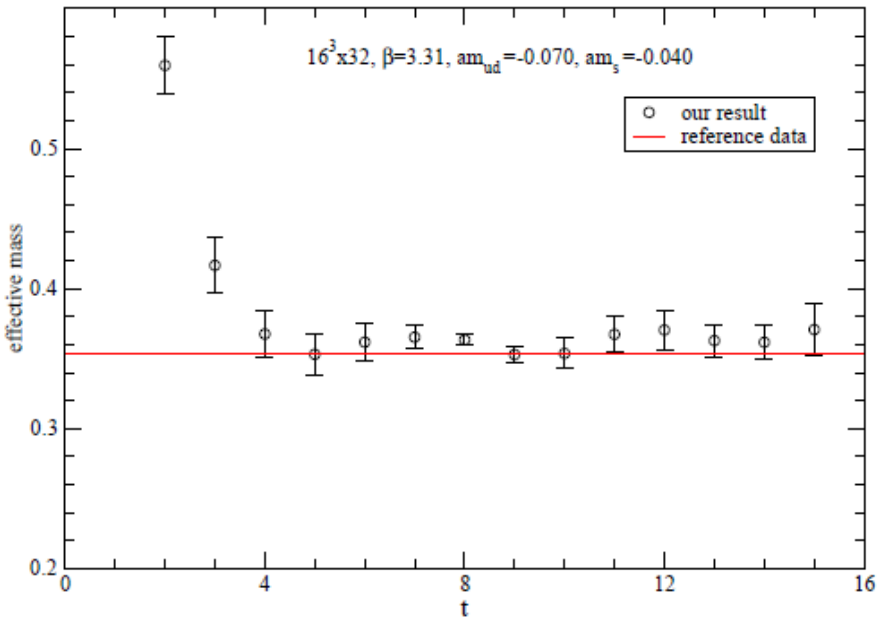
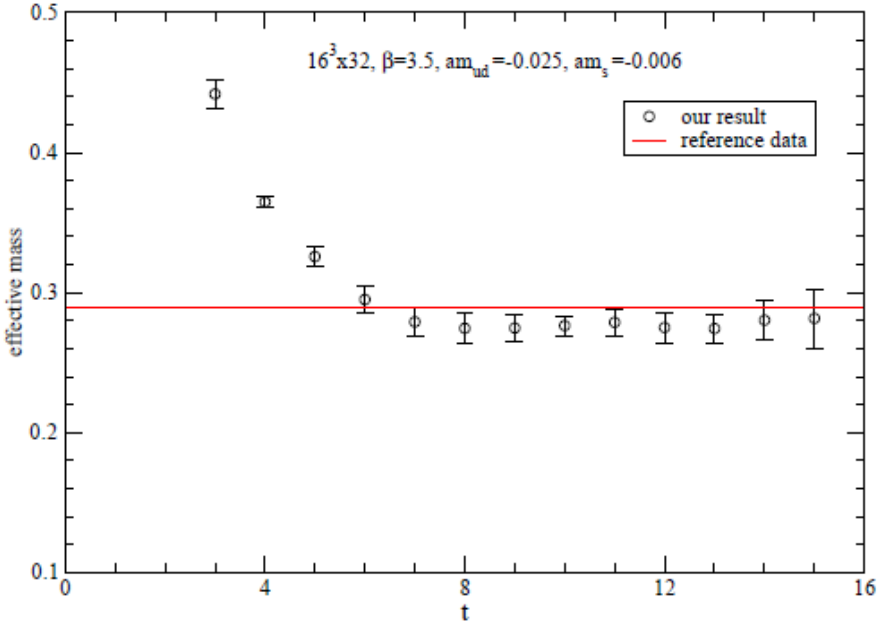
CONFIRMATION

- Example of comparison to literature
  Reference: BMW Colab. JHEP 1108(2011) 148
  Nf=2+1, 2 stout-HYP (2HEX), 16^3x32 lattice





BG/Q @KEK, 3% of peak performance, flat MPI for all the cores

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DEVELOPMENT

Trac/Subversion: joint development by the version control system

Subversion: version control system of code set

trac: project control system

Organized information using the wiki

← screen shot (trac)

↓ repository browser

WEB SITE

- Source Code
- Release information
- Progress of development
- Manuals / User's guide
- Confirmation reports

etc.

Please access to

http://suchix.kek.jp/bridge/Lattice-code/

(Japanese only now)

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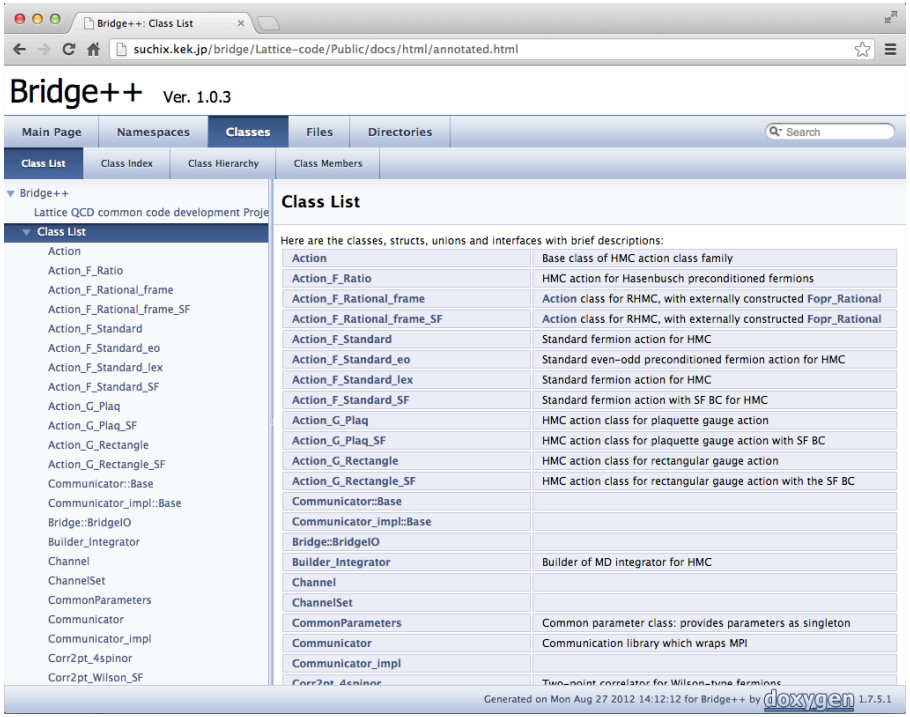
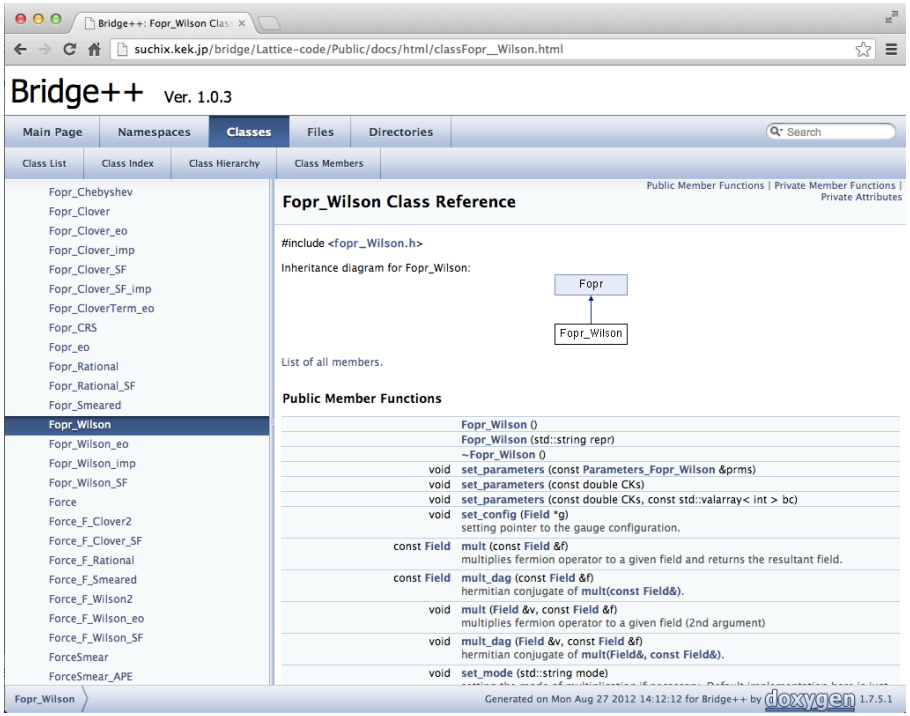
DOCUMENTATION

- First-step guide, implementation note, etc.
- doxygen

Class list → **function of each Classes**





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ROAD MAP

- **Action/Algorithms to be implemented**

  - Now Wilson/clover fermons are available in public version

  - Staggered (standard), domain-wall, overlap fermions are almost ready

- **Improvement of design**

  - General gauge group, fermion representations

- **Performance tuning**

  - On Hitachi SR, about 5%

  - On IBM Blue Gene/Q, less than 5% -— being improved

  - Shared memory parallelization

  - Framework to use accelerators: next page

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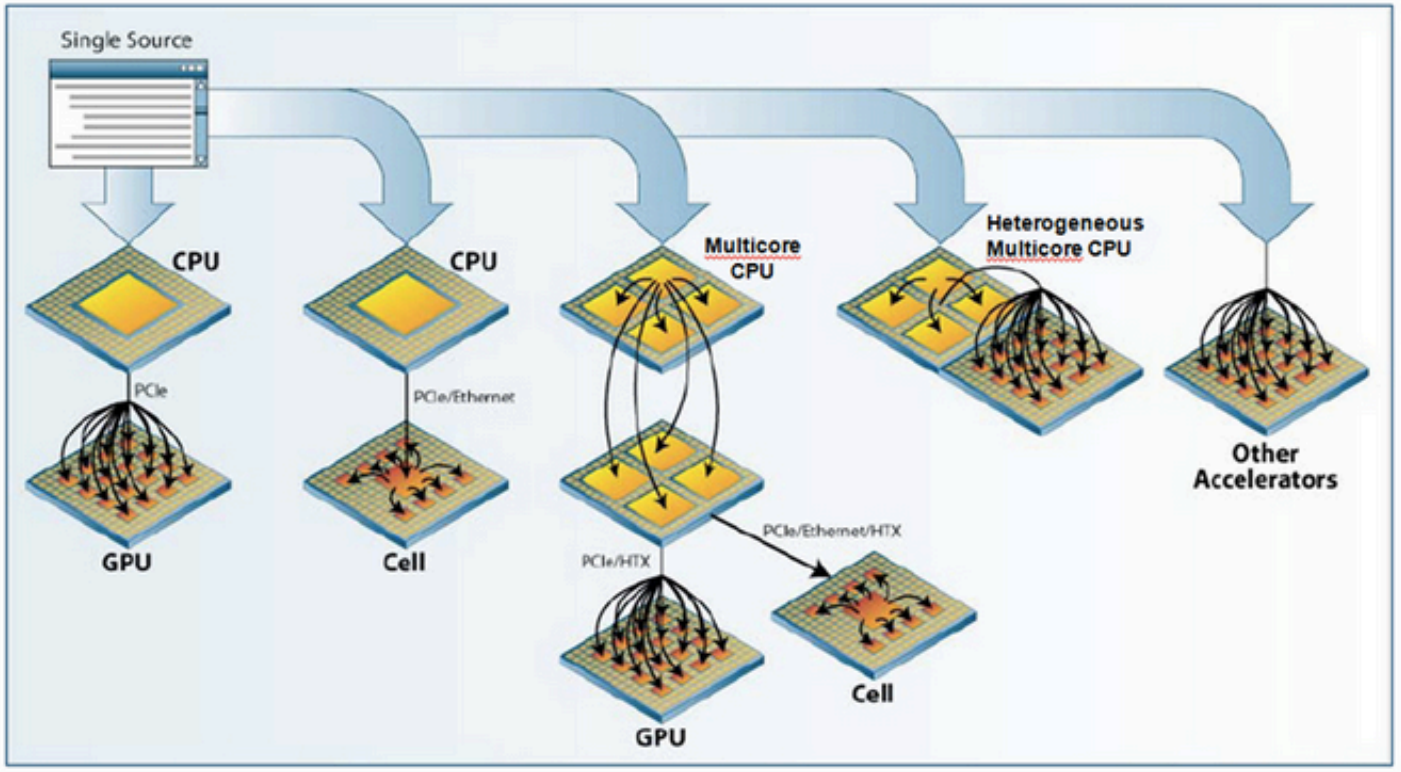
ACCELERATORS

- General framework to use various accelerators
  (GPGPU, Cell B.E., MIC, etc.)
  We employ OpenCL (implemented, now being tuned)

-- Open Computing Language (OpenCL) is a framework for writing programs that execute across heterogeneous platforms consisting of central processing units (CPUs), graphics processing units (GPUs), DSPs and other processors.



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SUMMARY

New lattice QCD code Bridge++ has been developed aiming at:

- Developing research environment
  - to skip unnecessary efforts of coding while getting high performance
  - to remove barriers of communication between researches/beginners
  - to share experiences, ideas and data

- Making use of knowledge of different fields
  - applied mathematics (algorithms)
  - computer science. software design

  One of the goals of this program

The project is still in the early stage.
We strongly need your suggestions, contributions, and feedbacks

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DEMONSTRATION

Thank you for your attention.

http://suchix.kek.jp/bridge/Lattice-code/