

Common code system for the lattice QCD simulations

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







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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!





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" <u>http://bridge.kek.jp/A04/</u> (H. Matsufuru's talk)

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

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





- 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





WHY COMMON CODE?

<u>Research environment may changes</u>

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







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



E 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)







• Example: solver and fermion operator

Class diagram: relation between classes

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







CONFIRMATION

 Example of comparison to literature Reference: BMW Colab. JHEP 1108(2011) 148 Nf=2+1, 2 stout-HYP (2HEX), 16³x32 lattice



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





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



lattice QCD 共通コードプロジェクト Bridge++

新衛與研究「実核宇宙連携による計算基礎科学に基づいた重層的物質構造の解明」および 計算基礎科学連携拠点 次世代スーパーコンピュータ戦略プログラム分野 5「物質と宇宙の活派と構造」(領域代表:青木慎也)では、 QCD (Quantum Chromodynamics) を含む格子ケージ環論のシミュレーションのためのコードを開発し ています。

様々な経子作用やアルゴリズムを適用可能で、ノートPCから超並列計算機表で幅広いアーキテクチャに対応し、最先端の研究に必要なパフォーマンスを実現でき、なお かつ使い慕いものを目指しています。2000年10月15日弦波大で1回自自フリーディズカッションを行って以来、勉強会などを重ねながら、設計、開発を続けていま す。興味のある方はな気軽にで参加下さい。また、開発に参加していただける方は経験的す教室します。

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Bridge++β コードセットの使い方

SVNユーザー登録

β版開発にはSVNユーザー登録が必要です。 こちらのUserIDをお持ちの方はbridge++SVNに既にアクセス可能です。 新規登録が必要な方は管理人までご連絡ください。 ◆**TracDI2インIDとは長なります。**TracoコインID登録については、**#Tracのユーザー登録**を参照してください。

Tracのユーザー登録

TracのユーザーIDの登録はご自分で行えます。下記(アカウントの作成)に沿って登録してください。 登録をしなくても閲覧は可能ですが、登録しログインする事によって、TracaのNik等が編集可能になります。 また、ユーザー作成時にメールアドレスを登録すると、自分に関係するパグ報告などがメールで送信されるようになります。

• アカウントの作成

コードの入手先

subversion: ⇒ http://code1.jldg.org/repos/bridge

\leftarrow screen shot (trac)

↓ repository browser

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👂 🛄 trunk] trunk				namekawa: merge 792:794, including YAML to Tests (part 1)	
属性 svn:ignore の設定値						
trunk/build						



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)





DOCUMENTATION

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

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function of each Classes

⊖ ⊖ ⊖ Bridge++: Class List ×		u ^m	O O Bridge++: Fopr_Wilson Clas: ×				
← → C f C f L suchix.kek.jp/bridge/La	ttice-code/Public/docs/html/annotated	d.html 🔂 🗐	← → C ff C suchix.kek.jp/bridge/Lattice-code/Public/docs/html/classFopr_Wilson.html				
Bridge++ Ver. 1.0.3			Bridge++ ver. 1.0.3				
Main Page Namespaces Classes	Files Directories	Q Search	Main Page Namespaces Classes	Files Directories	Qr Search		
Class List Class Index Class Hierarchy	Class Members		Class List Class Index Class Hierarchy	Class Members			
Bridge++ Lattice QCD common code development Proje	Class List		Fopr_Chebyshev Fopr_Clover	Public Member Functions Priv			
Class List Action	Here are the classes, structs, unions and	d interfaces with brief descriptions:	Fopr_Clover_eo	#include <fopr_wilson.h></fopr_wilson.h>			
Action_F_Ratio Action_F_Rational_frame	Action Action_F_Ratio	Base class of HMC action class family HMC action for Hasenbusch preconditioned fermions	Fopr_Clover_SF Fopr_Clover_SF_imp	Inheritance diagram for Fopr_Wilson:			
Action_F_Rational_frame_SF Action_F_Standard	Action_F_Rational_frame_SF	Action class for RHMC, with externally constructed Popr_Rational Action class for RHMC, with externally constructed Fopr_Rational	Fopr_CloverTerm_eo Fopr_CRS	Fopr_Wilson			
Action_F_Standard_eo Action_F_Standard_lex	Action_F_Standard Action_F_Standard_eo	Standard fermion action for HMC Standard even-odd preconditioned fermion action for HMC	Fopr_eo Fopr_Rational				
Action_F_Standard_SF Action_G_Plaq	Action_F_Standard_lex Action_F_Standard_SF	Standard fermion action for HMC Standard fermion action with SF BC for HMC	Fopr_Rational_SF Fopr_Smeared	Public Member Functions			
Action_G_Plaq_SF	Action_G_Plag	HMC action class for plaquette gauge action	Fopr_Wilson	Fopr_Wilson ()			
Action_G_Rectangle Action_G_Rectangle_SF	Action_G_Rectangle	HMC action class for praquette gauge action with a be	Fopr_Wilson_eo Fopr_Wilson_imp	Wilson_eo Topmotion (datasting cpr)			
Communicator::Base	Communicator::Base	HMC action class for rectangular gauge action with the SF BC	Fopr_Wilson_SF Force	void set_parameters (const double CKs) void set_parameters (const double CKs, const std::valarray< int > bc)			
Bridge::BridgeIO	Communicator_impl::Base		Force_F_Clover2	<pre>void set_config (Field *g) setting pointer to the gauge configuration.</pre>			
Builder_Integrator Channel	Bridge::BridgeIO Builder Integrator	Builder of MD integrator for HMC	Force_F_Clover_SF Force_F_Rational	const Field mult (const Field &f) multiplies fermion operator to a given field and	returns the resultant field.		
ChannelSet	Channel		Force_F_Smeared	const Field mult_dag (const Field &f) hermitian conjugate of mult(const Field&).			
Communicator	CnannelSet CommonParameters	Common parameter class: provides parameters as singleton	Force_r_wiison2 Force_r_Wilson_eo void mult (Field &v, const Field &f) multiplies fermion operator to a given field (2nd argument)		argument)		
Communicator_impl Corr2pt_4spinor	Communicator Communicator impl	Communication library which wraps MPI	Force_F_Wilson_SF ForceSmear	void mult_dag (Field &v, const Field &f) hermitian conjugate of mult(Field , const Field).			
Corr2pt_Wilson_SF	Corr2nt Asninor	Two-point correlator for Wilson-type fermions	ForceSmear_APE	void set_mode (std::string mode)			
		Generated on Mon Aug 27 2012 14:12:12 for Bridge++ by (1033)(30) 1.7.5.1	Fopr_Wilson	Generated on Mon Aug 27 2012 14:12:12 for B	ridge++ by (10) 1.7.5.1		







• 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





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.







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





DEMONSTRATION





Thank you for your attention.

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

Quarks to Universe in Computational Science, Nara, December13-16, 2012