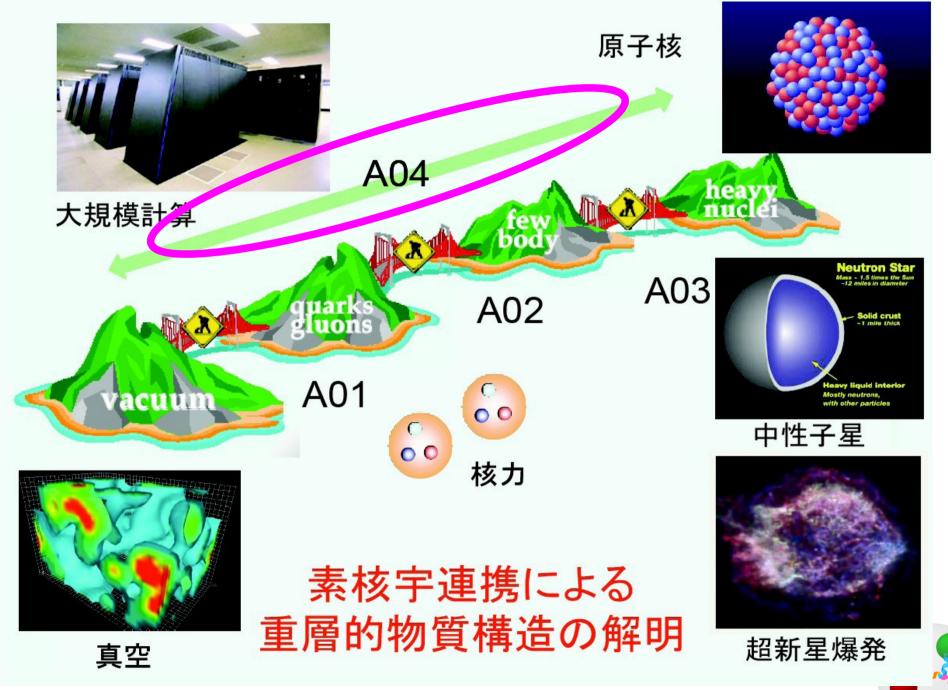
Activity of A04 team

Interdisciplinary algorithms and computer simulations

http://bridge.kek.jp/A04/



3 December 2011, workshop@Nemu-no-sato

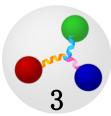


Goals

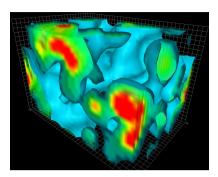
- Support researches in this area through development of algorithms, computational technologies and environments
- Understand physics over different scales from viewpoints of mathematical structure and algorithms

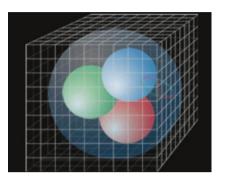
Approaches

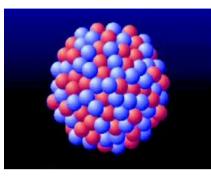
- Algorithms
- Architecture dependent techniques
- Environment (Data Grid)
- Common code (lattice QCD)

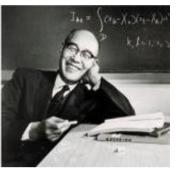


Members











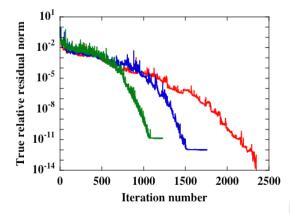
HM (KEK) Tomoteru Yoshie (Tsukuba) Takashi Kaneko (KEK) Shoji Hashimoto (KEK) Ken-Ichi Ishikawa (Hiroshima) Tatsumi Aoyama (Nagoya) Jun-ichi Noaki (KEK) Naoya Ukita (Tsukuba) Shinji Motoki (KEK)

Tetsuya Sakurai (Tsukuba) Hiroto Tadano (Tsukuba) Daisuke Takahashi (Tsukuba) Koichi Yabana (Tsukuba) Noritaka Shimizu (Tokyo)

Hideyuki Suzuki (Tokyo U. Science) Kosuke Sumiyoshi (Numazu Call. Tech.) Akira Mizuta (KEK)











Recent activity

Improving algorithms and parallel computation

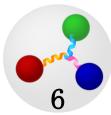
- Supernova explosion (Sumiyoshi, Sakurai, Imakura, HM)
 - Iterative linear algorithm for parallel comp.
 - talks by Sumiyoshi and Imakura
- Linear algorithms for lattice QCD (Sakurai, Tadano, et al.)
- General relativistic fluid dynamics/thermal radiation in the post process
 - tuning and parallelization (Mizuta)
- Lattice QCD common code (Talk by Noaki)
- In the following, some details of
- GPU computation
- KEKSC (announcement)
- Data Grid (JLDG)



Algorithm

• Goals:

- Sharing know-how of algorithms
- Collaboration with applied mathematicians
- Bases toward inter-field application
- Development of new algorithms
- Example of target algorithms
 - Linear equation solver, eigenvalue problem
 - Evolution equation, variational methods, Monte Carlo methods
- Algorithms suitable to each architecture:
 - For massively parallel/coarse grained parallel machines
 - For accelerator boards (GPGPU, Cell, etc.)
 - mixed precision algorithms
 - Less communication with host CPU



Computation on GPU

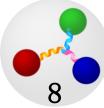
- GPU is now commonly used for numerical calculations
 - Ex. Lattice QCD: extensively used in practice
 - Many body / Integration / Multi-precision calculations
 - Many libraries are available
 - Now double prec. is enough fast / ECC available
- How to implement ?
 - CUDA by NVIDIA has been extensively used
 - CUDA Fortran now available in PGI compiler
 - OpenCL: common framework for multi-core computation applicable to NVIDIA, AMD, Cell, etc.
- Which application ?
 - Decomposed into large num. of independent computations
 - Less memory access, many arithmetic operations





Computation on GPU

- Running computation servers
 - Tesla cluster, Fermi/AMD GPU/Cell B.E. servers
 - Test bed for code development
 - Providing computational resources: Lattice QCD, multi-precision calculation, etc.
- Integration in nuclear eq. of state (Takano, Togashi +HM)
 - Code ported to OpenCL
 - Nvidia Tesla C2050 (double prec.)@KEK
 - Acceleration: 40 min \rightarrow 5-10 sec (roughly)
- Goals: sharing techniques and fundamental parts
 - Materials are compiled at our website
 - Prescription guide
 - Development of 'framework'
- If you are interested in, please contact us.
 - Direct contact or via JICFuS support:
 - You can ask whether your application MAY become fast.



KEK supercomputer

http://scwww.kek.jp/

KEKSC is now available / fully installed soon

- System-A in service at data center (~Jan)
- System-A+B: March 2012~
- System-A: Hitachi SR16000
 - Power7, 54.9 TFlops, 14TB memory
 - 56 nodes: 960GFlops, 256GB/node
 - Automated parallelization on single node
- System-B: IBM Blue Gene/Q
 - 6 racks (3 from March, 3 from Oct 2012)
 - 1.258PFlops, 96TB in total
 - Rack: 1024 nodes, 5D torus network 209.7TFlops, 16TB memory
- Application
 - Large-scale simulation program (http://ohgata-s.kek.jp/)
 - scbridge: for getting started for members in this project if you are interested in, please contact Noaki-san or HM





Data Grid



Computational Science requires advanced data handling

- archive large amount of data
- fast data transfer among SC sites
- research data sharing among collaborations nation (world)wide
- Japan Lattice Data Grid (JLDG)
 - provide fast data transfer via VPN on SINET4



http://www.jldg.org/

- connect major LQCD research sites
 (Tsukuba, KEK, RCNP, Hiroshima, Kanazawa)
- provide uniform file system (single directory-file tree) realized by Gfarm (Grid Data Farm)
- connecting to International Lattice Data Grid (ILDG) to provide public gauge configurations



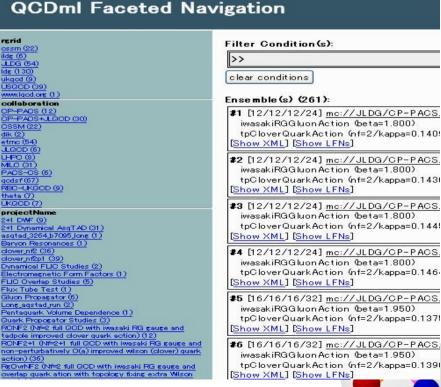
JLDG: peculiarity

User interface

- mount as a file system (only at U. Tsukuba)
- grid-ftp to servers (for other sites)
- direct file operations (ls, rm, mv ...) from client machine
- public data download via ILDG interface
- faceted navigation (ensemble search)

• File system

- user/group access control, cooperated with VOMS
- automatic file replica creation (among different machines)
- quota

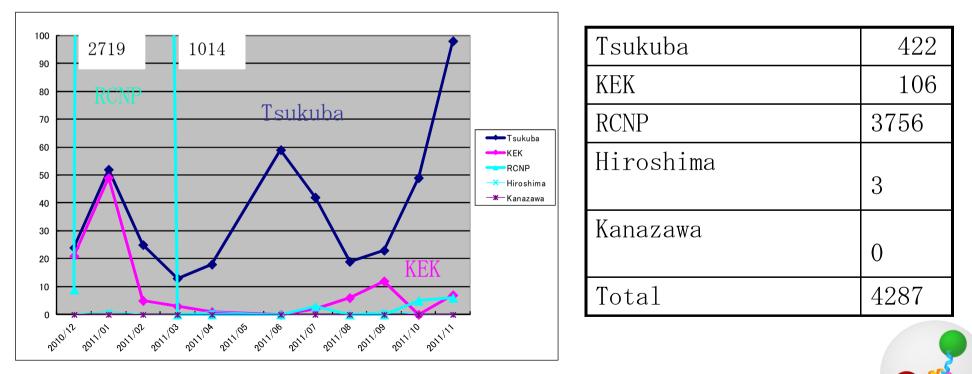




JLDG: status and statistics

• Status

- users: 4 research groups, O(60) users
- disks: 440TB (11 servers distributed over 5 sites)
- data: 3M files, 120TB
- public data: 54 ensembles, 70K config's, 12TB
- Statistics (# grid-ftp sessions, this year)





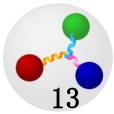
JLDG: future plan

• This FY

- new JLDG sites: U. Tokyo, Nagoya U.
- install more disks ~600TB (in Kansai area)

Next FY and on

- mounting JLDG file system (at several sites)
- improve stability/availability
- outsourcing of operation/maintenance
- application to other fields
- cooperation with HPCI data grid



Summary/outlook

• A04 team

Approaches from viewpoints of computational physics

- Algorithms
- Architecture dependent techniques
- Environment for data sharing
- Lattice QCD common code
- Outlook
 - Further collaborations are necessary
 - Increase practical applications
 - Accumulate documents and code
- If you are interested in, please contact us.
 - Direct contact for machine usage / collaboration
 - JICFuS support: www.jicfus.jp/field5/en/promotion/user/ prodides advices for programming, tuning, seeking for better algorithms, and so on

