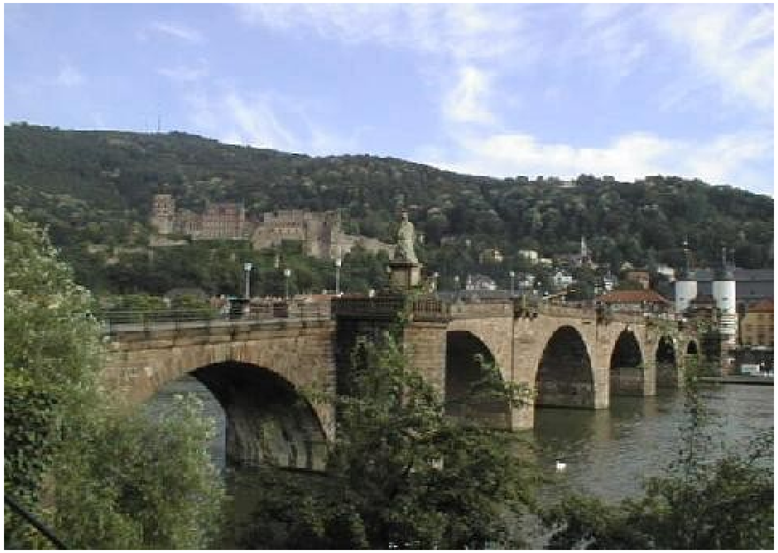
Lattice QCD in HPC



Hideo Matsufuru (KEK)

KEK-CSCS Joint Workshop, KEK, Japan, 29 October 2025

Hideo Matsufuru

- PhD : Hiroshima University, Japan (1998)
- Post doc.: Heidelberg, Osaka (RCNP), Kyoto (YITP)
- KEK Computing Research Center (2003-)
  Administration of supercomputer system (~2023)

Research interests

- Theoretical/computational physics
- Lattice QCD (elementary particle physics)
- High Performance computing
- Data grids

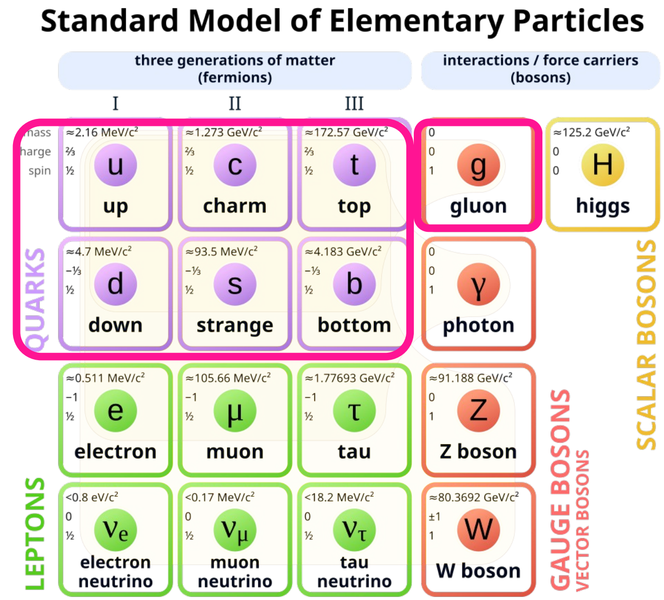
Contents

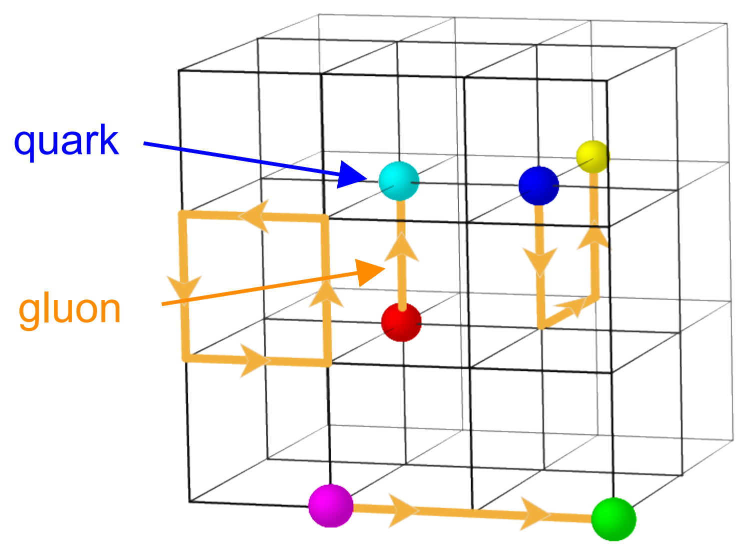
Summary

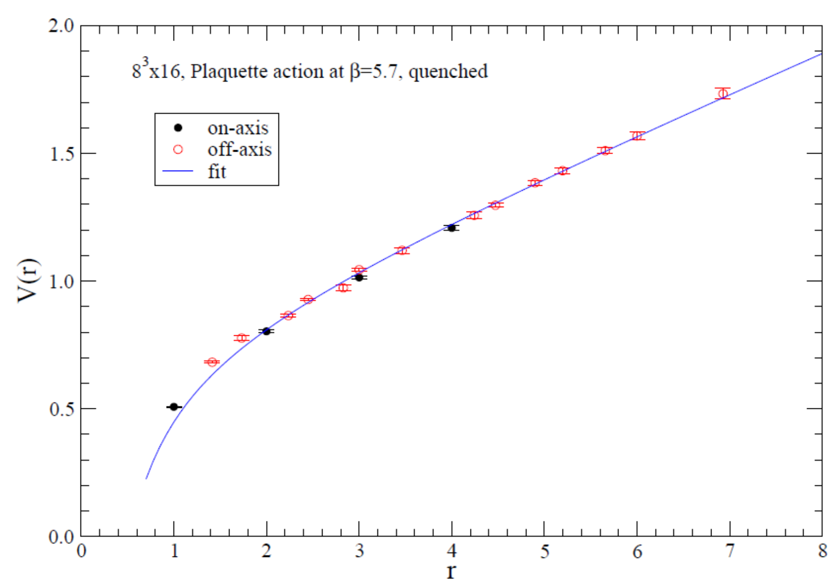
- Lattice QCD: computational elementary particle physics
  → only systematic approach to explore nonperturbative nature of QCD
- Lattice requires large computational resources
  → Need of High Performance Computing
- Gauge configurations are expensive and valuable data
  → Need of data grids: ILDG, JLDG

Lattice QCD simulations

- QCD (Quantum Chromodynamics)
  - Fundamental theory of the “strong interaction” among quarks and gluons
  - Difficult to solve due to strong coupling at long distance → perturbation is not applicable
- Lattice QCD simulations
  - Lattice QCD: fermion (quark) and gauge (gluon) fields on 4D Euclidean lattice (discretized spacetime)
  - Monte Carlo algorithm → physical quantities
  - Only general/quantitative approach to calculate QCD

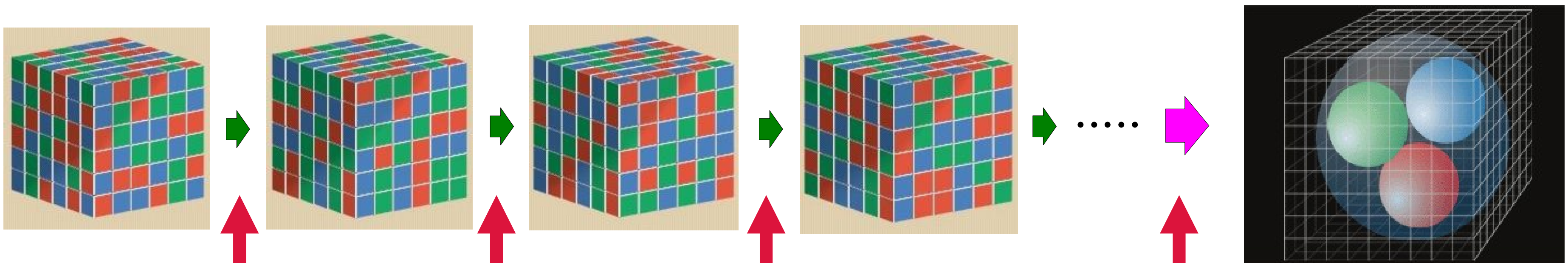






Lattice QCD simulations

- Monte Carlo algorithm → "gauge configurations"



At each step of Monte Carlo generation and measurement, a linear equation must be solved for a large sparse matrix by iterative solver

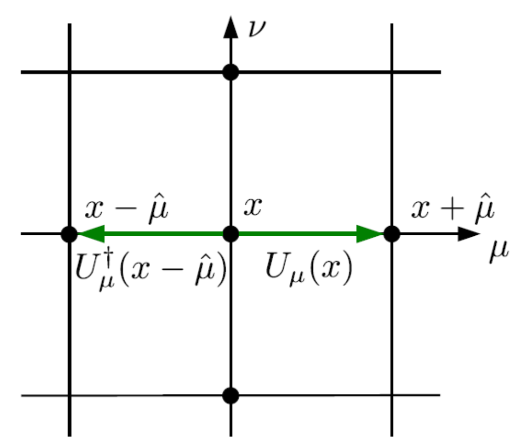
Fermion matrix of rank: 3 (color) x 4 (spinor) x #site → O(10^8)

Bottleneck of lattice QCD simulations

- Example of fermion matrix: Wilson fermion

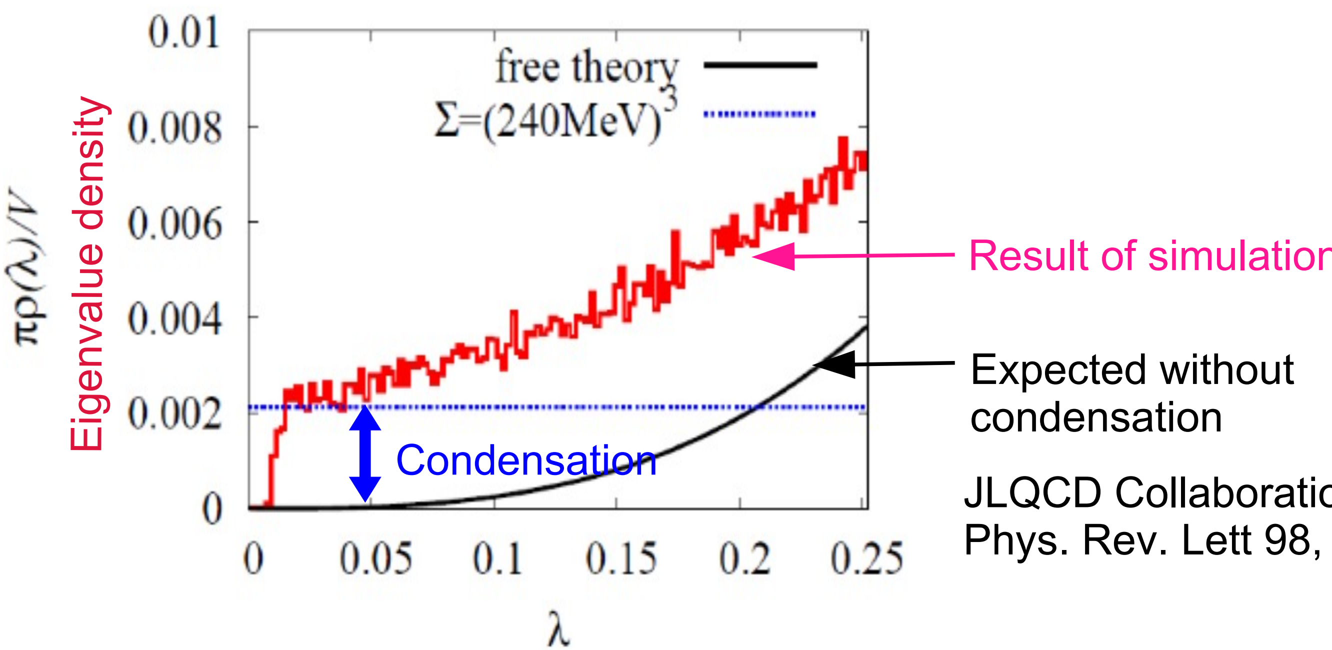
$$D_{x,y} = \delta_{x,y} - \kappa \sum_{\mu} \{(1-\gamma_\mu)U_\mu(x)\delta_{x+\hat{\mu},y} + (1+\gamma_\mu)U_\mu(x-\hat{\mu})\delta_{x-\hat{\mu},y}\}$$

  - $U_\mu(x)$: 3x3 complex matrix (gauge field)
  - γ_μ : 4x4 matrix (permutation of components)
  - κ : hopping parameter (related to quark mass)
- Coupling with nearest neighbor sites: 9-point stencil



Lattice QCD simulations

- Application of lattice QCD
  - Precision calculation of hadronic process → verification of standard model
  - Nature of QCD: finite temperature/density phase diagram
  - Exploring candidate models beyond standard model
- Example result: nature of QCD vacuum
  - QCD "vacuum" is not vacant, but quark-antiquark pairs condensate
  - "Chiral symmetry" is spontaneously broken → quark acquires effective mass
  - 98% of mass of matter (protons and neutrons) comes from this mechanism

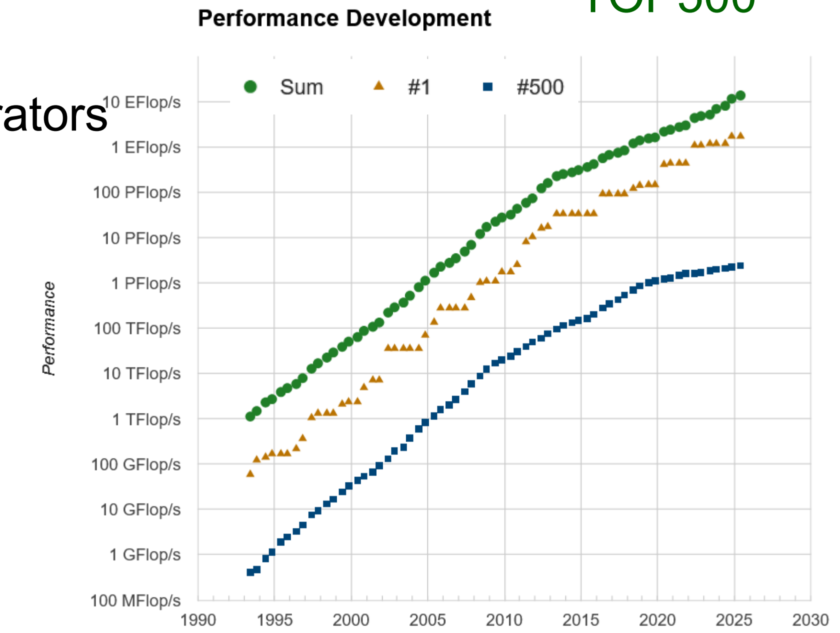


JLQCD Collaboration (H.Fukaya et al.), Phys. Rev. Lett 98, 172001 (2007)

Lattice QCD and HPC

- Lattice QCD has been a typical HPC benchmark
  - Vector architecture, massive parallel, SIMD, multi-core, many-core, GPU and other accelerators
  - Dedicated machines were developed
    - QCDPAX, CP-PACS (U.Tsukuba)
    - QCDOC (IBM+BNL+...) → Blue Gene
  - Pioneering work on GPU
    - I. Egri et al.,"*Lattice QCD as a video game*", Comput.Phys.Commun. 177 (2007) 631-639

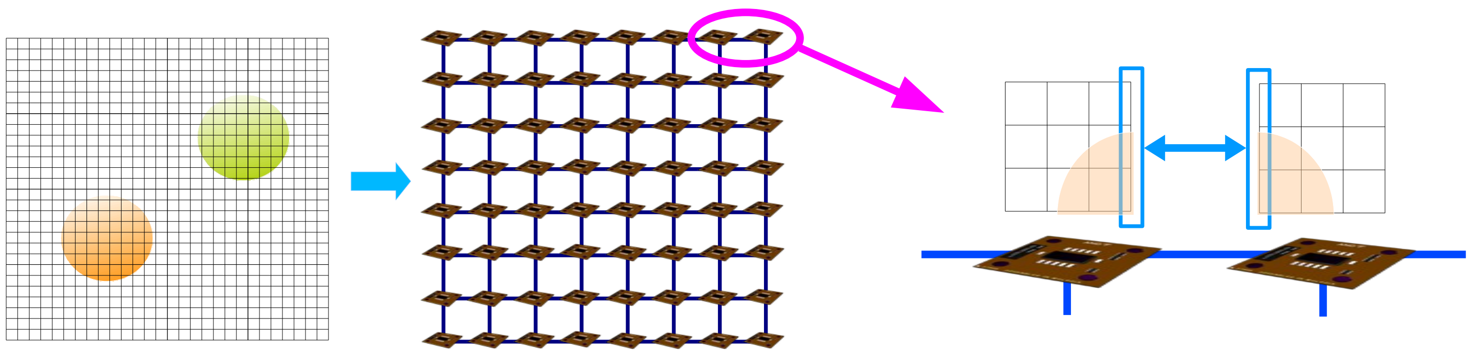
TOP500



- Performance tuning
  - Distributed memory parallel system: message passing (MPI etc.) → Minimize Communication overhead
  - Shared memory multi-core: thread parallelization (OpenMP, etc.)
  - Vector architecture: vectorization of long loops
  - SIMD processors
  - GPU and accelerators: many core threads of O(1K) ~ O(10K) → Offloading bottleneck tasks

Lattice QCD and HPC

- Massively parallel systems
  - Balance of computation and communication is important
  - Specific topology of interconnect network
  - Low-level communication library (instead of MPI) may achieve better performance



Intel Paragon @Hiroshima
(56 nodes, 4.2 Gflops)
1993--1998

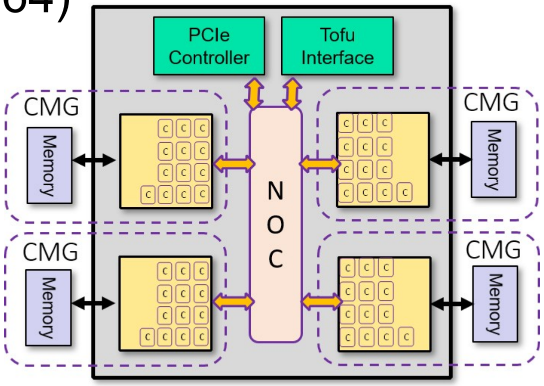
IBM Blue Gene/L @KEK
(57.3 TFlops)
2006-2011

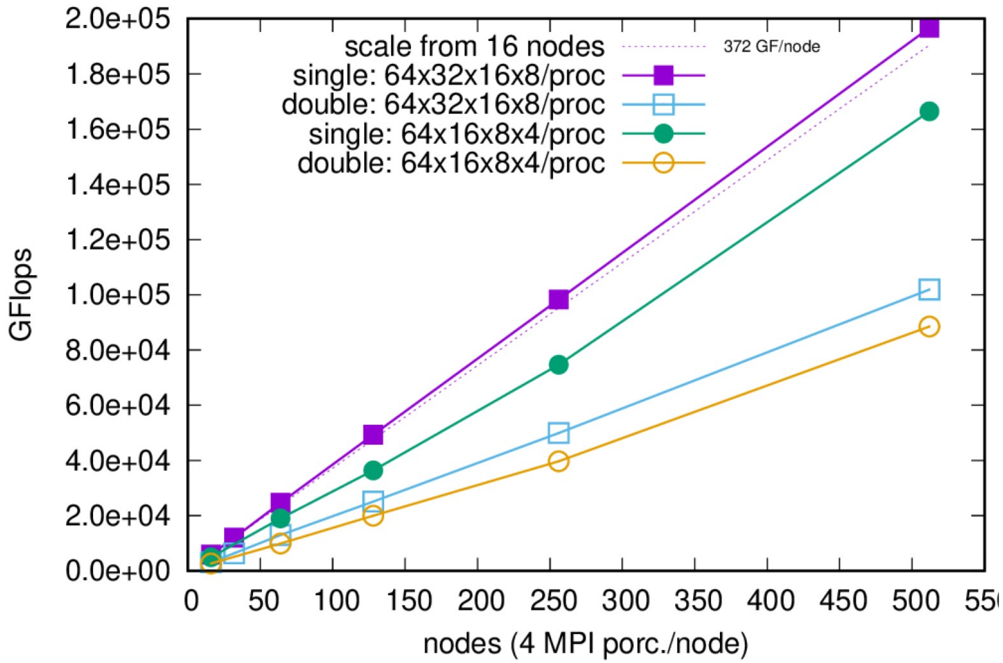
IBM Blue Gene/Q @KEK
(1.258 PFlops)
2012-2017

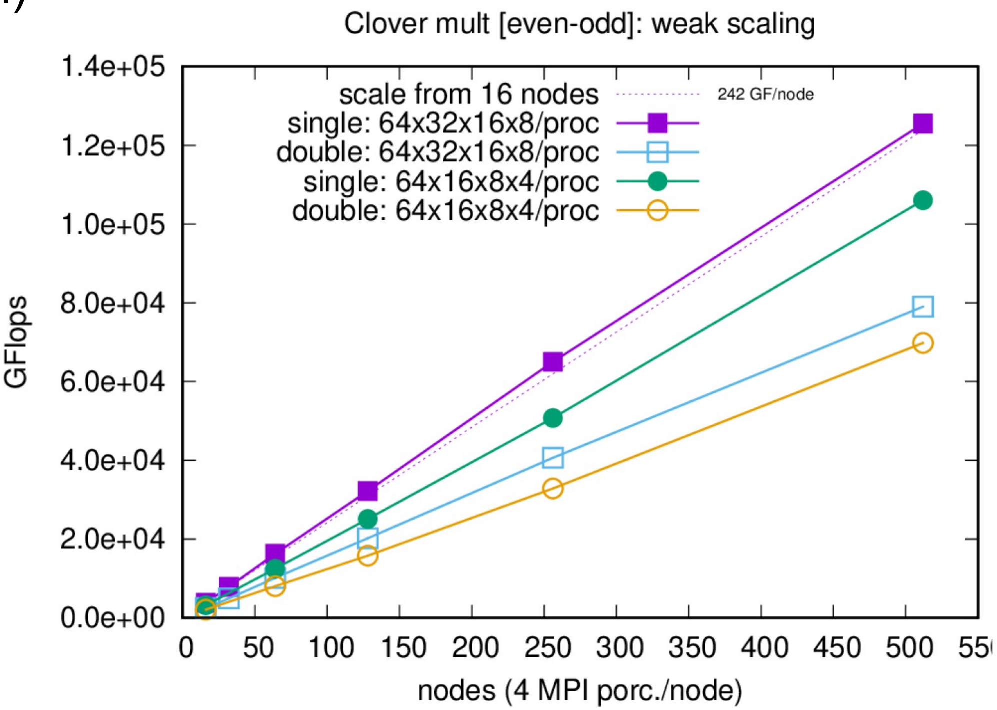
Fugaku @RIKEN CCS
(537 PFlops) 2020~
https://www.r-ccs.riken.jp/en/fugaku/

Performance on Fugaku

- Supercomputer Fugaku (RIKEN)
  - Total peak performance: 537 PFlops (FP64)
  - A64FX processor, 48 compute cores
  - 3.34 TFlops/processor, 1024 GB/s
  - Tofu Interconnect D (28 Gbps x 2 x10)
- Performance: weak scaling plot
  - Clover (improved Wilson) fermion
  - Matrix multiplication (Single precision)



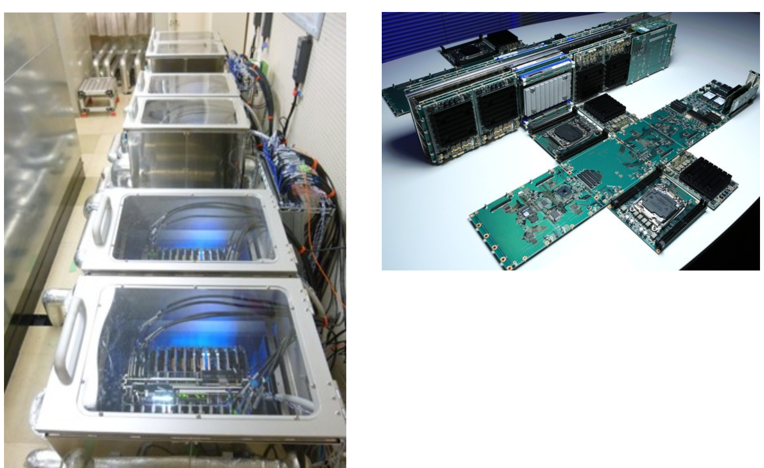




Lattice QCD and HPC

- Accelerators: GPU, PEZY-SC
  - Offloading bottleneck tasks to device
  - Implementation:OpenACC, OpenMP (directives), CUDA, OpenCL, etc (APIs).
  - Minimize data transfer between host and device
  - Many-cores of O(1K)-O(10K) → parallelization to many threads
  - Recent systems adopt GPUs
    - Miyabi at JCAHPC (U. Tokyo+Tsukuba) has started (NVIDIA GV200)
    - Next system at Univ. Tsukuba (AMD GPU)
    - FugakuNEXT (planned 2030~) : next Japanese flagship (NVIDIA GPU)
  - Developing/porting fast GPU code is urgent subject

PEZY-SC on Suiren system@KEK



Miyabi @JCAHPC

Code development

Lattice QCD code Bridge++

- General purpose code set for simulations of lattice gauge theory
- C++, object-oriented design

- Development policy
  - Readable: for beginners
  - Extendable: for testing new ideas
  - Portable: works on many machines
  - Practically enough high performance

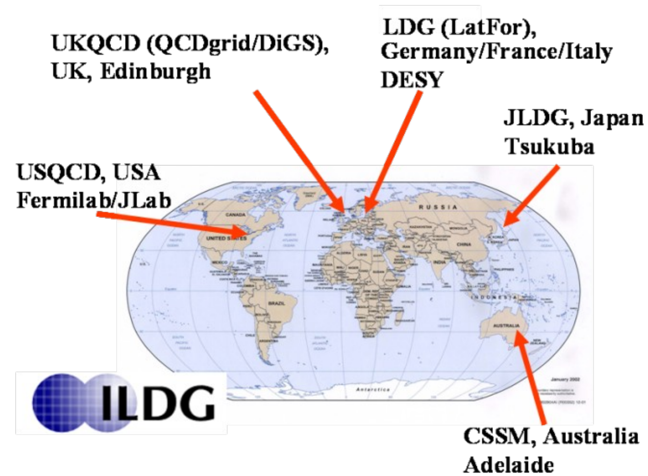
  - Project launched in October 2009, first public release in July 2012
  - Latest version: 2.1.0 (13 September 2025)
- How to enable achieve portability and high performance simultaneously?
  - Out solution: implement robust generic code and optimized code for specific architecture separately and enable them to run simultaneously

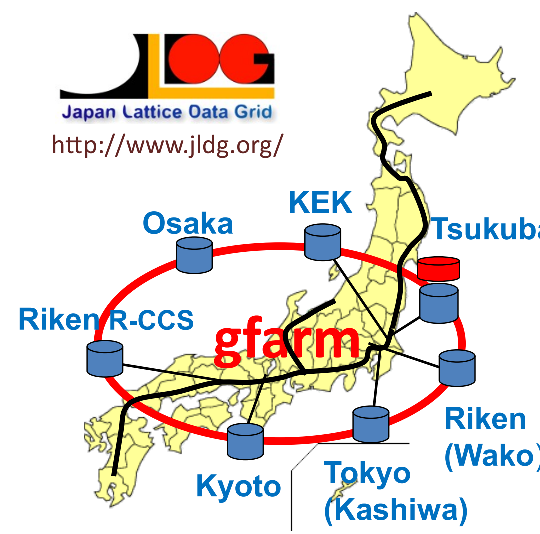
    → Bottleneck parts can be replaced with optimized code
  - Optimized code for Fugaku and GPU are aveilable

Data Grids

- Data grids for Computational elementary particle physics
  - Gauge configurations
    - Expensive to generate
    - Various physical quantities can be calculated

    → Worth to share
- ILDG (International Lattice Data Grid)
  - International activity to share lattce QCD data
- JLDG (Japan Lattice Data Grid)
  - Infrastructure to share data of lattice and related field in Japan
  - Regional grid of ILDG

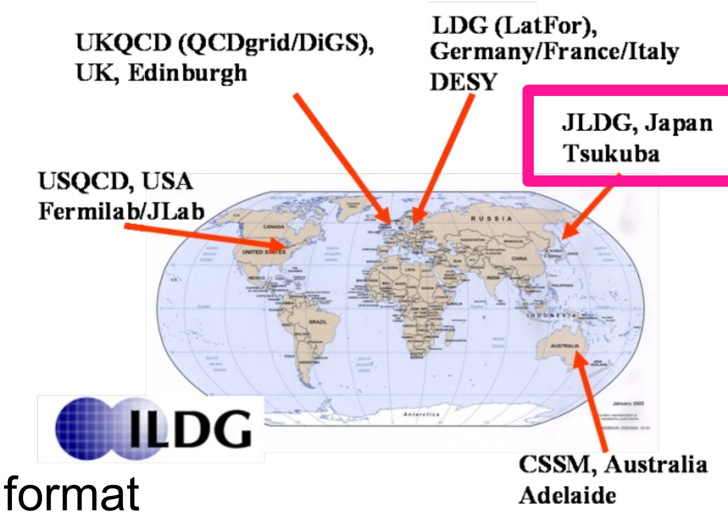


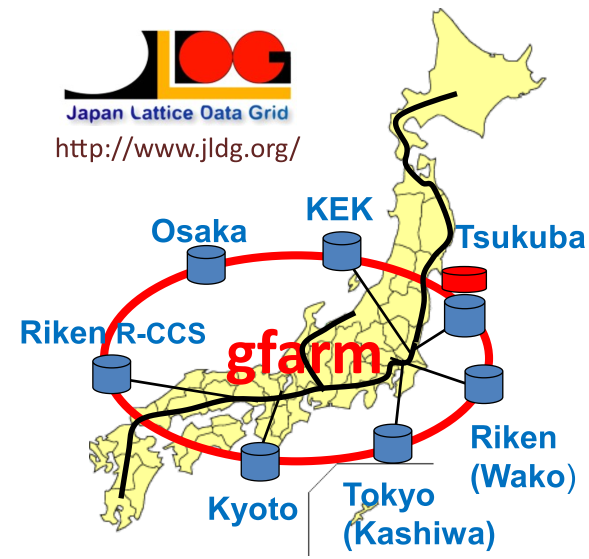


Introduction to ILDG

https://hpc.desy.de/ildg/

- Organized to share lattice QCD data (configurations)
  - Activity started in 2002
- Grid of grids
  - Resources are provided by regional grids
  - JLDG play a role of Japanese regional grid
- Organization
  - Board (representative from regional grids)
  - Metadata Working Group
    → Spcifying description of metadata (QCDml), file format
  - Middleware Working Group
    → Spcifying data access interface, authentication
- Activity
  - Recently rebooted as ILDG 2.0
  - Hands-on workshops (2023, 2025)
  - Data sessions in Lattice conference
  - Update of metadata/middleware issues





Data sharing

- FAIR principle for scientific data sharing

  M. Wilkinson et al., Sci Data 3 (2016) 160018

  - Findable : unique and persistent ID, rich metadata, searchable
  - Accessible : retrievable by ID, open protocol, persistently accessible metadata
  - Interoperable : (meta)data with broadly applicable language
  - Reusable : with clear and accessible license – missing in QCDml (ver.1.x)

- File format and metadata
  - File format – common binary data format
    - In which order the data are arranged
    - Packing software: LIME
  - Metadata → data base: Metadata Catalog
    - Ensemble : actions, parameters, license (ver.2.0), ...
    - Configuration: history, URI (Uniform Resource Identifier), checksum/plaquette, ...
    - How to describe?

      → XML specified by XML schema : QCDml (QCD markup language)

Japan Lattice Data Grid

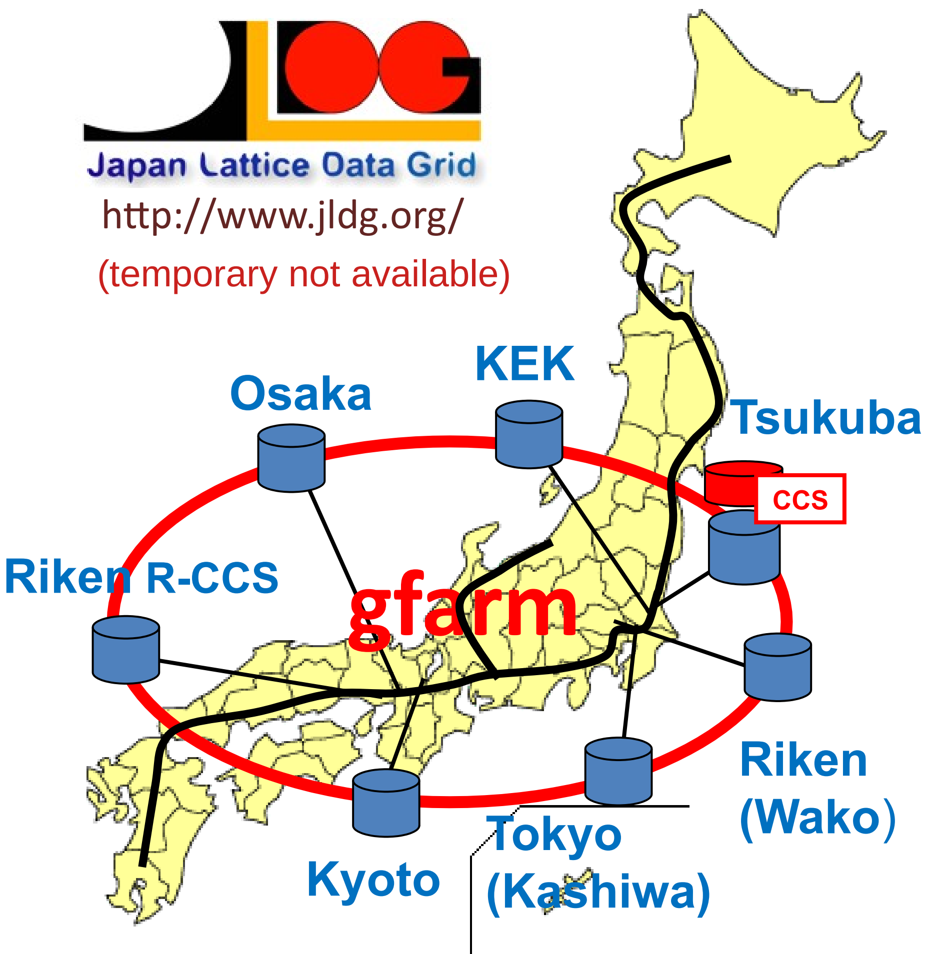
Cf. T. Amagasa et al., J. Phys. Conf. Ser. 664 (2015) 042058

- Data Grid for lattice QCD and related science (nuclear/astrophysics)
  - Sharing public data and fast data transfer within collaborations

Japan Lattice Data Grid

http://www.jldg.org/

(temporary not available)



- Operation officially started in May 2008
- Constructed on VPN HEPnet-J/sc
  - On SINET operated by NII (National Inst. of Informatics)
- Gfarm grid file system
  - User can access as if single file system
  - Automatic replication
- Operated by JLDG team (members from sites and groups)
- Resources (as of Aug 2024)
  - Total storage: 21 PB, 11.3 PB used (87%)
  - Total number of files: >200M
- Regional grid of ILDG

Summary/outlook

Summary

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  → Need of data grid: ILDG, JLDG