Lattice QCD on supercomputers with Chinese CPU

Ying Chen

Institute of High Energy Physics
Chinese Academy of Sciences

ACAT2022, Oct. 25, 2022, Bari Italy

Outline

I. An overview of lattice QCD
II. Domestic supercomputers in China
III. Lattice QCD applications
IV. Summary

I. An overview of lattice QCD

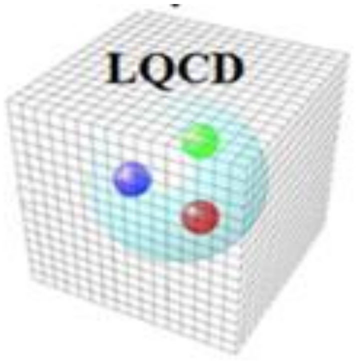
1. Lattice QCD —— ab initio nonperturbative method for QCD at the low energy scale

- **Standard Model (SM): QCD+EW**
- **QCD is nonperturbative at the low energy scale.**
  Model independent solutions are desired——Lattice QCD （LQCD)
- **LQCD is very relevant to (high energy frontier, high luminosity frontier, cosmology frontier)**
  Hadron physics (hadron spectroscopy, hadron structure)
  Precision test of SM
  New physics search (BSM)

A.S. Kronfeld et al., "Lattice QCD and Particle Physics" (Snowmass 2021), arXiv: 2207.07641 (hep-lat)
Z. Davoudi et al. ,"Lattice Gauge Theory" (Snowmass 2021), arXiv: 2209.10758 (hep-lat)

2. Formalism of Latttice QCD

- **Path integral quantization on finite Euclidean spacetime lattices**



$$Z = \int DU \det M[U]\ e^{-S_g[U]}$$

$$\left\langle \hat{\mathcal{O}}[U,\psi,\bar{\psi}] \right\rangle = \frac{1}{Z}\int DU \det M[U]\ e^{-S_g[U]}\mathcal{O}[U]$$

Very similar to a statistical physics system

Monte Carlo simulation——importance sampling according to

$$\mathcal{P}[U] \propto \det M[U]\ e^{-S_g[U]}$$

- **A typical high performance computing field:**
  - **nearest neighbor interaction** $\int d^4x_E\ \bar{\psi}(\gamma\cdot D+m)\psi \to \bar{\psi}M[U]\psi$
  - **tremendous degrees of freedom** $L^3\times T\times 12$ **(**$\sim 10^8$ **for** $48^3\times 96$ **)**
  - **Monte Carlo simulation**

Computing intensive——frequently solving the sparse matrix problem (Hotspot)

$$M[U]X = Y$$

II. Domestic supercomputers in China

- **Before 2016, Most of Supercomputers in China were constructed using commercial CPUs, such as IBM made, Intel made, HP made, etc..**

  Symmetric multiprocessing (SMP)

  Heterogenous (CPUs, CPU+KNLs, CPU+GPUs)

- **After 2016, Supercomps with home-made CPUs appeared**

Tianhe-II
(100P, CPU: Matrix 2000)

Sunway-TaihuLight
(125P, CPU: SW26010)

- **Towards to exascale supercomputers**
    - There are several hardware architectures in plan
    - Prototypes:

      Heterogeneous at nodes —— CPU + accelerator,

      Heterogeneous in chips —— Many-core system (Sunway series, etc.)

- **It is urgent to establish the software ecosystem**
    - New architecture, requires more users
    - No sophisticated compiler
    - Few tools for software developers

- **Lattice QCD applications**

III. Lattice QCD Applications

1. A CPU+GPGPU heterogenous cluster

- **Easy for codes to be transplanted**
- **Code1: Chroma+QUDA (ROCm-devel branch),**
- **Code 2: GWU package (through χQCD Collaboration**

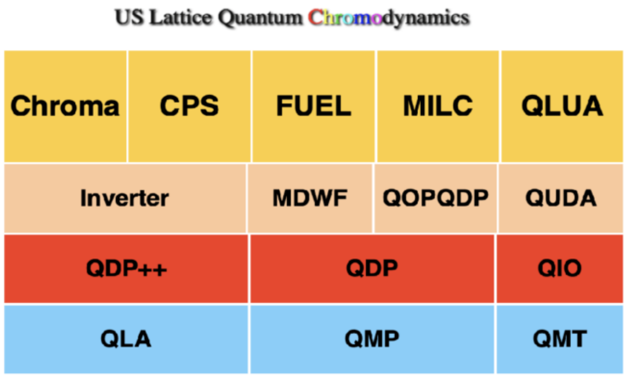


Figure 1: The SciDAC Layers and the software module architecture.

http://usqcd-software.github.io

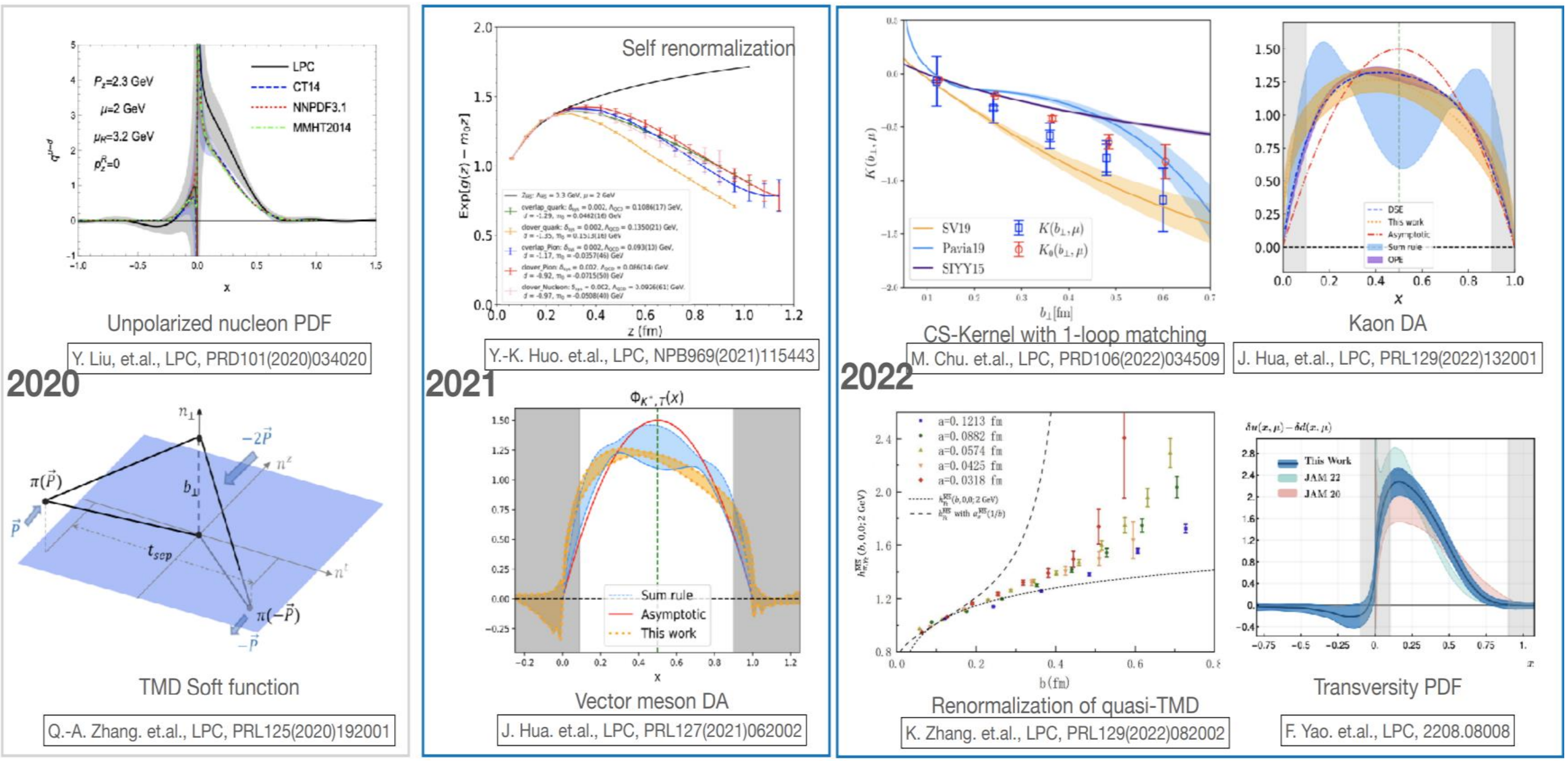
Fermion actions	Propagator	Configuration generation
Clover	Done (Multgrid)	Done (Multgrid)
Twisted mass	Done (Multgrid)	N/A
Staggered	Done (Multgrid)	TODO
Domain wall	TODO	Based on CPS+QUDA
Overlap	Done (Deflated CG)	N/A

Y. Bi, et.al, Lattice2019, 2001.05706

K. Zhang, et.al, Lattice2021, 2201.09004

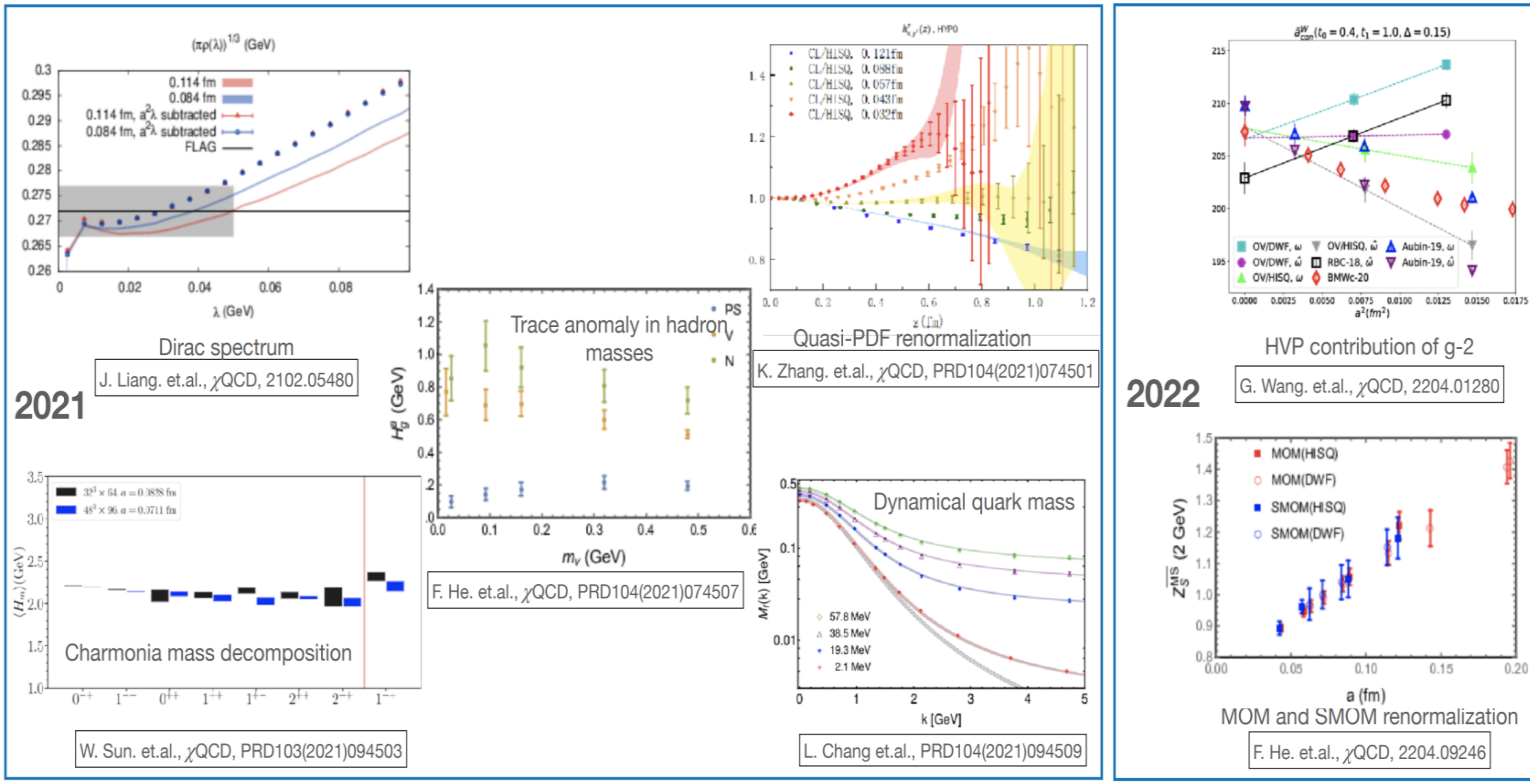
- **Some applications**

Hadron structures (PDF, DA etc.) using the Chroma + GUDA package.



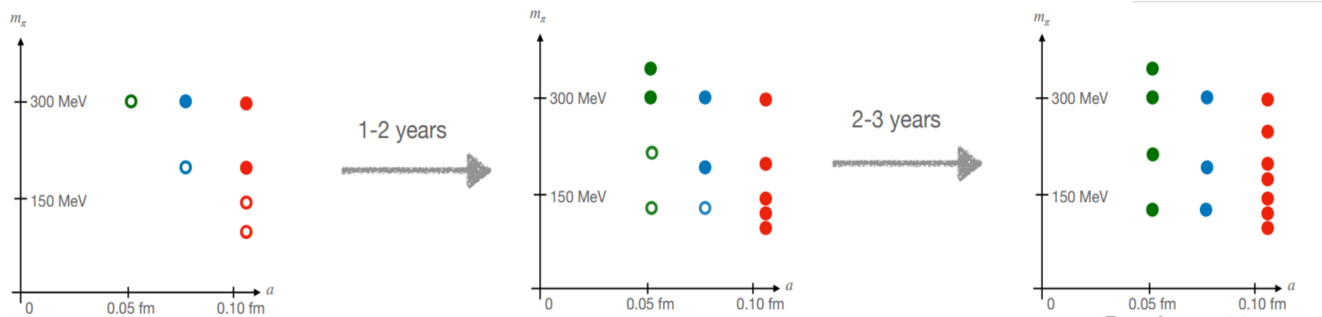
Based on Large Momentum Effective Theory (LAMET)
(X. Ji et al., Rev. Mod. Phys. 93 (2021)3, 035005)

Some results using GWU codes.



Overlap fermions on Domain wall fermion gauge ensembles generated by RBC/UKQCD and gauge ensembles with HISQ (MILC Collab.)

- **Configuration generation**
  - Gauge configurations are fundamental data for LQCD studies
  - The control of systematics requires different gauge ensembles with different lattice spacing, different quark masses and different volumes



Current status

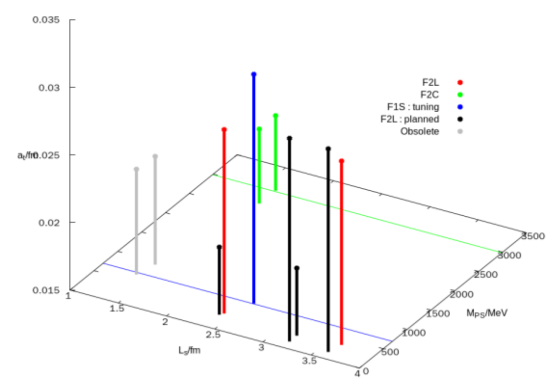
Present FLAG "Green star" requirement

Requirement to control all the systematic uncertainties

Configuration sets on isotropic lattices: ready (closed) and to-do (open)

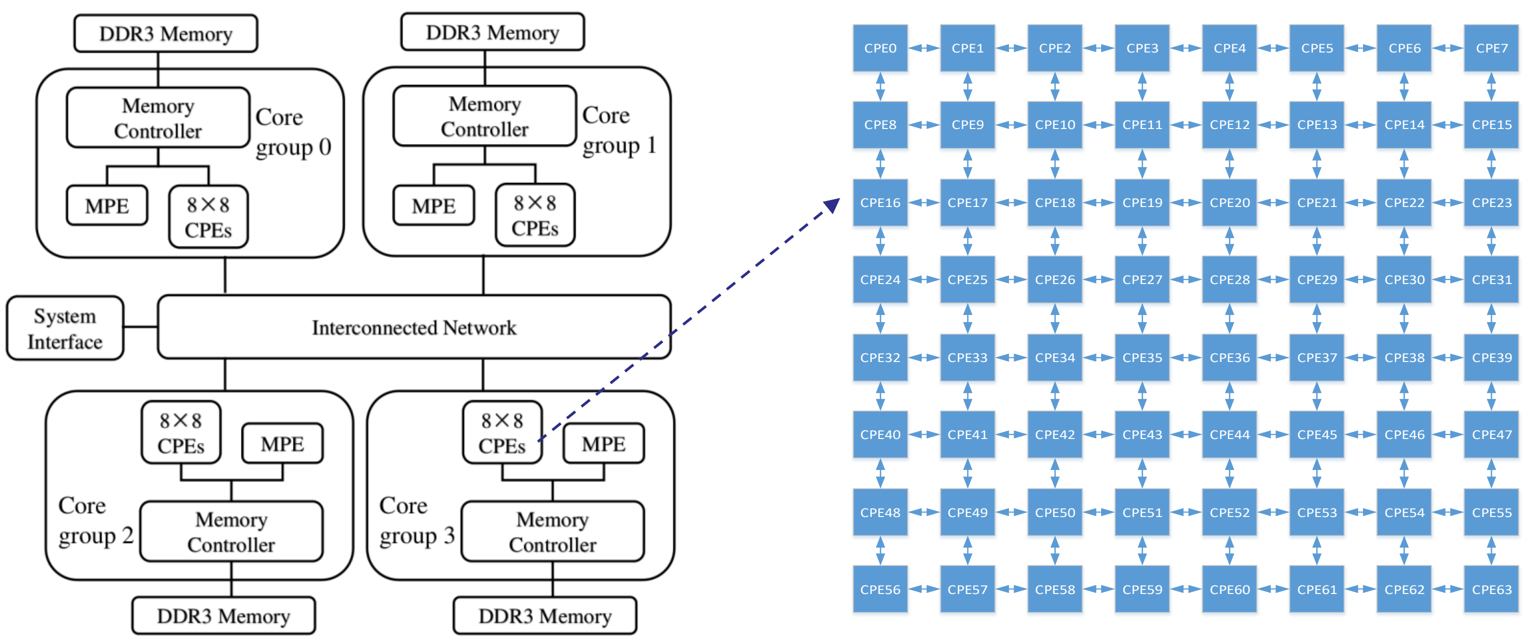
- Gauge ensembles are also generated on anisotropic lattices:

  To be used for studies of
  - hadron spectroscopy
  - hadron-hadron scatterings



2. Code development on Sunway-TaihuLight

- Sunway-TaihuLight has 40960 SW26010 processors
- Each SW26010 is a heterogenous Many-core processor
  - 4 core groups (CG), 32GB memory
  - 1 CG = 1 management processing element (MPE)
    - + 1 computing processing element (CPE) cluster of 64 CPEs
- Peak speed ~ 125 PFLOPS or 93 PFLOPS (Linpak)
- Node layout:



- **Code development**:

- Data partitioning
  each node has a sublattice.

- MPE handles the MPI and I/O
  communications among nodes

- Small bandwidth, Small L1 cache

- Data size at CPE is very limited:
  largest sublattice 16^4

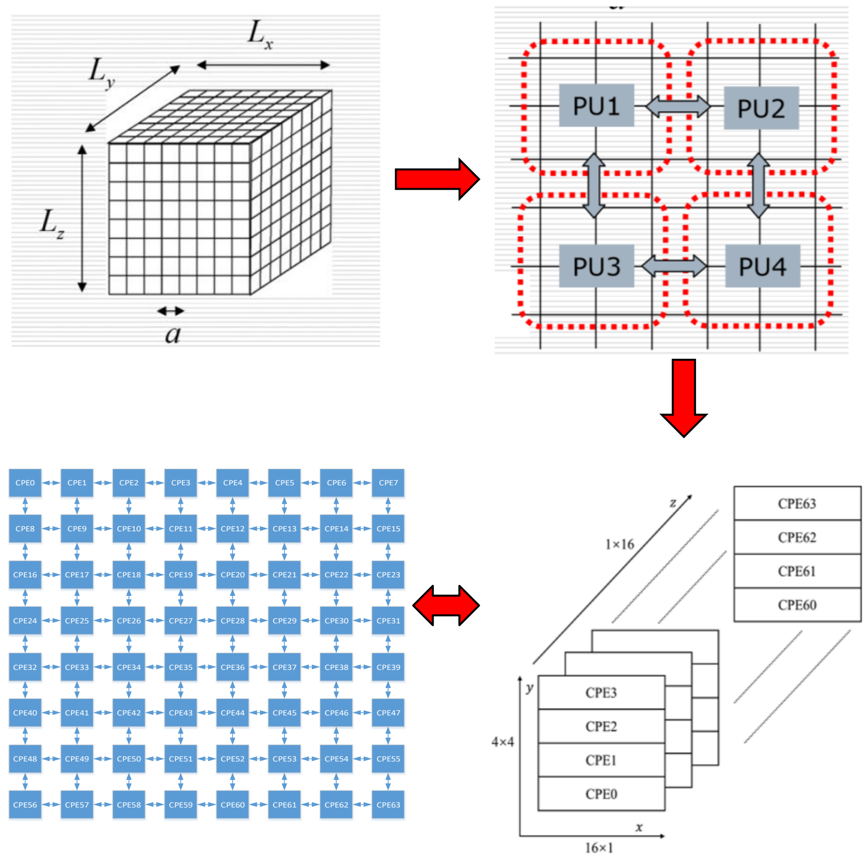
- Data slicing at CPE

- Workflow: balance computing
  and data exchange with MPE

- Manual and CVM optimization

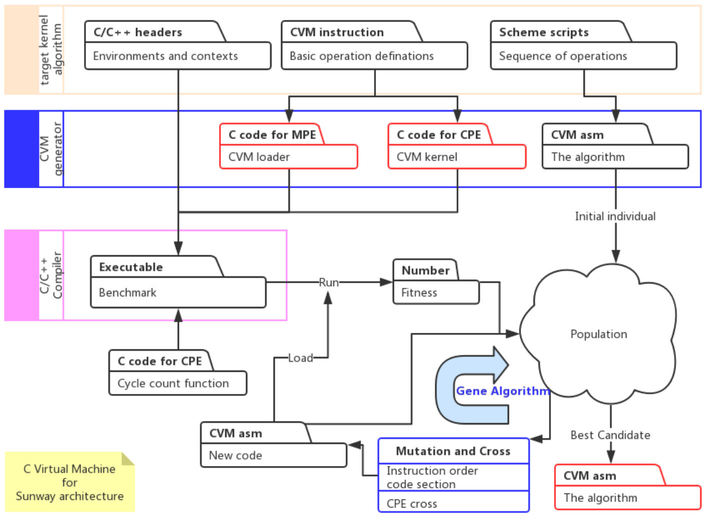
- Performance not good enough

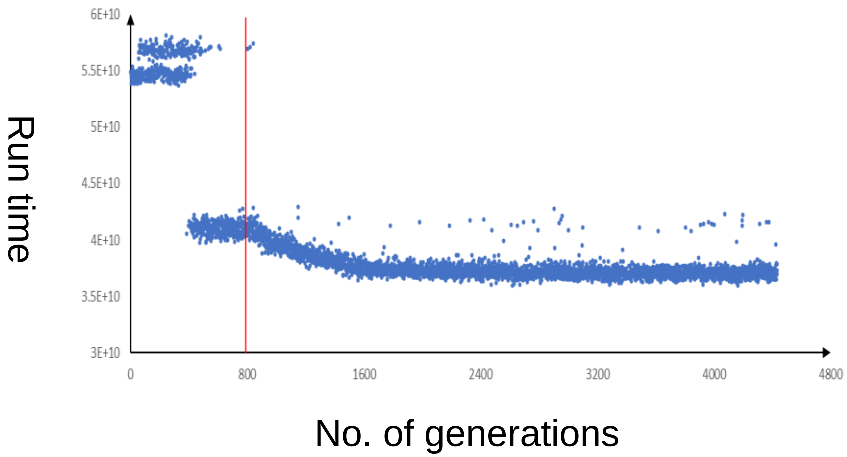
Courtesy to Ukawa



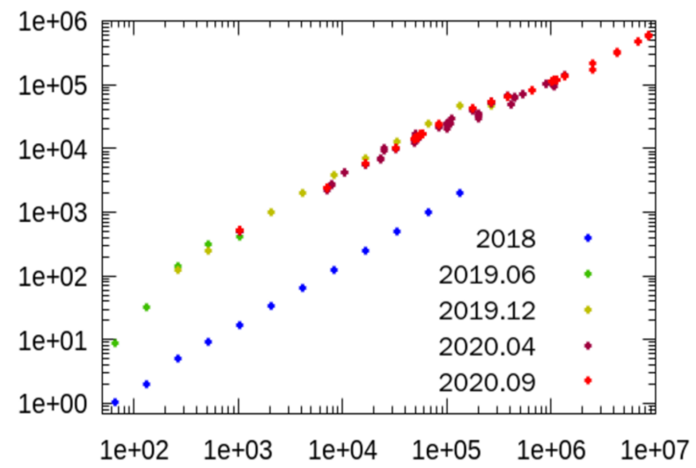
16^4 sublattice on one CPE cluster

- **Automatic optimization scheme—— C Language Virtual Machine (CVM)**
  - C code decomposed into basic operations
  - Different sequences of operations may give the same results
  - CVM assembles the operators into algorithms
  - Preference selective genetic algorithm
  - New code
  - After the manual optimization, CVM achieves roughly 13% additional speedup.
  - This is supposed to be done by compiler, but we have to do it by ourselves.





- **Performance progress**
- **Maximal job scales 8.52M cores (80% of the machine)**
- **Achieves 0.62 PFLOPs performance**
- **Note that HPCG measures 0.48 PFLOPs for sparse matrix system**



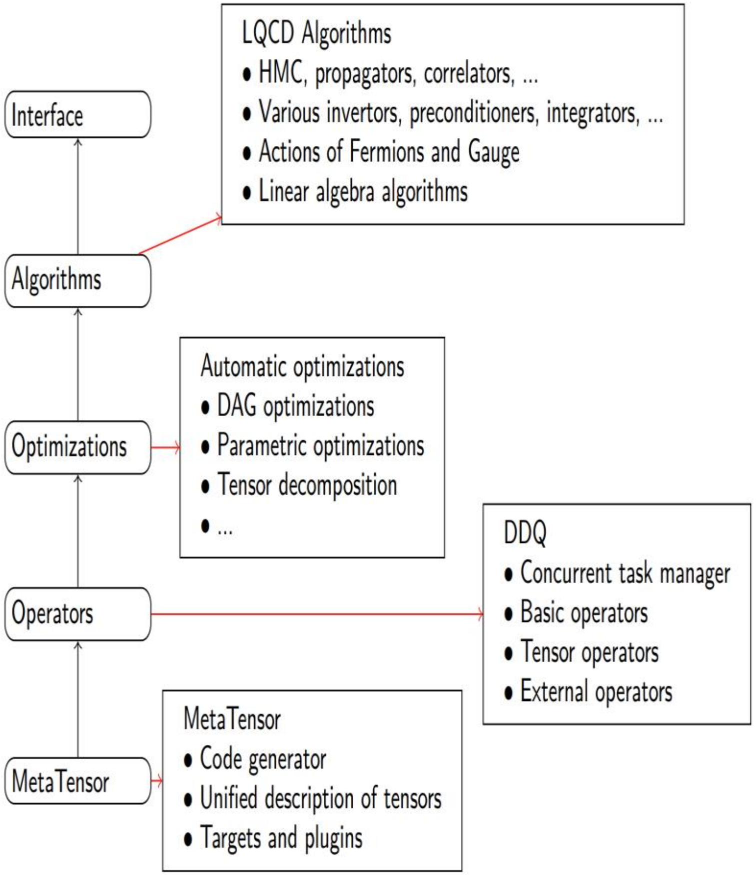
	CPU	Core number	Peak speed （Tflop/s)	LinPack（dense）		HPCG（sparse）	
				Peak (Tflop/s)	Efficiency （%）	Peak (Tflop/s)	Efficiency （%)
Fugaku	ARM A64FX	7,299,072	513,854.7	415,530	80.9	13366.4	2.60
Summit	NV V100	2,397,824	200,794.9	143,500	71.5	2925.75	1.46
Sierra	NV V100	1,572,480	125,712.0	94,640	75.3	1975.67	1.43
Sunway	SW26010	10,649,600	125,435.9	93,015	74.2	480.85	0.383
Tianhe-2A	Matrix-2000	4,981,760	100,678.7	61,444.5	61.0	580.11	1.71
HPC5	NV V100	669,760	51,720.8	35,450.0	68.5	860.32	1.66

https://top500.org/lists/hpcg/hpcg-november-2020

3. A new software framework for lattice QCD

- Five layers, open sockets for future modules on each layer.
- MetaTensor:
  A metaprogramming tool translate tensor expressions into C/C++ codes.
- Operator layer:
  A task manager “DDQ” can arrange all operators according to their dependence.
- Optimization layer:
  A tranparent layer, sockets are open for various automatic optimization algorithms.
- Algorithm layer:
  Contains algorithms needed by LQCD. Algorithms are written with scripts of operators and tensor expresssions.
- Interface:
  Contains a GUI which is easy to use.

Platform independent framework!



Summary

- **Lattice QCD is important for particle physics.**
- **High precision calculations of lattice QCD require massive computing resources.**
- **Supercomputers (SS) in China is an opportunity for lattice QCD studies.**
- **Homemade SS in China is not to be used efficiently at present.**
- **The ecosystem of Chinese SS need to be established.**

Thanks for your attention!