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Improving usability of DFT codes by using GUI software C-Tools

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C-TOOLS

Outline

- RIST in HPCI
- About C-Tools
  - the purpose of the development
  - the functions
- Simulation by using C-Tools
  - Run Quantum Espresso (PWscf) in K computer

RIST

HPCI : High Performance Computing Infrastructure

- Established as Japanese integrated high performance computing infrastructure in 2011
- Variety of computer systems are connected via high speed academic backbone network and provided as ***HPCI*** resources to users in Japan and overseas

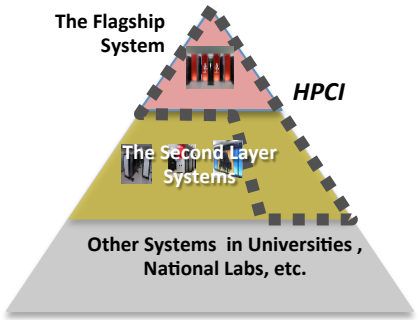
FY2017 Allocated computing resources

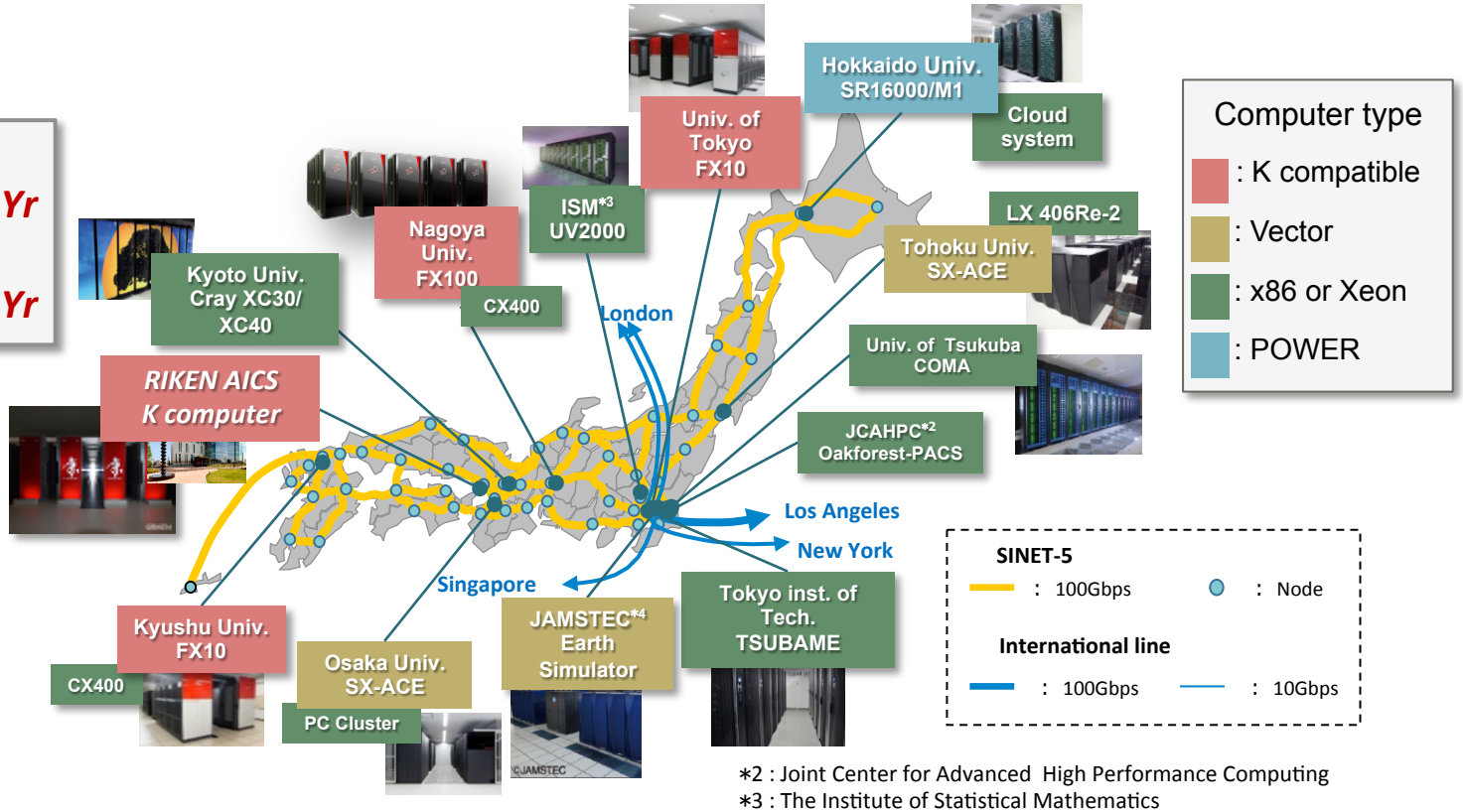
K computer

~4 Pflops x Yr

Other systems in total

~5.6 Pflops x Yr





*2 : Joint Center for Advanced High Performance Computing
*3 : The Institute of Statistical Mathematics
*4 : Japan Agency for Marine-Earth Science and Technology

HPCI Framework

Government (MEXT*1)

Act on the Promotion of Public Utilization of the Specific Advanced Large Research Facilities

Basic Policies on the Promotion of Public Utilization of the ***K computer***

Designation & Funding

Designation & Funding

Collaboration

RIKEN *AICS2 & *HPCI* facilities**

RIST

Computer resources and their operation

- Project secretariat
- Resources awarding and allocation
- Users support and consulting

Suggestions to HPCI program

Japanese & worldwide HPC communities

Feedback for HPCI project operations

Suggestions to HPCI program

***HPCI* Consortium of Japan**

Representative of HPC user communities

*1 : Ministry of Education, Culture, Sports, Science and Technology, *2 :Advanced Institute for Computational Science

Top Five Application Software Used in HPCI

field	ranking	software	number of projects		
			total	academia	industry
Bio & Life science	1	GROMACS	**17**	15	2
	2	GENESIS	**10**	10	0
	3	MODYLAS	**6**	6	0
	4	AMBER	**5**	4	1
	5	SiGN	**4**	4	0
Material science & Chemistry	1	GROMACS	**10**	9	1
	1	LAMMPS	**10**	4	6
	1	MODYLAS	**10**	8	2
	4	Quantum ESPRESSO	**9**	6	3
	4	NTChem	**9**	9	0
Environment, Disaster mitigation & prevention	1	SCALE	**9**	9	0
	1	NICAM	**8**	8	0
	3	LETKF	**7**	7	0
	4	OpenFOAM	**6**	2	4
	5	GAMERA	**5**	5	0
Engineering & Manufacturing	1	FrontFlow/blue	**12**	3	9
	2	OpenFOAM	**11**	2	9
	3	LANS3D	**8**	7	1
	3	LS-DYNA	**8**	3	5
	5	FrontFlow/red	**7**	2	5

red: overseas open-source software (OSS)

green: Japanese national projects software (open-source or in-house)

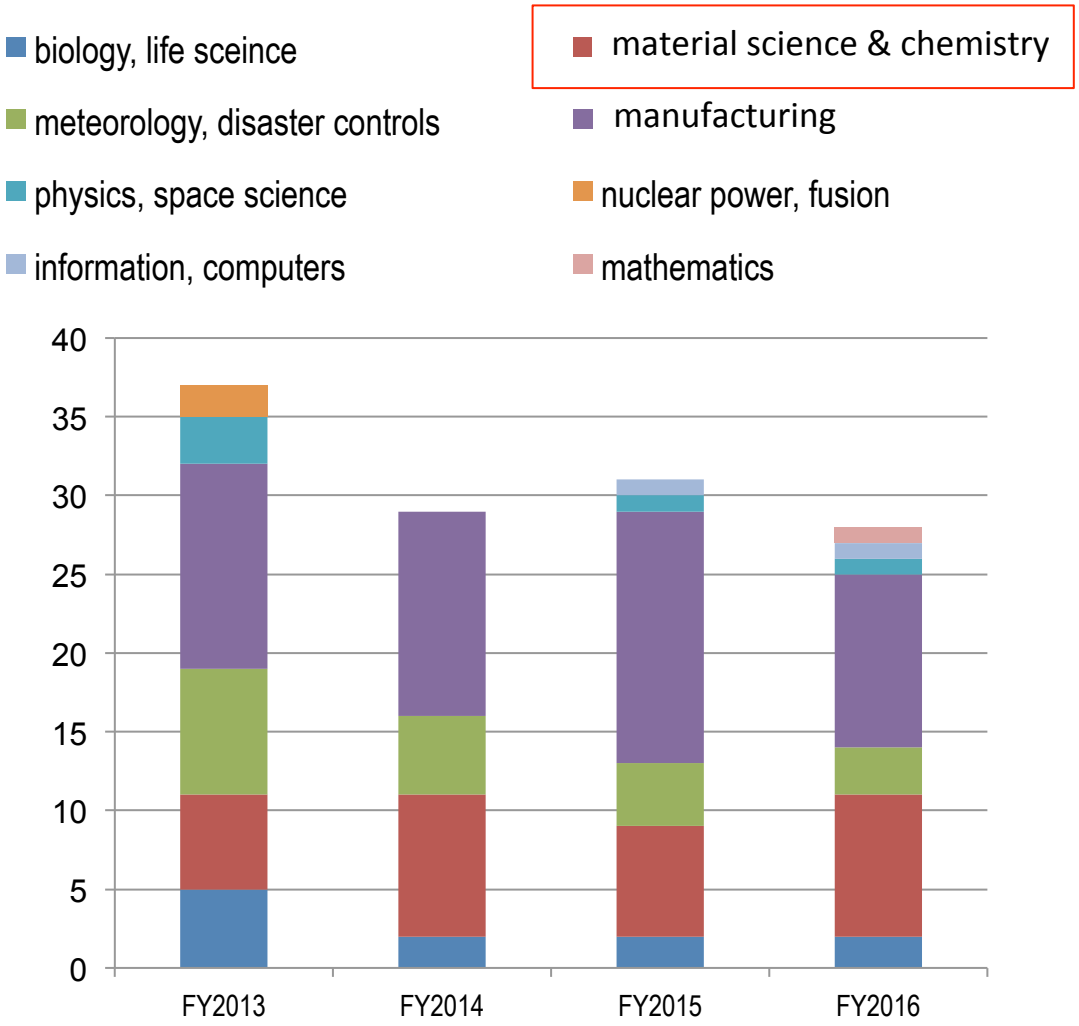
black: Commercial or in-house software

From the application forms in FY2016 and user reports in FY2015

OSS is widely used and becoming important tool in HPCI

Application Program Support

- Consultation
- Diagnosis
- Program Tuning
  - profiling
  - bottleneck removal
  - better algorithms



Number of supported applications

We support 30 projects and work on applications from several different fields.

Cf. Number of HPCI projects ~200

User Support) Example : Optimizing Quantum ESPRESSO

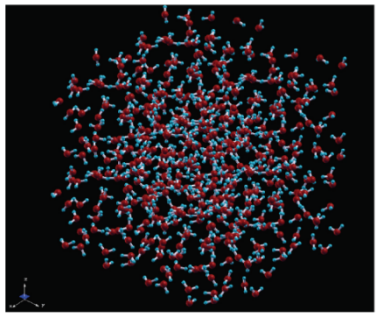
- Users' demand on Quantum ESPRESSO (QE)
  - To achieve better execution performance and parallel scaling

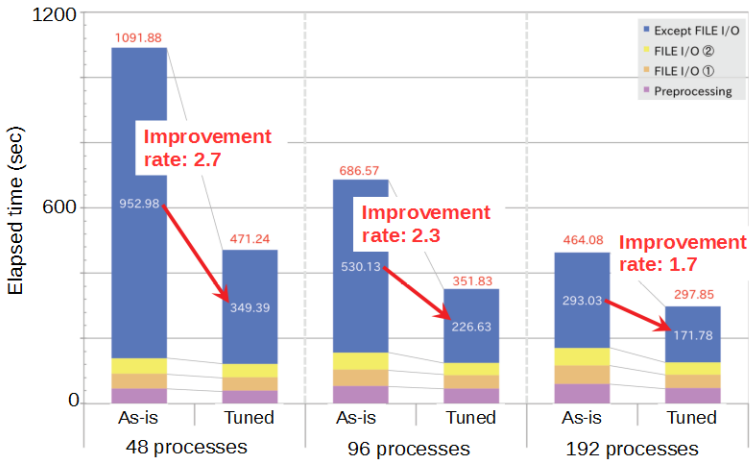
- User support of QE in K computer
  - Optimization of CP package (Car-Parrinello MD)
    - Key 1: Usage of fast collective MPI communication algorithm in K computer
    - Key 2: Reduction of instruction costs in matrix multiplication routines

2.7 times as fast as the original

  - Building binaries (ver.5.1.1) suitable for K computer
    - available for all the users
    - including our tuned CP package

Case study: 512 water molecules



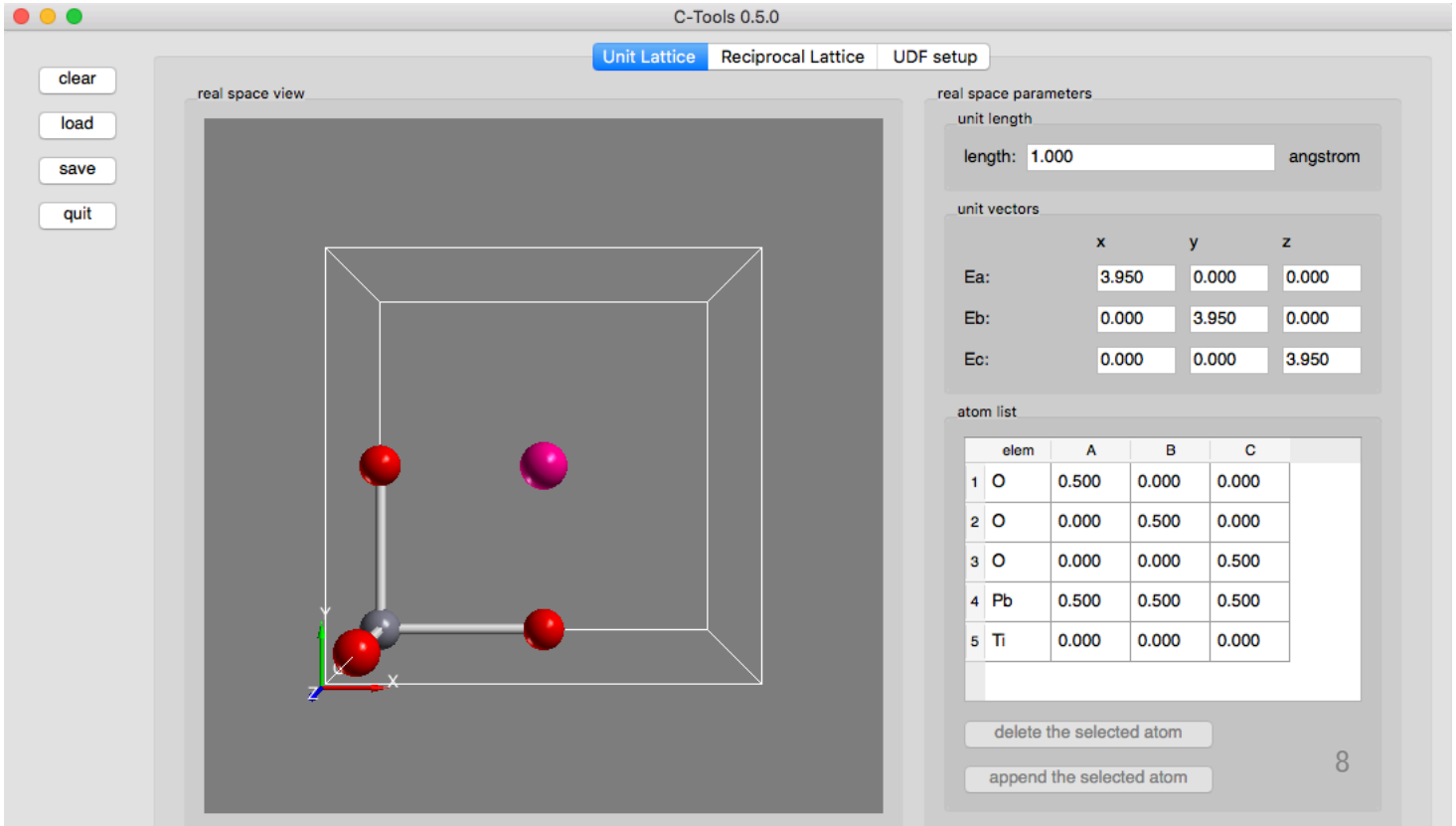


contributing to *ab initio* MD simulation of lithium ion batteries by FUJIFILM Co. Ltd. (hp150090)

About C-Tools

- C-Tools can produce input files of supported DFT codes via user friendly parameter adjustment using three-dimensional computer graphics (3DCG) and graphical user interfaces (GUI).
- Input file conversion between supported DFT codes
  There are a variety of DFT codes with each strength, and to combine the strength we have to transfer among the codes.

opening screen



C-TOOLS

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C-Tools: Supported DFT codes (5 codes)

- plane-wave pseudo-potential
  - xTAPP [1]
  - VASP [2]
  - Quantum Espresso (PWscf) [3]
- the pseudo-atomic localized basis
  - OpenMX [4]
- the real-space difference method and a pseudo-potential method
  - RSDFT [5]

[1] Yoshihide Yoshimoto, TAPP consortium tapp@cms.phys.s.u-tokyo.ac.jp. http://xtapp.cp.is.s.u-tokyo.ac.jp/

[2] http://www.vasp.at.

[3] http://www.quantum-espresso.org.

[4] T. Ozaki, H. Kino, J. Yu, M.J. Han, N. Kobayashi, M. Ohfuti, F. Ishii, T. Ohwaki, H.Weng, Computer code OpenMX. http://www.openmx-square.org/.

[5] J.-I. Iwata, D. Takahashi, A. Oshiyama, B. Boku, K. Shiraishi, S. Okada, and K. Yabana, J. Comput. Phys. **229**, 2339 (2010).; http://ma.cms-initiative.jp/ja/listapps/rsdft/.

C-TOOLS

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[load]

Structure files
CIF (Crystallographic Information File)
XYZ (Chemical file format)

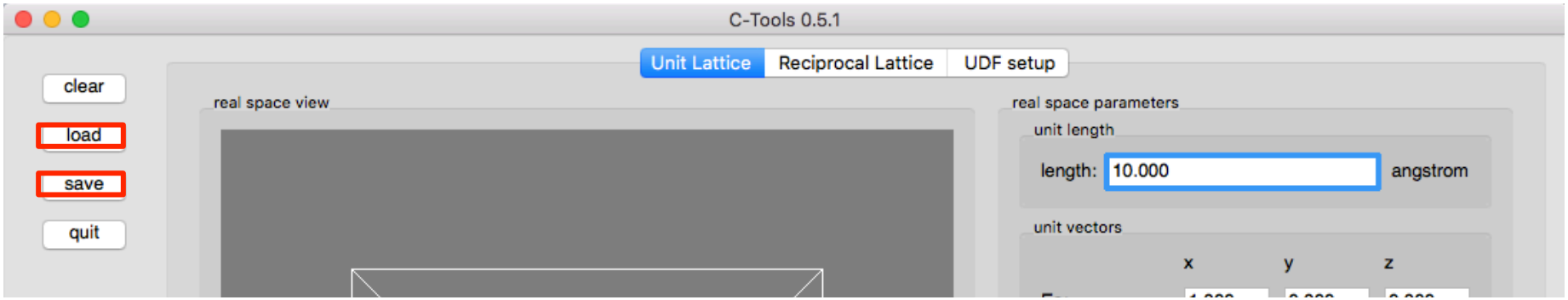
The input files can be easily created by clicking the [load] and [save] botton

output

Creating Input files automatically

[save]

Input files
xTAPP
OpenMX
RSDFT
VASP
PWscf



C-TOOLS

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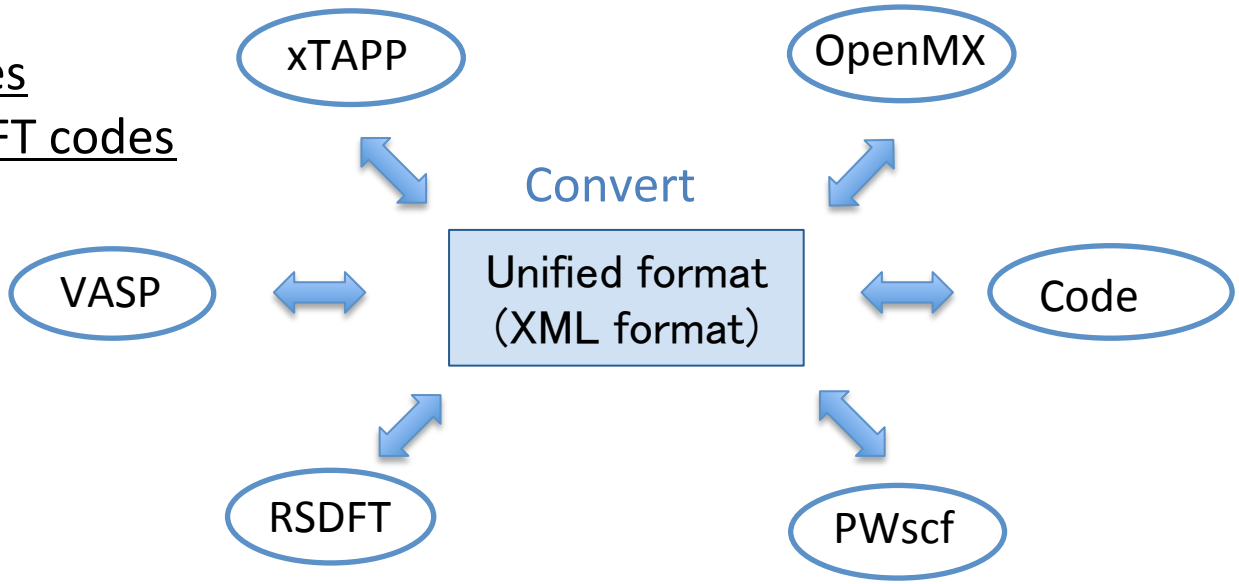
Convert the input files between different DFT codes



xTAPP	Unified format (XML format)	VASP

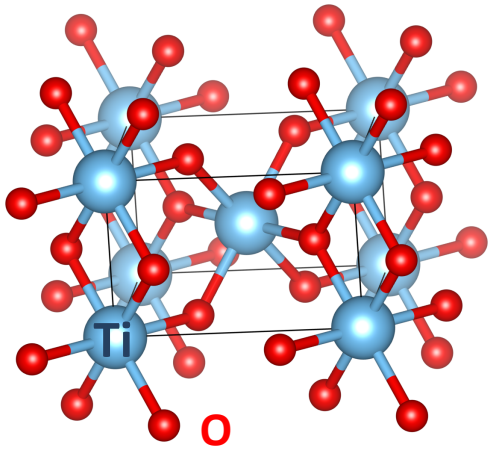
# main data 	
&tappinput
scf_converge = 1.0E-10,
scf_number_iter = 40,
number_band = 28,
lattice_factor = 9.2850,
lattice_list =
1.0, 0.0, 0.0,
-0.5, 0.866, 0.0,
0.0, 0.0, 1.1001,
number_atom = 9,
number_element = 2,
/
	<?xml version="1.0" encoding="UTF-8"?>
	<Unified_DFT_Format>
	<Common_Parameters>
	<Calculation_Settings>
	<Calculation_Type> Energy </Calculation_Type>
	<Continue> No </Continue>
	<Accuracy> Normal </Accuracy>
	<Energy_Converge> 1.0E-10 </Energy_Converge>
	<Electron_Max_Iteration> 40 ron_Max_Iteration>
	<Number_Band> 28 </Number_Band>
	<Smearing> ON </Smearing>
	<Symmetry> ON </Symmetry>
	<Force_Converge> 1.0E-3 </Force_Converge>
	</Calculation_Settings>
		# SCF input for VASP
		SYSTEM = Quartz
		EDIFF = 0.1E-03
		NELM = 60
		NBANDS = 28
		IMIX = 4
		ISMEAR = 1
		ISYM = 1
		NSW = 0
		EDIFFG = 0.1E-02

Simulation by using C-Tools

rutile TiO_2

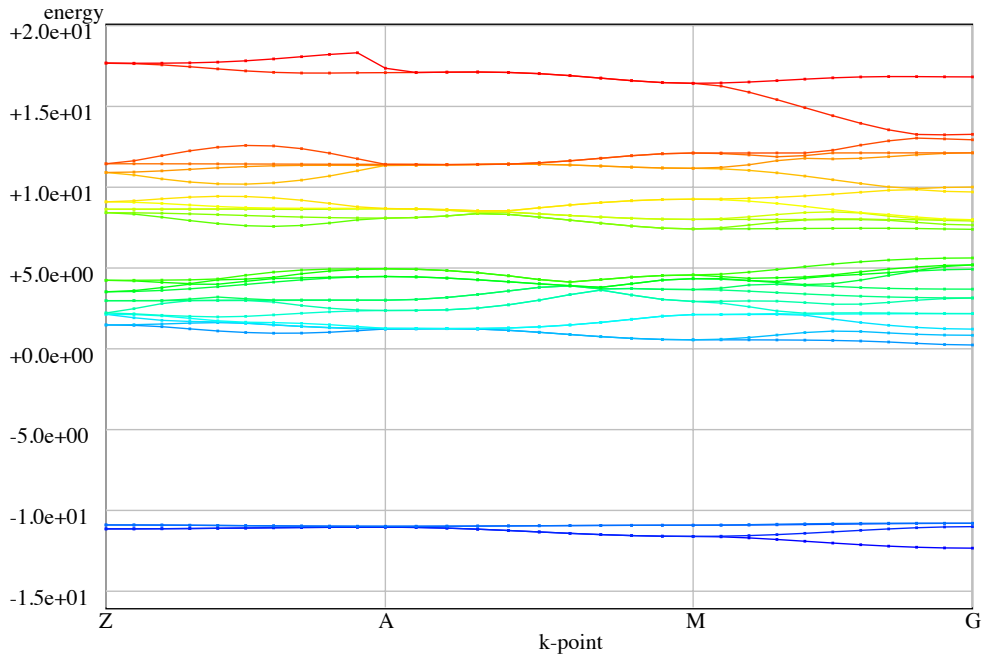
Structure file（cif）

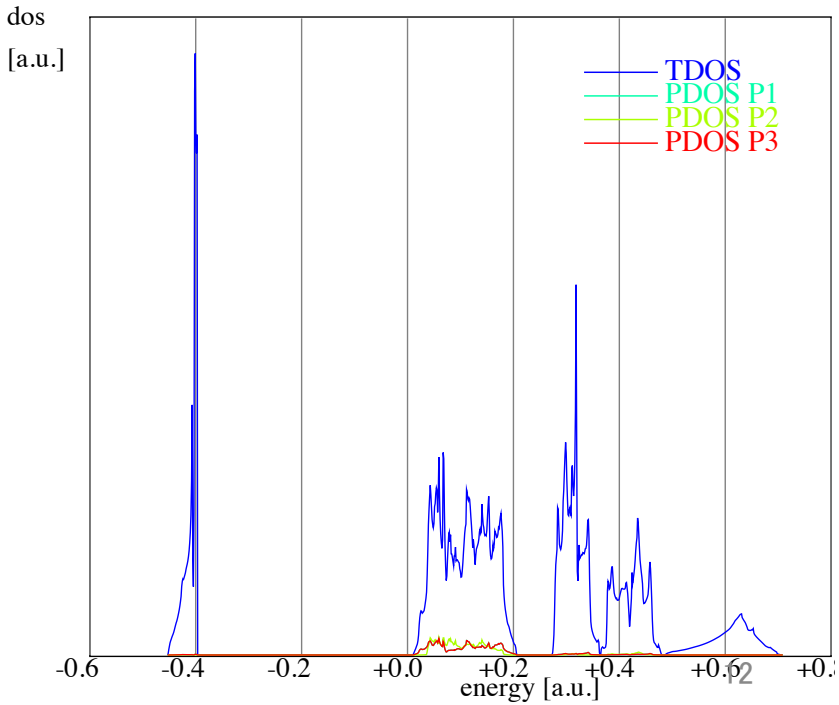
[number of atoms] Ti : 2, O : 4
[space group] $P4_2/mnm$



Creating a xTAPP input file by C-Tools

The results





Run DFT code packages in HPCI

- the codes should be properly compiled in HPCI
  - Investigating the proper compile options
- the codes should properly run in HPCI

  （→ We need to measure the performance of the codes in HPCI）
  - Specifying the number of nodes, MPI processes, threads
  - Specifying the runtime options　(If the code has the options)

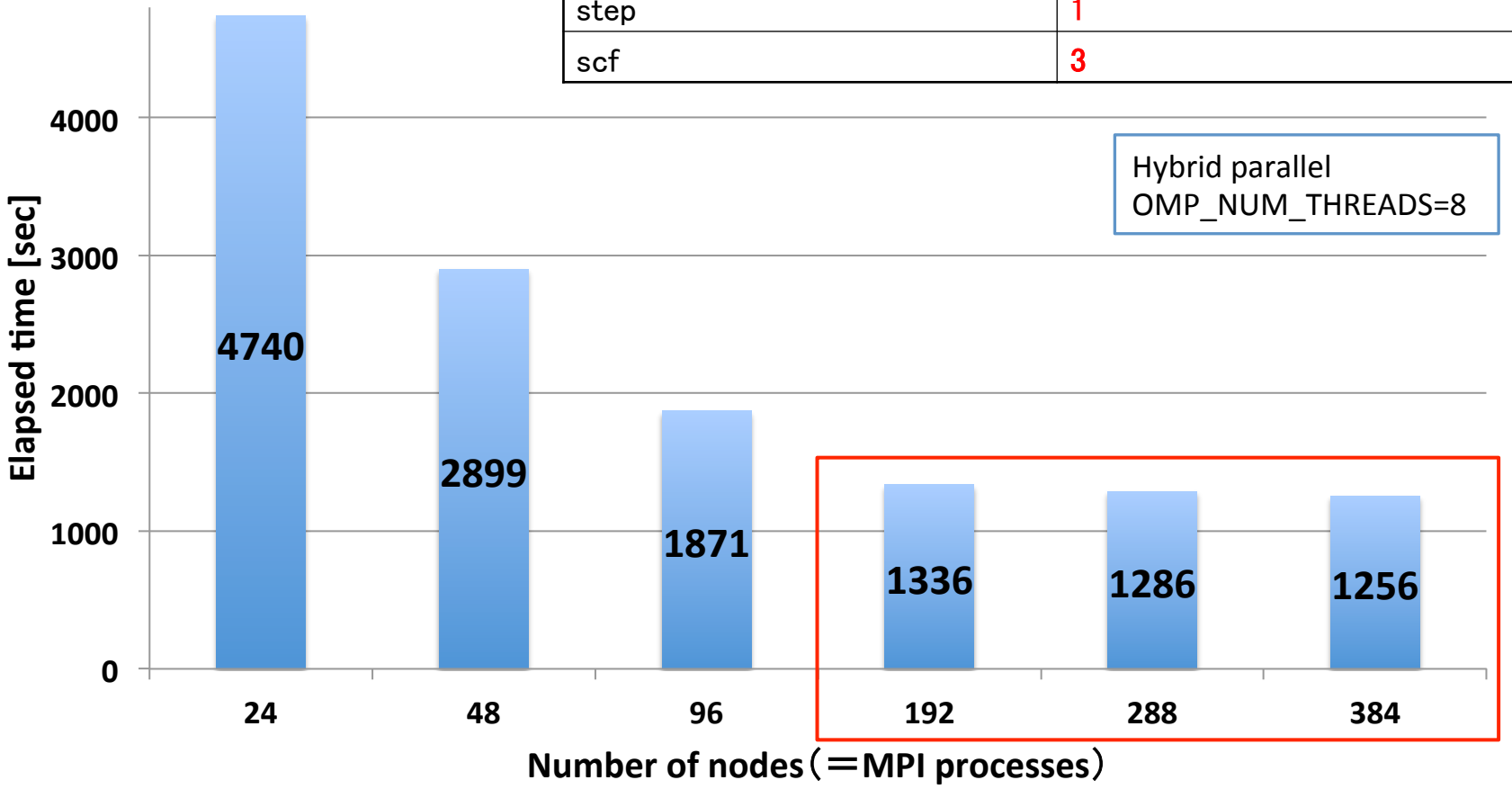
If the code does not run properly,

- It takes too much calculation time
- Computing resources are consumed needlessly

Run Quantum Espresso (PWscf) in K computer (1)

Creating Input file by C-Tools

Target	rutile TiO_2 + impurity hydrogen
Size	217 atoms per unit cell
exchange correlation functional	GGA(PBE)
k point	3 x 3 x 3 (irreducible: 14 points)
step	1
scf	3

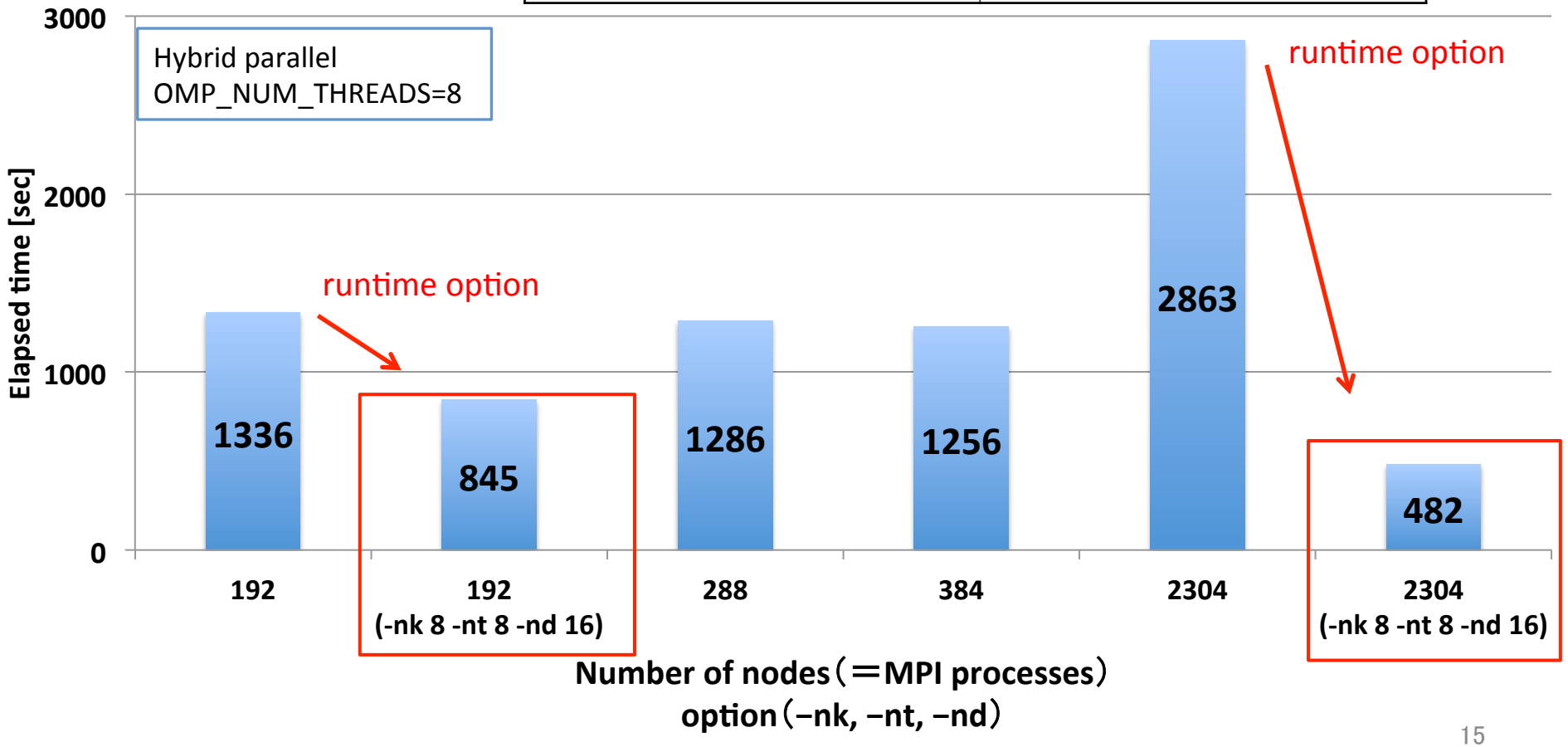


- MPI processes = 192 → saturation

Run Quantum Espresso (PWscf) in K computer (2)

runtime option
–nk : k-point parallel
–nt : FFT parallel
–nd : subspace Hamiltonian

Target	rutile TiO_2 + impurity hydrogen
Size	217 atoms per unit cell
exchange correlation functional	GGA(PBE)
k point	3 x 3 x 3 (irreducible: 14 points)
step	1
scf	3



Summary

Improving usability of DFT codes by using C-Tools

- Creating Input files by C-Tools
  - Running a simulation
  - Investigating the performance of Quantum Espresso (PWscf) in K computer

Target	rutile TiO_2 + impurity hydrogen
Size	217 atoms per unit cell

→ Optimal execution
nodes (= MPI processes) : 192
theareds : 8
runtime options : (−nk 8 −nt 8 −nd 16)

→ The scalability changes depending on the size of calculation targets.
We need to check the performance every time when the size changes.

C-TOOLS

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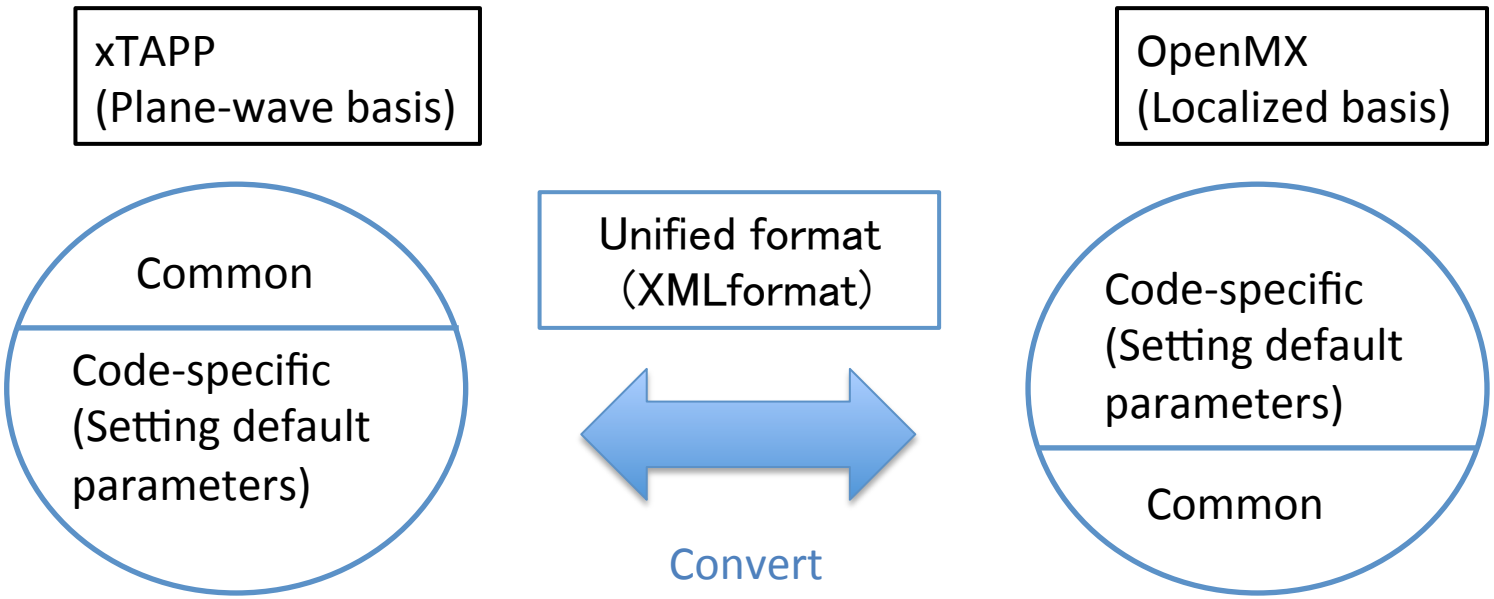
Unified format



- Basic parameters of common
- Setting default parameters (recommendation values) for the unique function of each code
- Detailed settings for each code