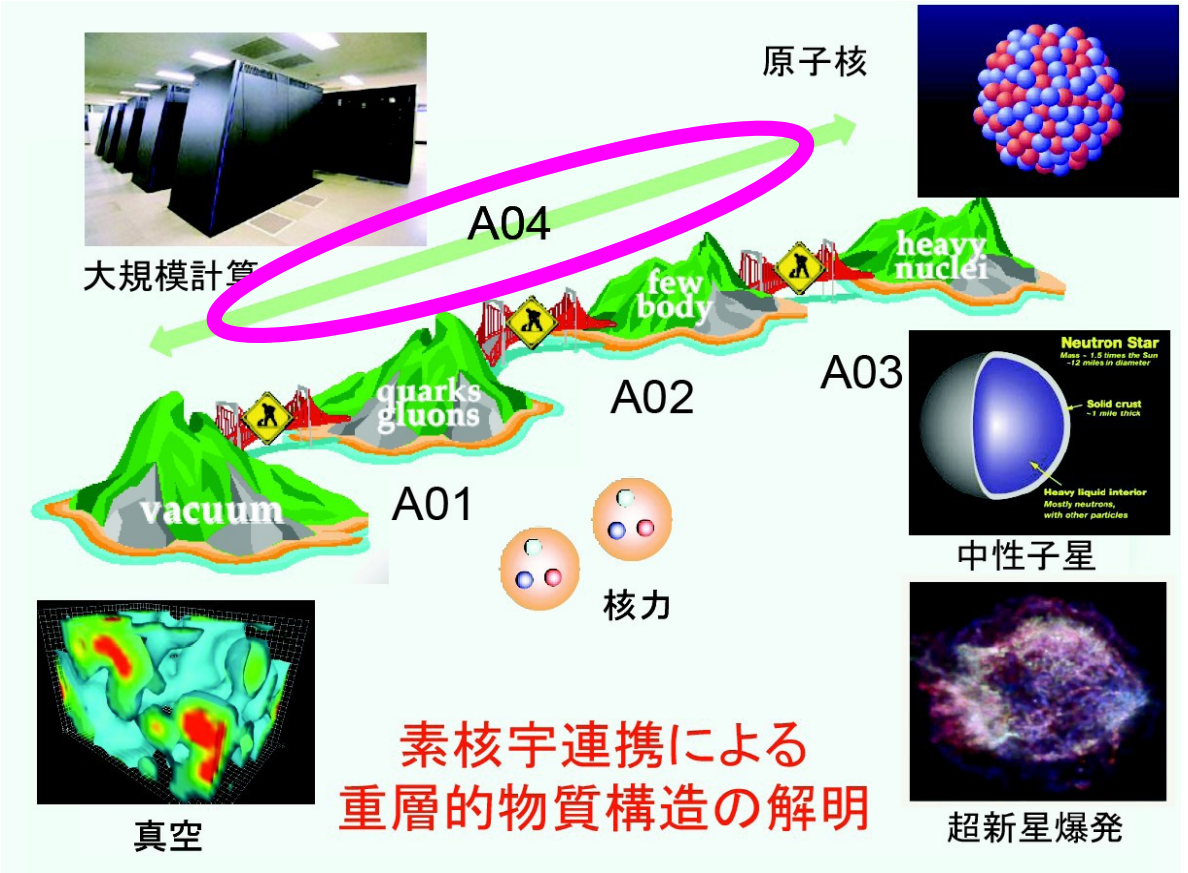
Computational physics project (A04) report

Interdisciplinary algorithms and computer simulations

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



Hideo Matsufuru (KEK)

QUCS 2012, 13-16 December 2012, Nara

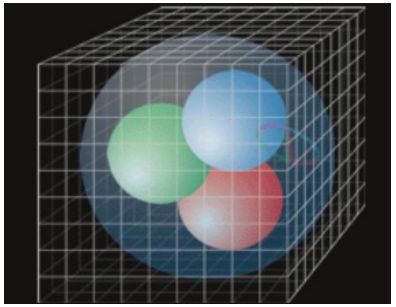
Goals

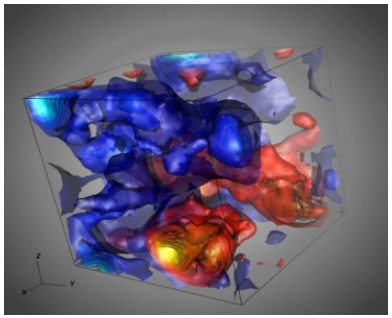
- Support projects in this area through promoting collaboration and developping algorithms, computational techniques and environment
- Understand physics over different scales from viewpoints of computational physics

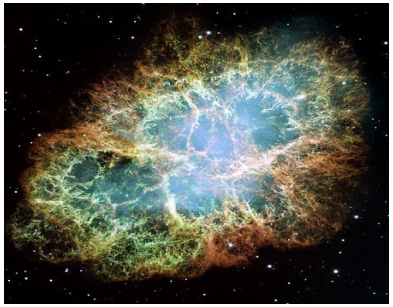
Approaches:

- Algorithms
  - Sharing information/know-how
  - Collaboration with applied mathematitians
  - Development of new algorithms
- Architecture (computaional techniques)
  - Find out best architecture
  - Fully make use of processor's performance
  - Support porting/tuning
- Environment (Data Grid)
- Lattie QCD common code (software engineering)

Members







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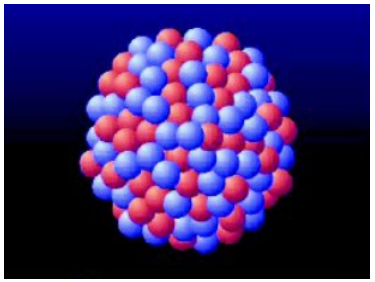
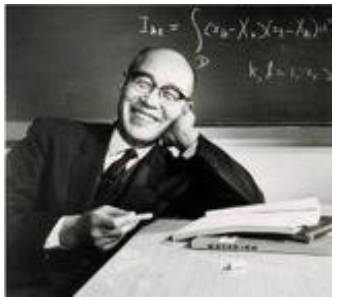
Tomoteru Yoshie (Tsukuba)
Takashi Kaneko (KEK)
Shoji Hashimoto (KEK)
Ken-Ichi Ishikawa (Hiroshima)
Tatsumi Aoyama (Nagoya)
Jun-ichi Noaki (KEK)
Naoya Ukita (Tsukuba)
Shinji Motoki (KEK)

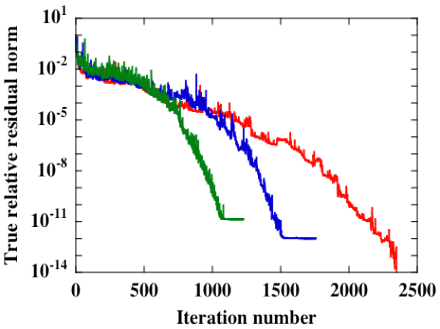
Kazuhiro Yabana (Tsukuba)
Noritaka Shimizu (Tokyo)

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

Tetsuya Sakurai (Tsukuba)
Hiroto Tadano (Tsukuba)
Daisuke Takahashi (Tsukuba)







Related proposed project

- H21-22, H23-24: T.Sakurai

  Large-scale numerical linear algorithms for elementary particle, nuclear, and astrophysics
- H21-22: T.Ishikawa

  Study of dedicated system for computation of higher order corrections
  - Multi-order precision computation
  - Dedicated hardware
  - Computations more than double precision needed
  - Cf. Multi-precision forum: http://suchix.kek.jp/mpcomp/

Interdisciplinary algorithms

- Matrix analyses of linear problems
  - Supernova/lattice QCD
  - Advices/hint to Bridge++ code
- Seminar series (2010,2011)
  - Relativistic hydrodynamics (A.Mizuta)
  - Krylov subspace method (T.Sakurai)
  - Dynamical Density Matrix Renormalization Group (K.Iwano, KEK)
  - (TD) DFT (K.Yabana)
- “Door to High Performance Computing”
  - Compilation of information/know-how
  - Wiki, under development (forever...)
  - Supported by SPIRE Field 5
  - Large contribution by A.Imakura for linear solver algorithms: advice to choose best algorithm

Interdisciplinary algorithms

- Supernova explosion (Sumiyoshi, Sakurai, Imakura, HM)
  - MPI paralleized
  - Algorithm improvement
    Weighted Jacobi preconditioner for iterative solver

  → Talks by Imakura (Sat 15th) and Sumiyoshi (Sun 16th)
- Relativistic hydrodynamics (A.Mizuta, talk on Sun 16th)
  - Development of 3D/2D relativistic hydrodynamic code
  - Nice lecture note (published in Genshikaku-kenkyu)
- Also see
  - Talk by K-I. Ishikawa
  - Poster by T.Kaneko

Architecture

- Running GPGPU servers
  - Totally 12 servers were installed:
    NVIDIA Tesla/Fermi, AMD Radeon, Cell B.E.
  - For prgram development and practical computation
  - Many flavor phsics (most heavily used)
    several papers/proceedings published
    → N.Yamada's talk (Sun 16th)
  - Supernova EOS project: next page
  - Multi-precision computation
  - Developement of OpenCL programs
    → bases of supernova EOS, Bridge++
- Lectures (by bender companies)
  - CUDA programming
  - CELL B.E. Programming
- Workshop (Jun 2009)
- School on accelerator board (Dec 2009)

Acceleration by GPGPU

Supernova-EOS Project (Togashi's talk)

Construction of a new nuclear Equation of State (EOS) table for supernova simulations with the variational method

In this study, the expectation values of the three-body Hamiltonian with the degenerate Fermi-gas wave function $<H_3^{\alpha}>_F$ are necessary for various densities and proton fractions.

The three-body Hamiltonian

$$H_3^{\alpha} = \sum_{i<j<k}^{N} V_{ijk}^{\alpha}$$

V^{α}_{ijk} : the component of the UIX three-body potential ($\alpha = 2\pi$, R)

These expectation values $<H_3^{\alpha}>_F$ are expressed as double integrals of analytic functions.

Computation on GPU

- Code ported to OpenCL
- Nvidia Tesla C2050 @KEK

Acceleration is attained with GPU. (40 min → 5-10 sec)

Architecture

Recent techinologies that may be efficient:

(just for information)

- HMPP/Open ACC
  - If you don't like OpenCL nor CUDA ...
  - Directive based framework to use accelerators
- XMP: directive based parallelization
  - If you don't like MPI ...
  - Directive based framework for distributed memory parallelization
  - Developed in Tsukuba Univ. etc.
  - Introductory slide is available in Bridge++ website (by M.Sato, Tsukuba Univ.)
- To be tested before the end of project

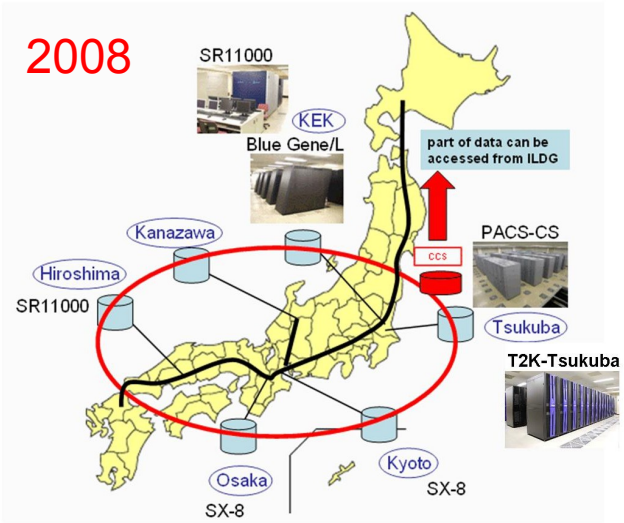
Data Grid

- Advanced computational environment is necessary
  - Large amount of data (lattice QCD, etc.)
  - Fast data transfer among SC sites
  - Sharing data inside/among collaborations
- Japan Lattice Data Grid (JLDG)

  http://www.jldg.org/

  - Provides public data and high speed data transfer
  - Official service started May 2008
  - Tsukuba, KEK, Osaka RCNP, Hiroshima, Kanazawa, (Kyoto)
    + Tokyo (Kashiwa), Nagoya
  - Virtual private network on SINET
  - Gfarm grid file system: ver.1 → ver.2
    FUSE mount (NFS-like) is now possible
- Continuously being improved
- User group and stored data are increasing
  - Lecture for users (27 Jan 2010)
- Application to other field?

Japan Lattice Data Grid



New site:
- Tokyo (Kashiwa)
- Nagoya

New support:
- SPIRE Field 5

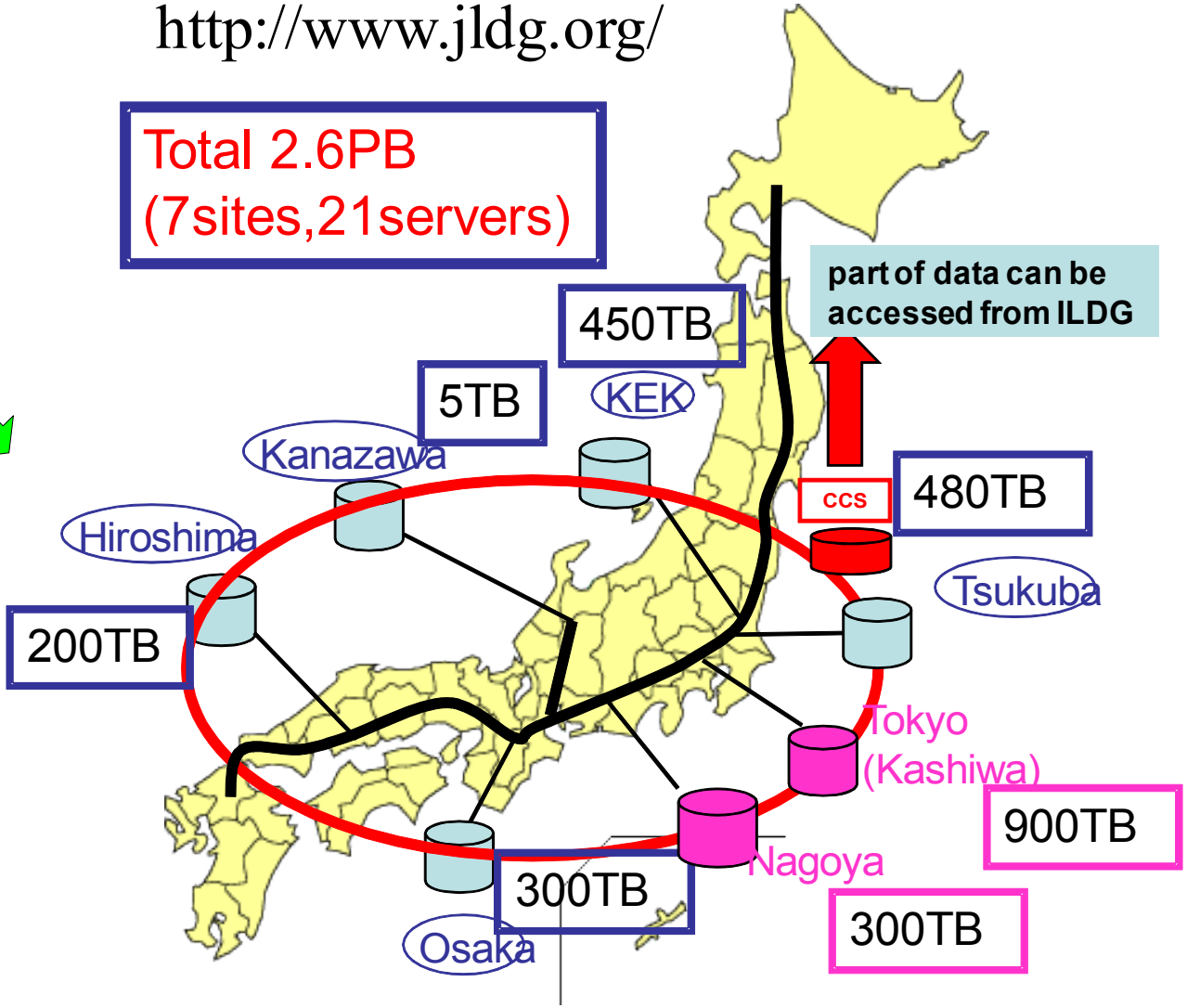
Storage:
- 260TB → 2.6PB

Japan Lattice Data Grid

http://www.jldg.org/

As of 2012/12

Total 2.6PB
(7sites,21servers)



Lattice QCD common code

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

- Now ver.1.0 is public [24 July 2012]
- Development started in Autumn 2009
- Object oriented, C++, MPI parallelized
- Still in active development phase:
  Your advices/contributions are welcome !

- Why new code ?
  - Maintenance by ourselves
  - Detailed documents
  - Share ideas and skills in software design and algorithms
- Goals
  - High performance: on massively parallel, accelerators, etc.
  - Easy to understand for beginners
  - Easy to modify/extend for new ideas
- Details: S.Motoki's talk (Sat 15th)

Summary/outlook

- A04 team
  - Approaches from viewpoints of computational physics
  - Algorithms
  - Architecture dependent techniques
  - Environment for data sharing
  - Lattice-common code (software engineering)

- Outlook
  - This kind of activity is effective and may help your work
  - Not the end, but basis for further communication
  - SPIRE Field 5 continues similar activity
  - Please visit “Door to HPC” or JICFuS consult and give your comment !