



Effective Performance of K Computer in Life Science Applications

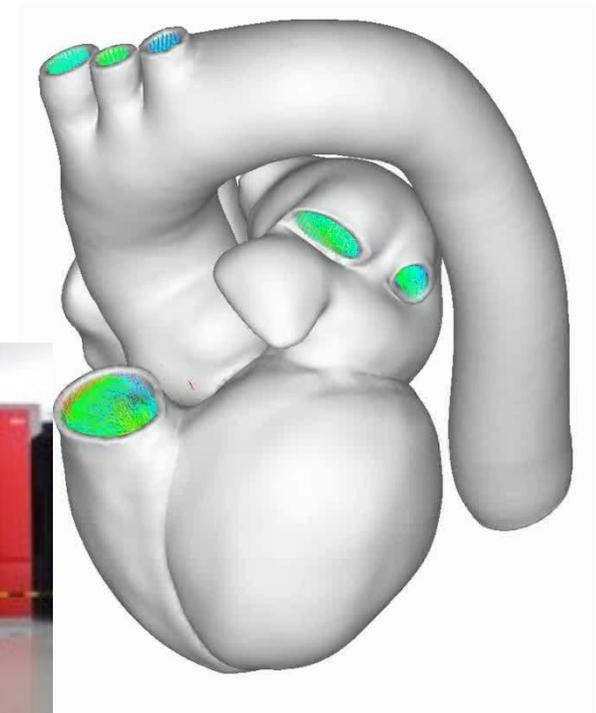
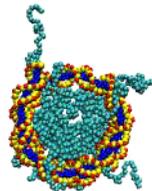


Ryutaro Himeno

ISLiM: Next Generation Integrated Simulation of Living Matter
Computational Science Research Program

RIKEN

himeno@riken.jp





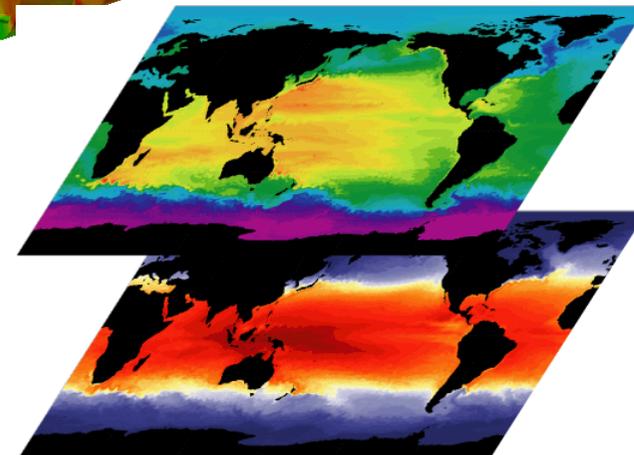
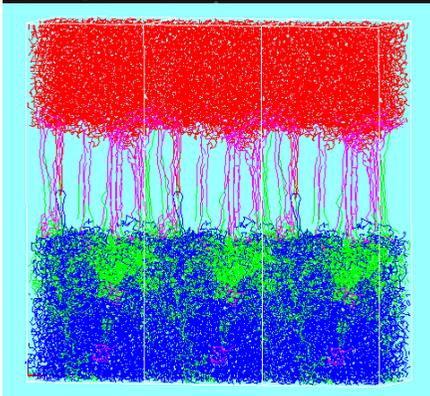
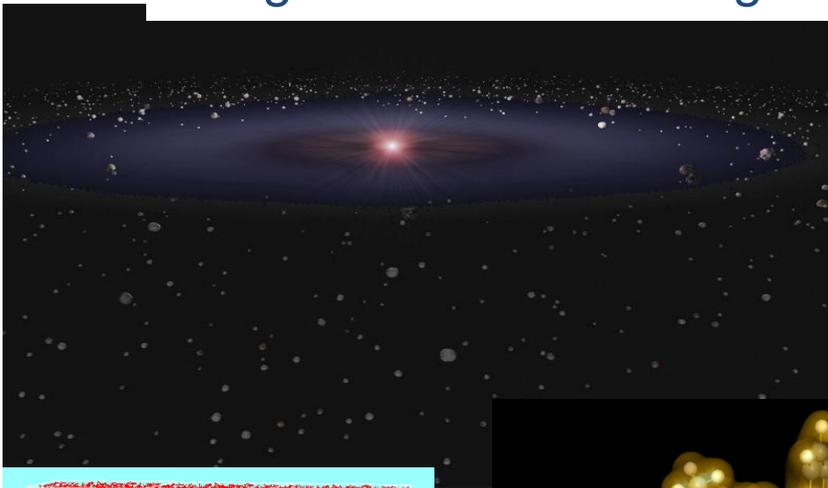
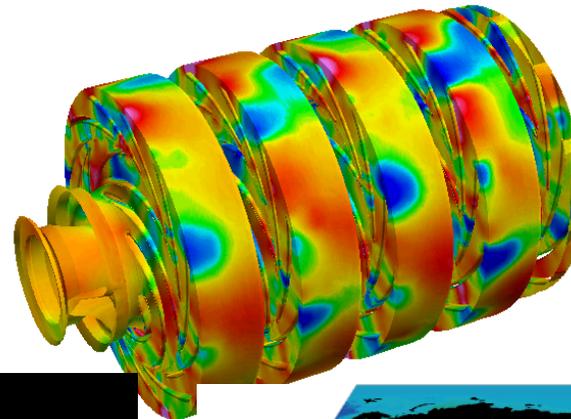
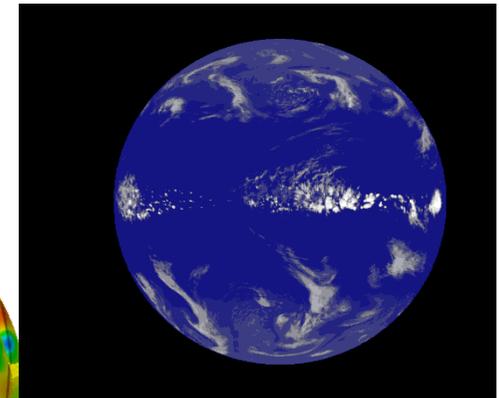
ISL λ I

Co-design: Target applications and BM suit



The application software committee started selecting target applications for making a benchmark suit in January, 2006.

21 codes were selected in March and NextBMT suit was developed. We evaluated the rough system design with 7 well scaling codes out of 21.





Characteristics

Shown in 2009



Hybrid Supercomputer System composed of Scalar and Vector Units

Vector unit is suitable for continuum physics simulation

Scalar unit is suitable for Data Base application, particle-based simulation

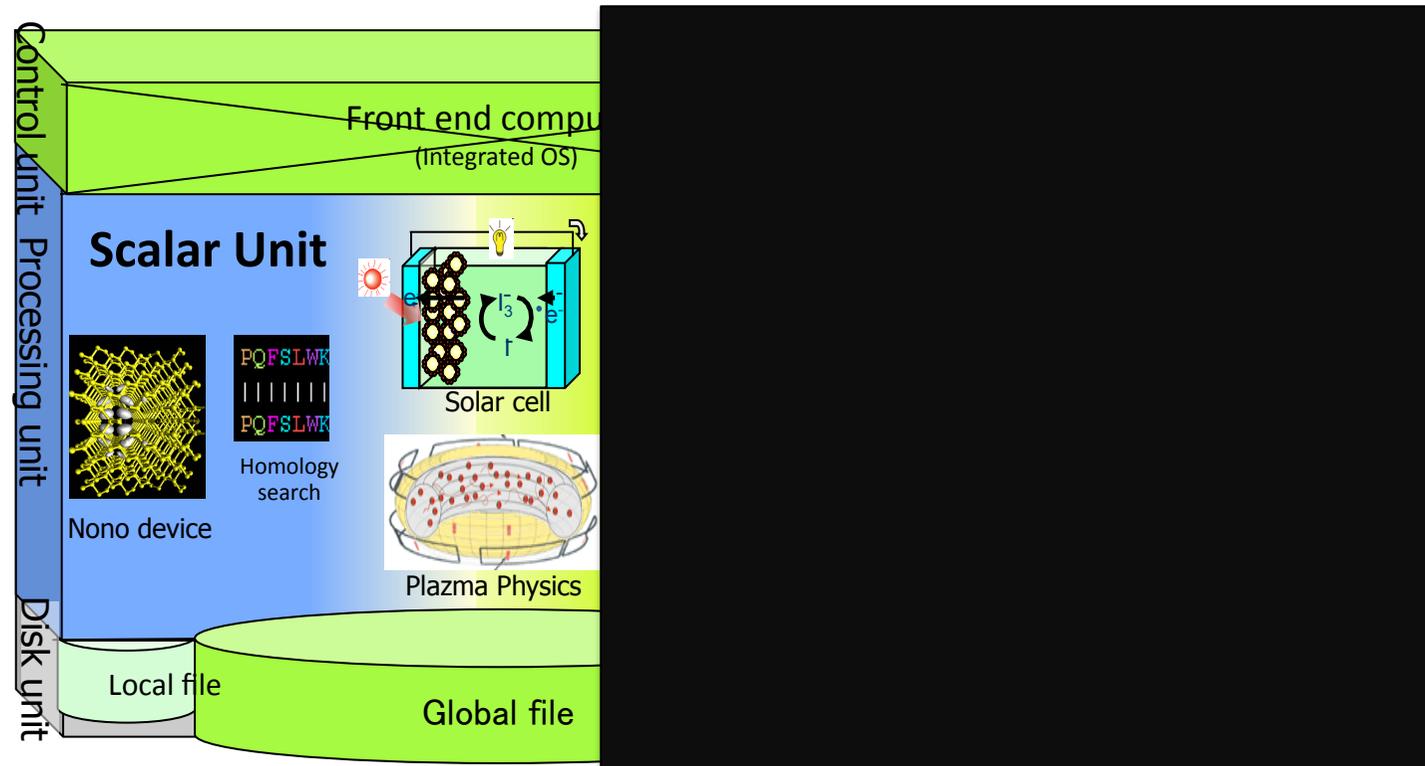
Hybrid system has both strong points for users to choose better units for different applications

Scalar Unit

Data base, homology search

Similarity with PC

- high speed low power CPU
- New strong network for enormous parallelism





Schedule of the Next-generation supercomputer R&D project



		FY2006	FY2007	FY2008	FY2009	FY2010	FY2011	FY2012	
System		Conceptual design		Detailed design		Prototype, evaluation	Production, installation, and adjustment		
Applications	Next-Generation Integrated Nanoscience Simulation	Development, production, and evaluation						Verification	Start operation in Fall
	Next-Generation Integrated Life Simulation	Development, production, and evaluation						Verification	
Buildings	Computer building		Design	Construction					
	Research building		Design	Construction					



ISLIM

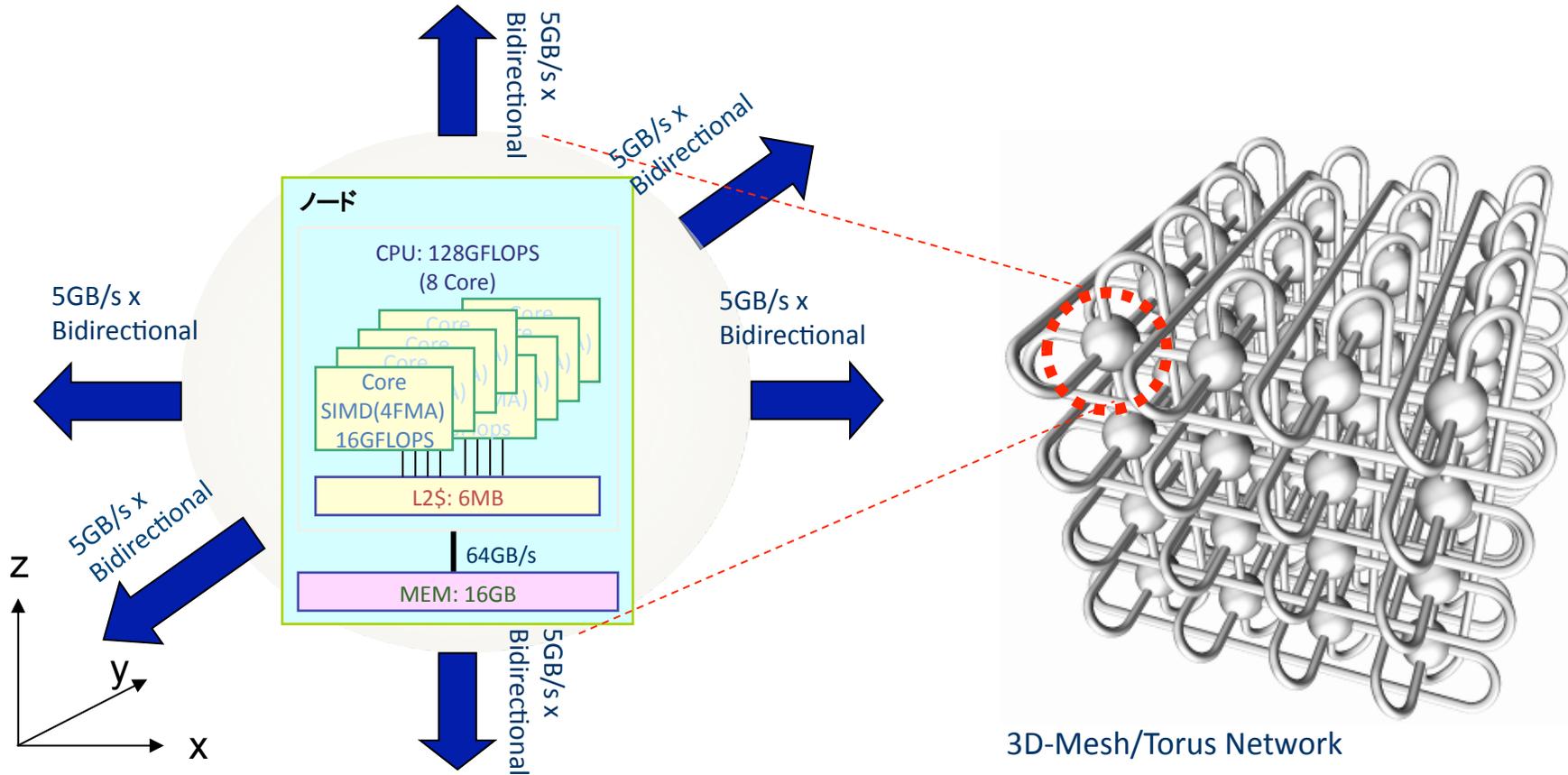
京 = "K" means 10^{16}

K-Computer System

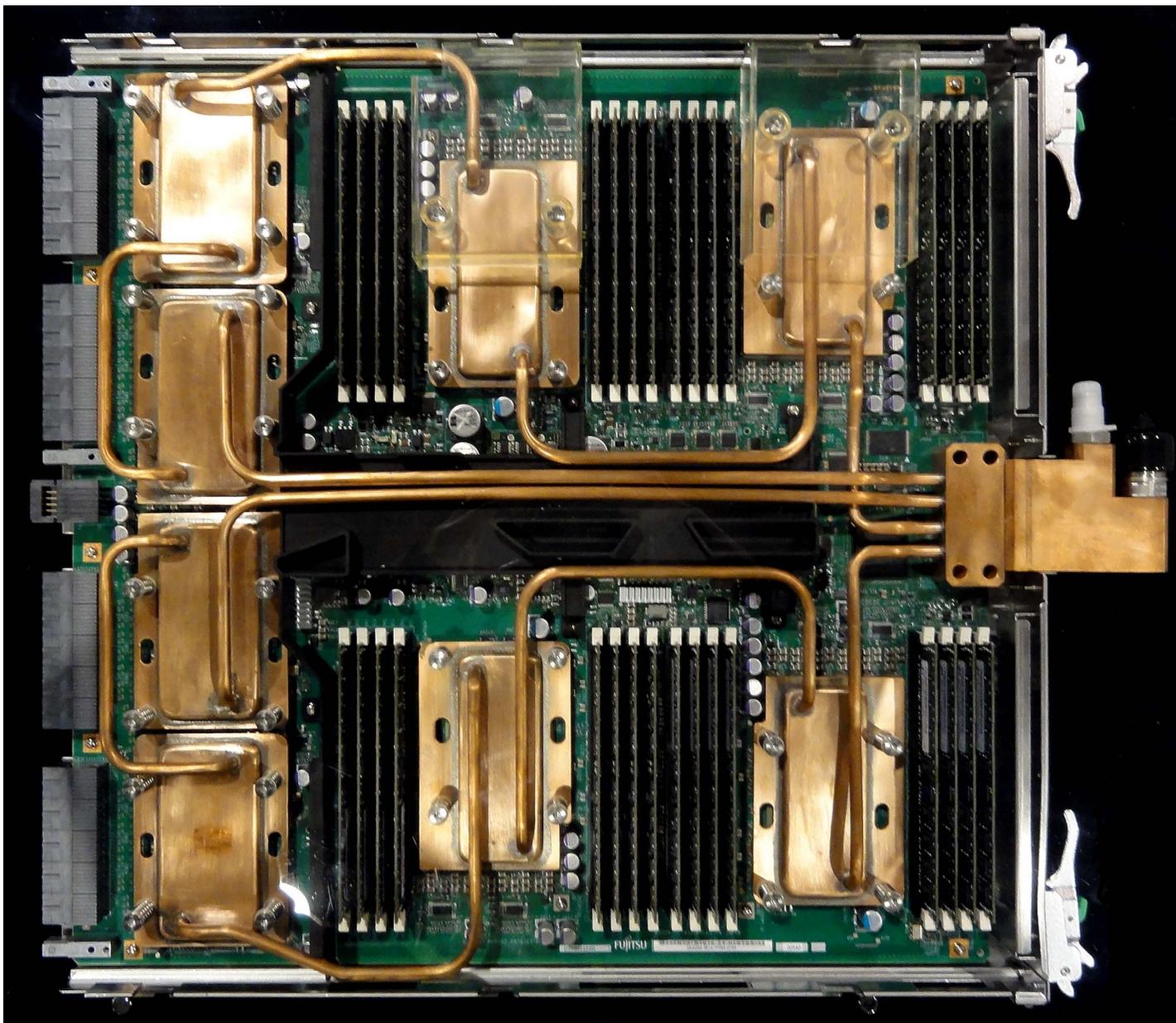


- Number of nodes : > 80,000
 - Number of Processors: > 80,000
 - Number of Cores: > 640,000
- Peak Performance: > 10 PFLOPS
- Memory Capacity: > 1PB (16GB/node)

- Network: Tofu interconnect (6-dim. Mesh/Torus)
 - User view: 3D-Torus
 - Bandwidth: 5GB/s bidirectional for each six direction
 - 4 Simultaneous Communication
 - Bisection Bandwidth: >30TB/s (bidirectional, nominal peak)



System Board of K computer



K Computer System



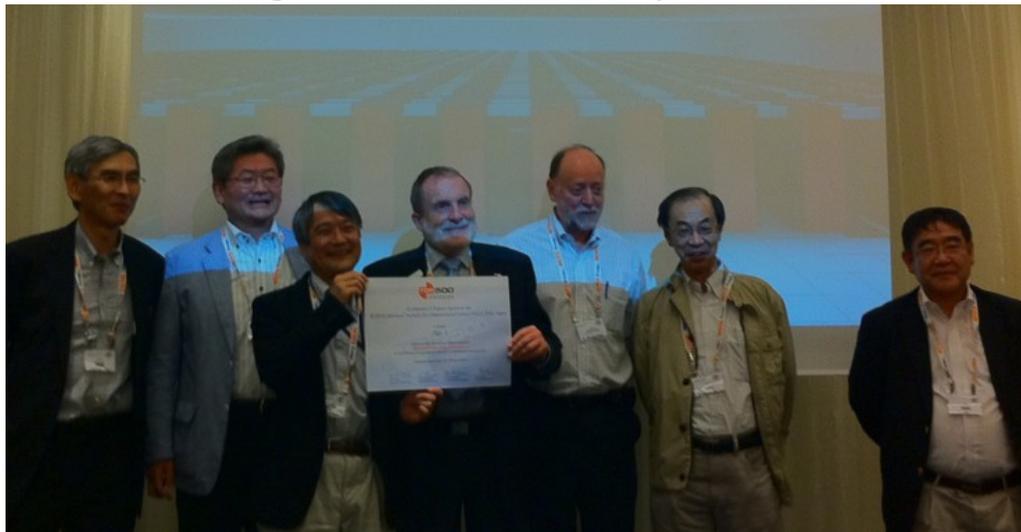
Still in progress for starting operation in coming fall.
Testing file system, Job manager, compiler, libraries, etc.



K-computer, the fastest, ISC2011



- 8.16 PetaFLOPs, 3-times performance of the 2nd supercomputer
- High effective performance
- High reliability



Fujitsu Lunch Party at ISC2011





SC2011



*K computer, a Fujitsu System at the
RIKEN Advanced Institute for Computational Science (AICS), Kobe, Japan*

新井直之

is ranked

No. 1

運川博昭

奥田基

村野和雄

堀越知一

among the World's TOP500 Supercomputers

with 10.51 PFlop/s Linpack Performance

村田聖雄

on the TOP500 List published at the SC11 Conference, November 15, 2011

榎野龍太郎

Congratulations from the TOP500 Editors

木村康則

Hans Meuer

Hans Meuer
University of Mannheim

Erich Strohmaier

Erich Strohmaier
NERSC/Berkeley Lab

Jack Dongarra

Jack Dongarra
University of Tennessee

Horst Simon

Horst Simon
NERSC/Berkeley Lab



Next-generation Supercomputer R&D project and Life Science Grand Challenge



		FY2006	FY2007	FY2008	FY2009	FY2010	FY2011	FY2012
System		Conceptual design		Detailed design		Prototype, evaluation	Production, installation, and adjustment	
Applications	Next-Generation Integrated Nanoscience Simulation	Development, production, and evaluation						Verification
	Next-Generation Integrated Life Simulation	Development, production, and evaluation						Verification
		Life Science Grand Challenge: ISLiM						
Buildings	Computer building		Design	Construction				
	Research building		Design	Construction				



Grand Challenge in Life Science at 1st stage

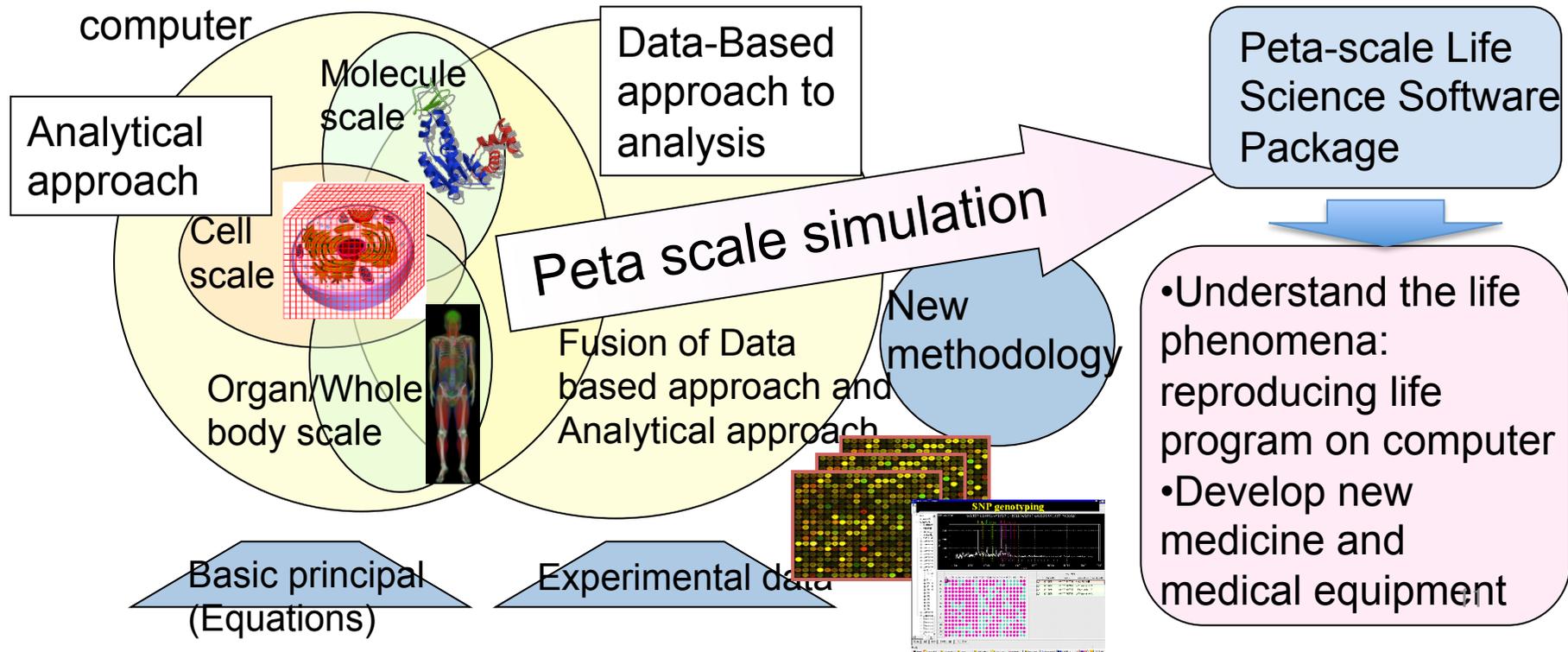


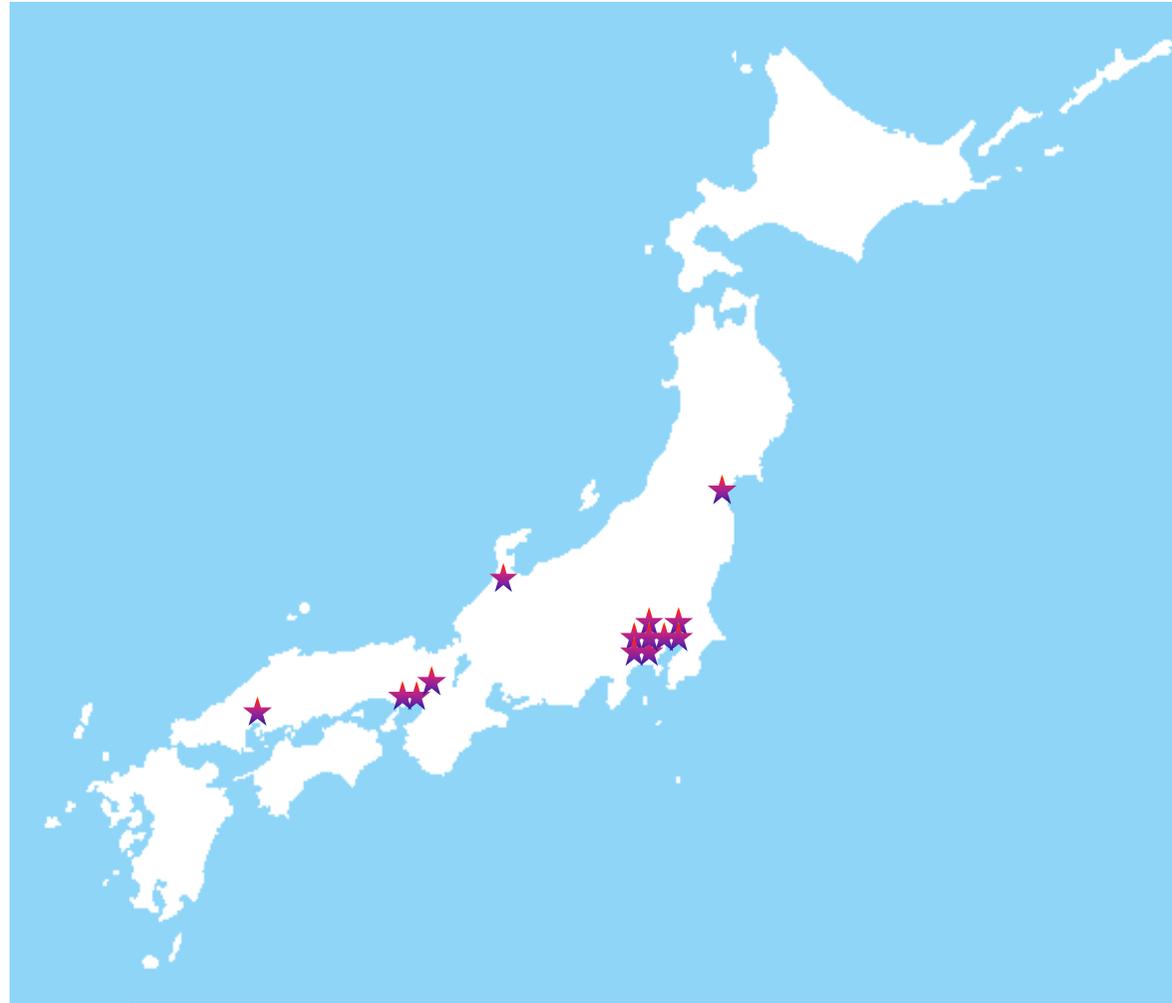
Goal

Understand the life phenomena: reproducing life program on computer
Develop new medicine and medical equipment

Approach

combination of analytical approach and Data-driven approach on Peta-scale computer



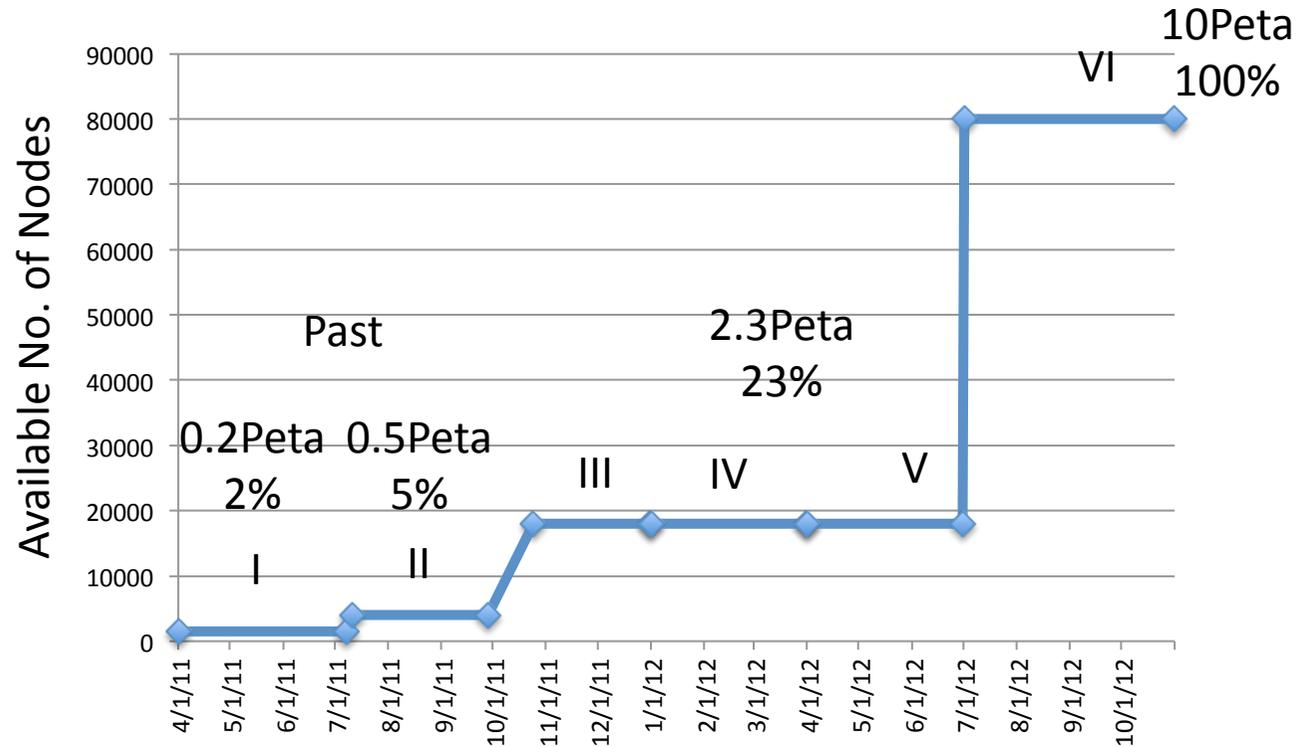


Organization 13
 (RIKEN, U. of Tokyo, Osaka U., Kyoto U. Tohoku U.,
 Tokai U., JAIST, Chiba U., Keio U. Yokohama City U.,
 Kobe U., TiTch, ISM)
 About 200 person, including 60 postDoc

Developing Software

	Applications	No. of application Software
Molecule scale	MD, Quantum Chemistry, Coarse Grain MD	9
Cell scale	Voxel-based multi-compartment transport-diffusion simulator	1
Organ/whole body scale	Heart sim., Lung sim., HIFU sim., Fluid-structure sim. for blood flow,	6
Brain & neural system	Neural sim., whole brain sim., cortical micro circuit sim.,	5
Data based analysis	Whole genome association study, data assimilation, prediction of protein-protein interaction, genome sequencer data processing, Haplotype whole genome association study	9
HPC	Parallel middleware, parallel visualization software, high-speed software core library	4

Test operation of K computer



	I	II	III	IV	V	VI
Date	2011/4/1	2011/7/11	2011/10/24	2012/1/1	2012/4/1	2012/7/1
Available nodes	1536	3840	18000	18000	18000	80000



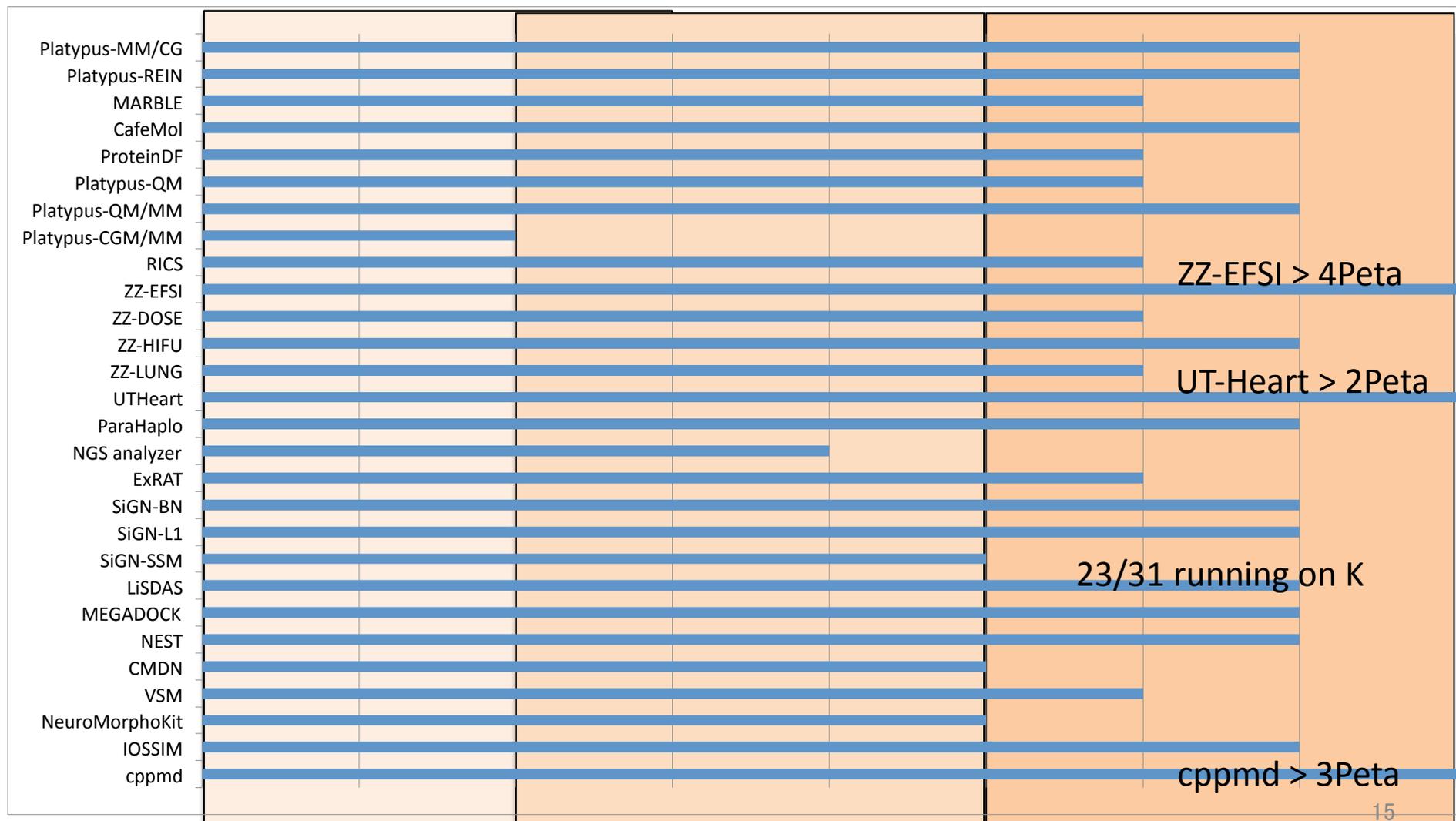
Current status of development



Phase I < 256

Phase II < 8192

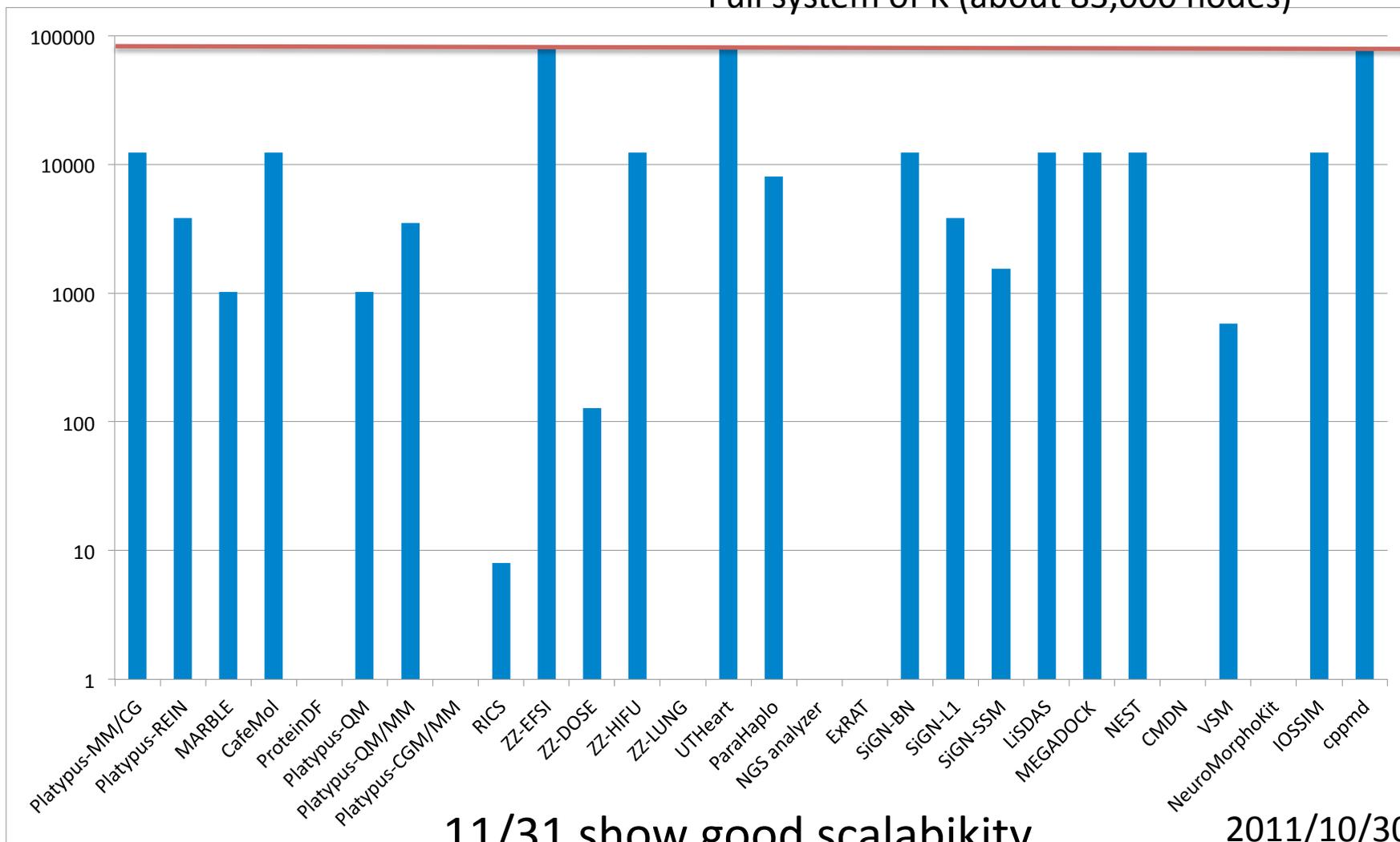
Phase III on K



Goal: > 1 Pata FLOPS

Tested max node no. on K

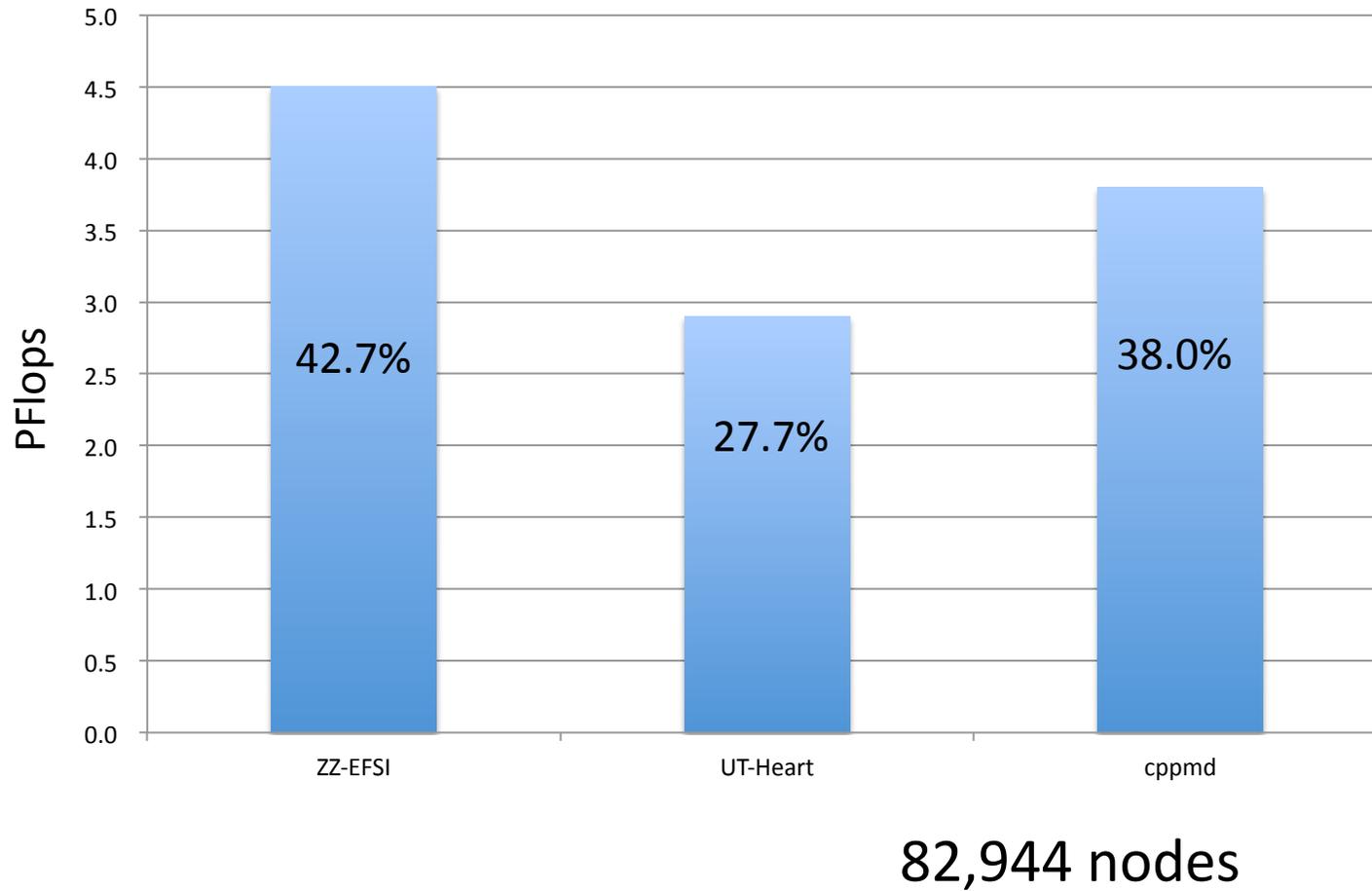
Full system of K (about 83,000 nodes)



11/31 show good scalability
over 10,000 nodes

2011/10/30

Measured performance on K computer using full system



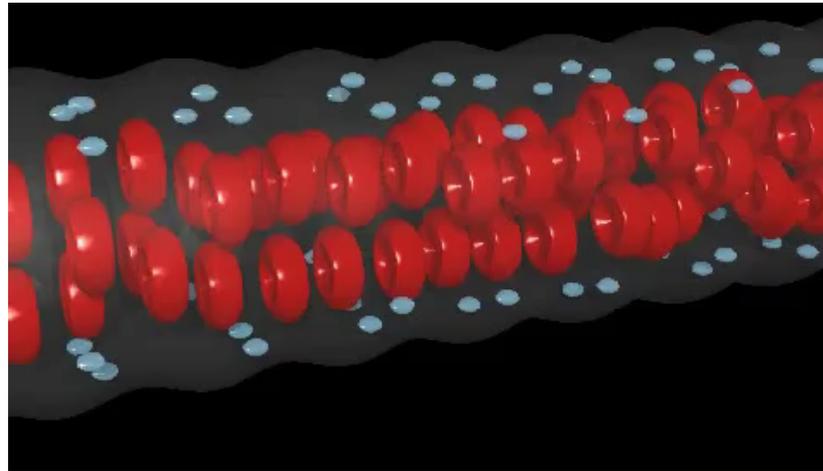


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Multi-scale simulation of clotting



Blood flow simulation including huge number of red blood cells and platelets

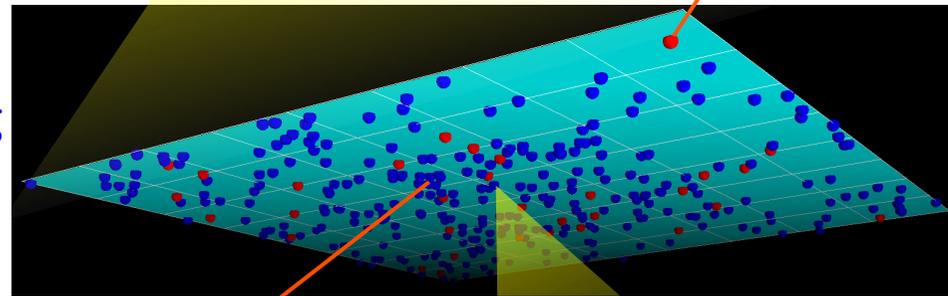


vessel wall

red blood cell

platelet

Dynamic Monte Carlo simulation of connecting between platelet and vessel wall



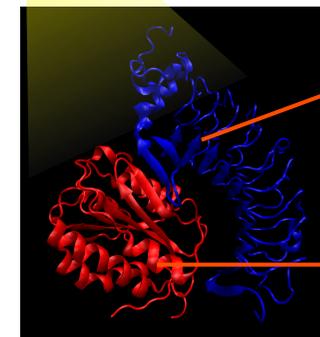
GPIb α -vWF bond

GPIb α

Current status : capillary scale

K will make it possible to simulate **coronary arteries** in a few milli-meter

MD simulation of interaction between ligand and receptor



GPIb α N-terminal

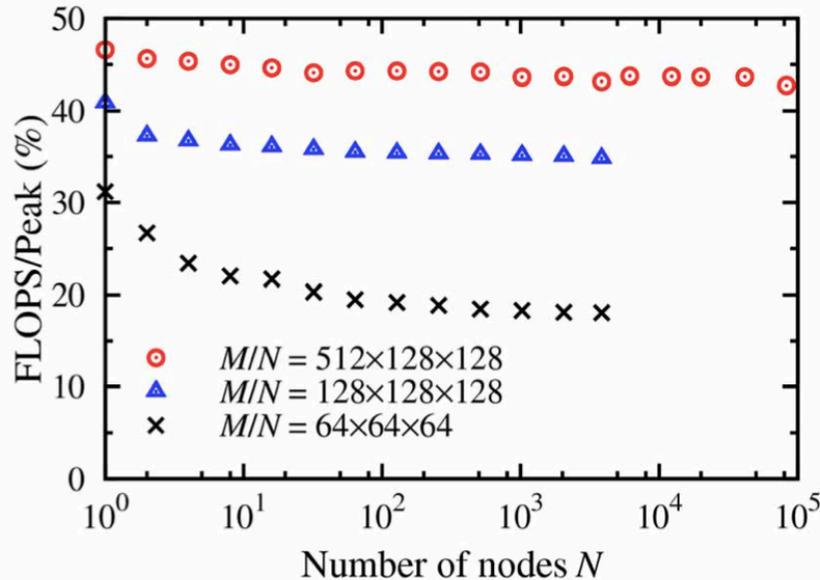
vWF A1 domain



Weak Scaling on K: ZZ-EFSI



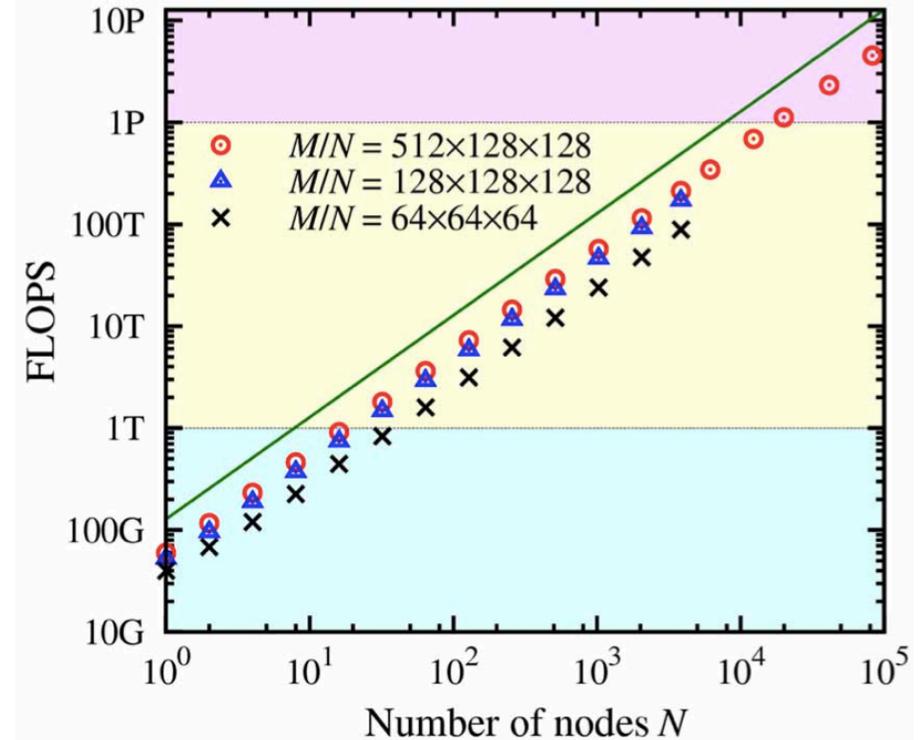
weak scaling (実効性能)



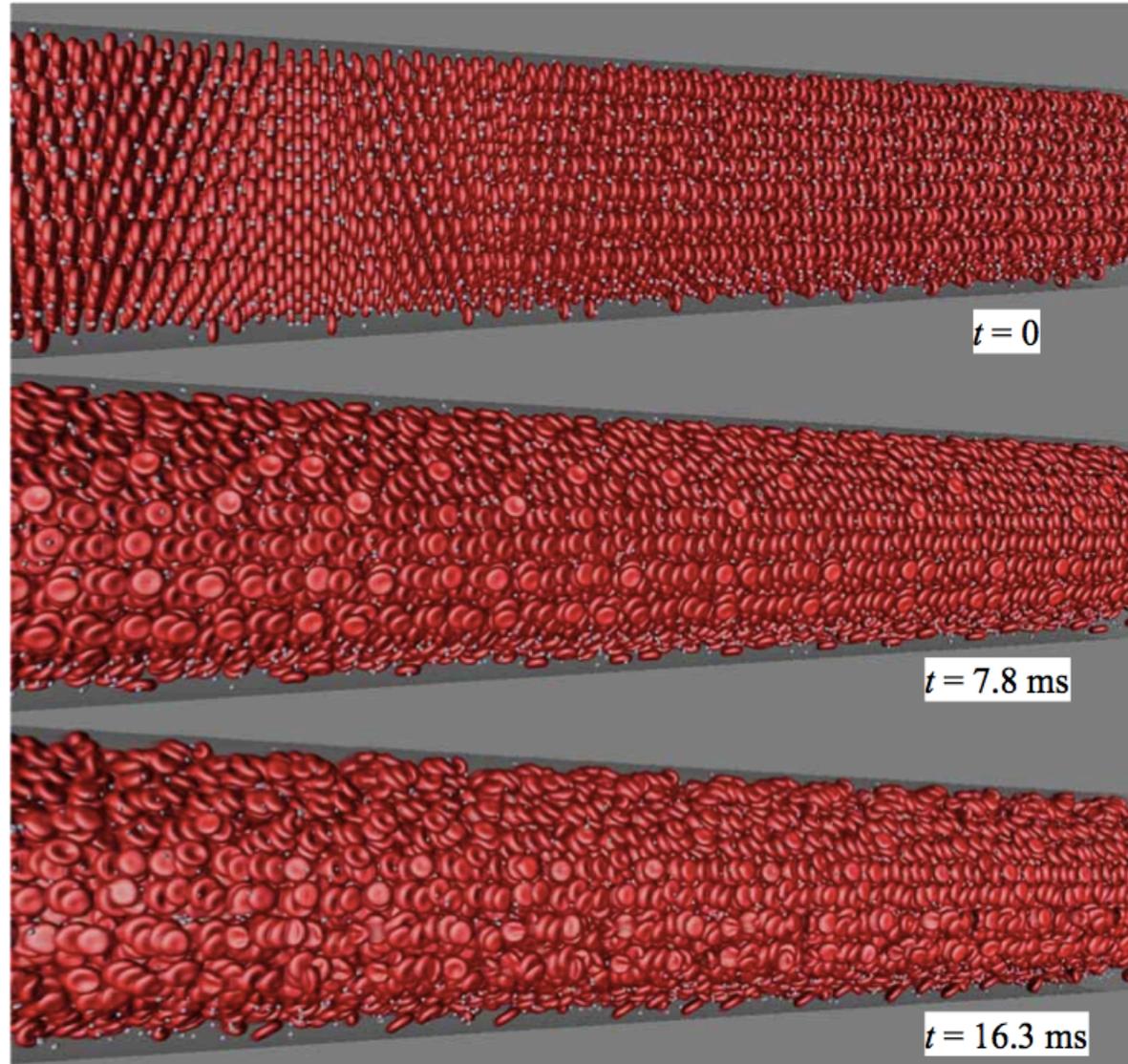
Changing solvers in ZZ-EFSI

- Using FFT to solve Poisson equation on PC
- Multi-color SOR on PC Cluster
- On K computer which has 80,000 CPUs
Implicit solver \rightarrow explicit solver using quasi-compressible formulation
less communication

weak scaling (性能)

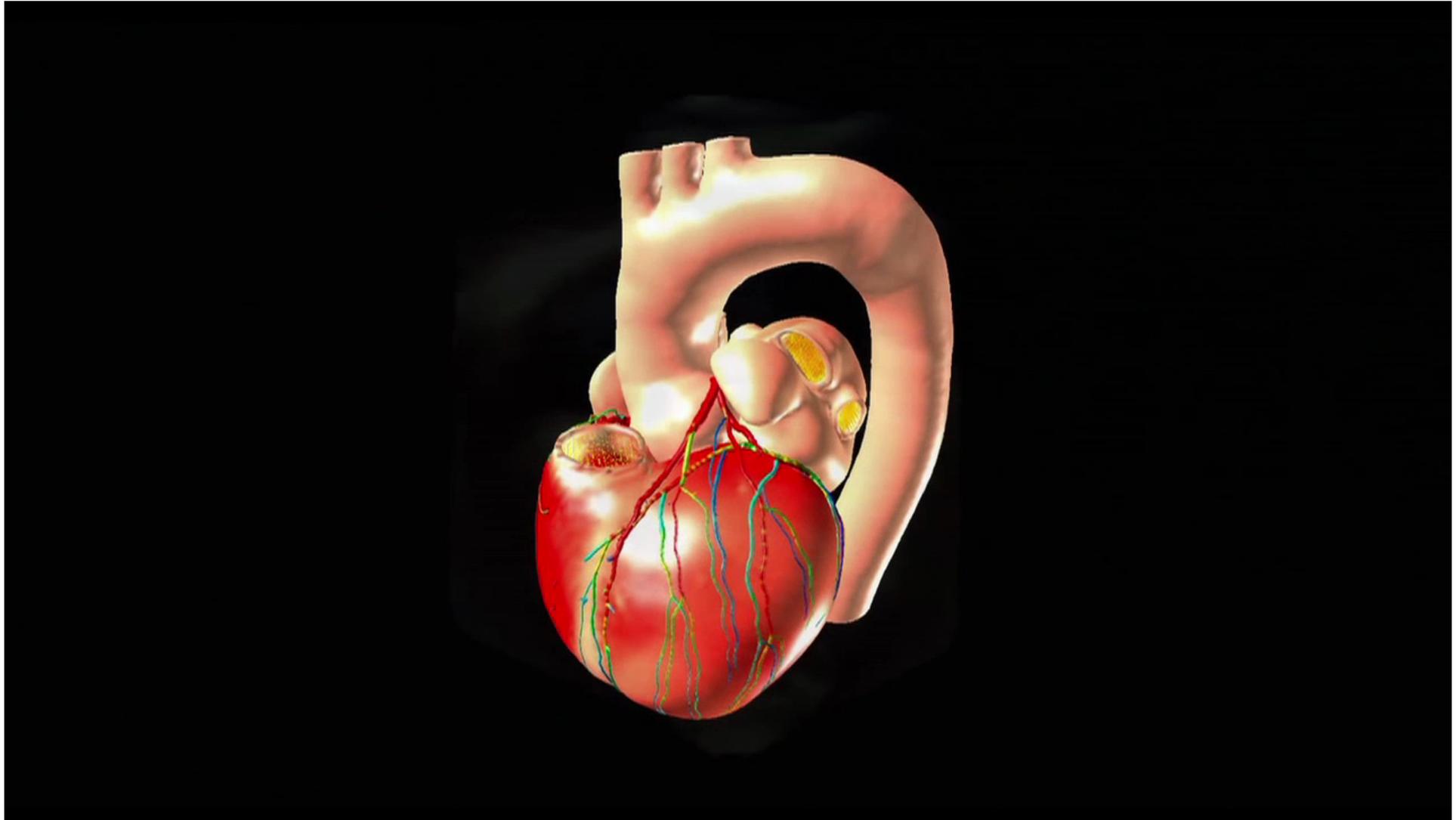


Visualized data:ZZ-EFSI





Heart Simulation

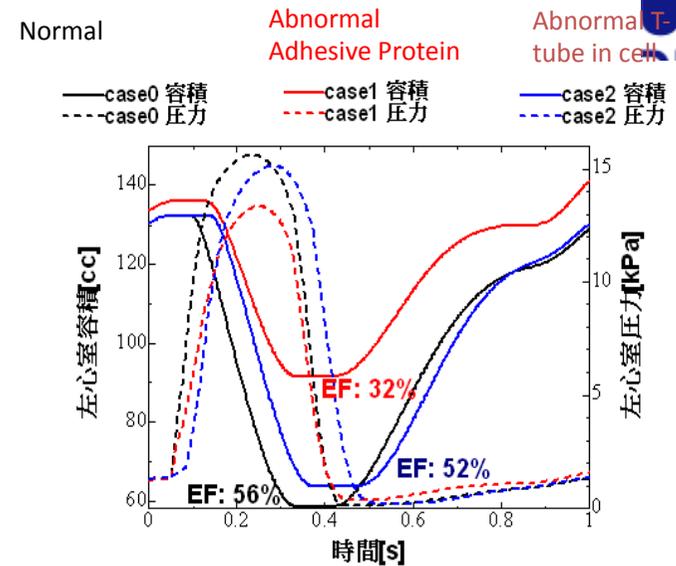
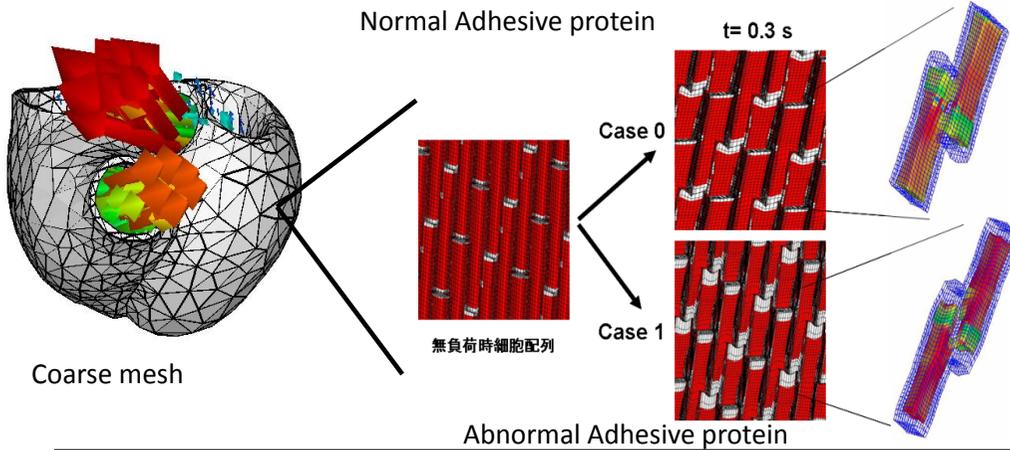




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Multi-scale Heart Simulator: *UT-Heart*

Simulation on RICC 8,000 cores



K-computer will enable us to simulate

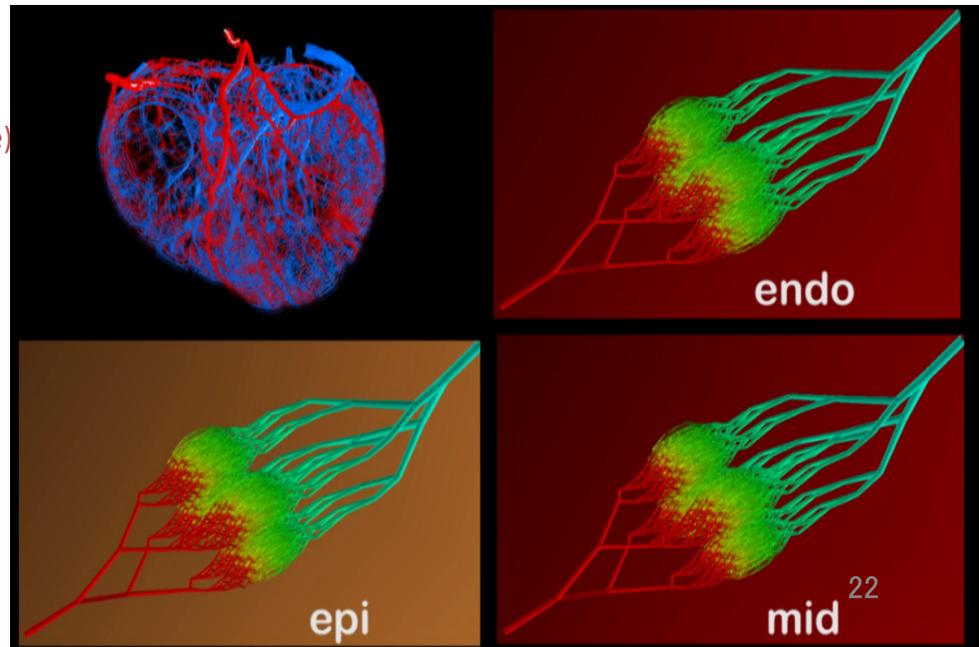
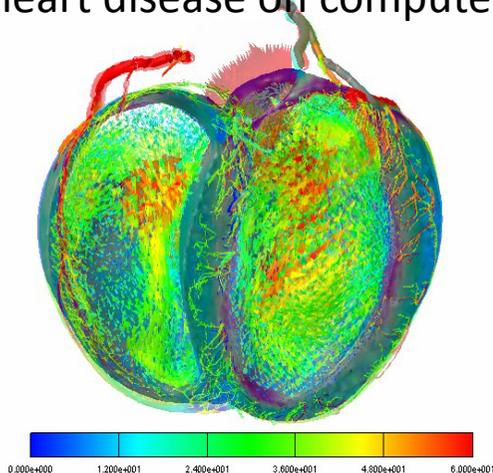
- 1) Coronary artery circulation with capillary
 - 2) Metabolism in cell
- to realize ischemic heart disease on computer

Normal condition : Blood from aorta reaches capillary bed in 4 beats

Simulated movie shows sudden occlusion causes shortage of Oxygen first then shortage of ATP

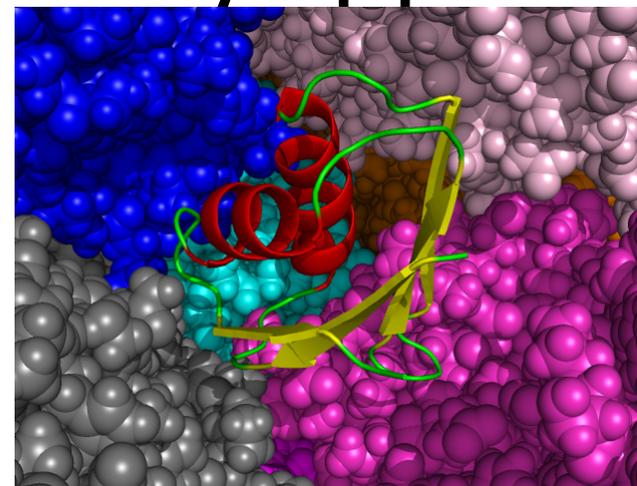
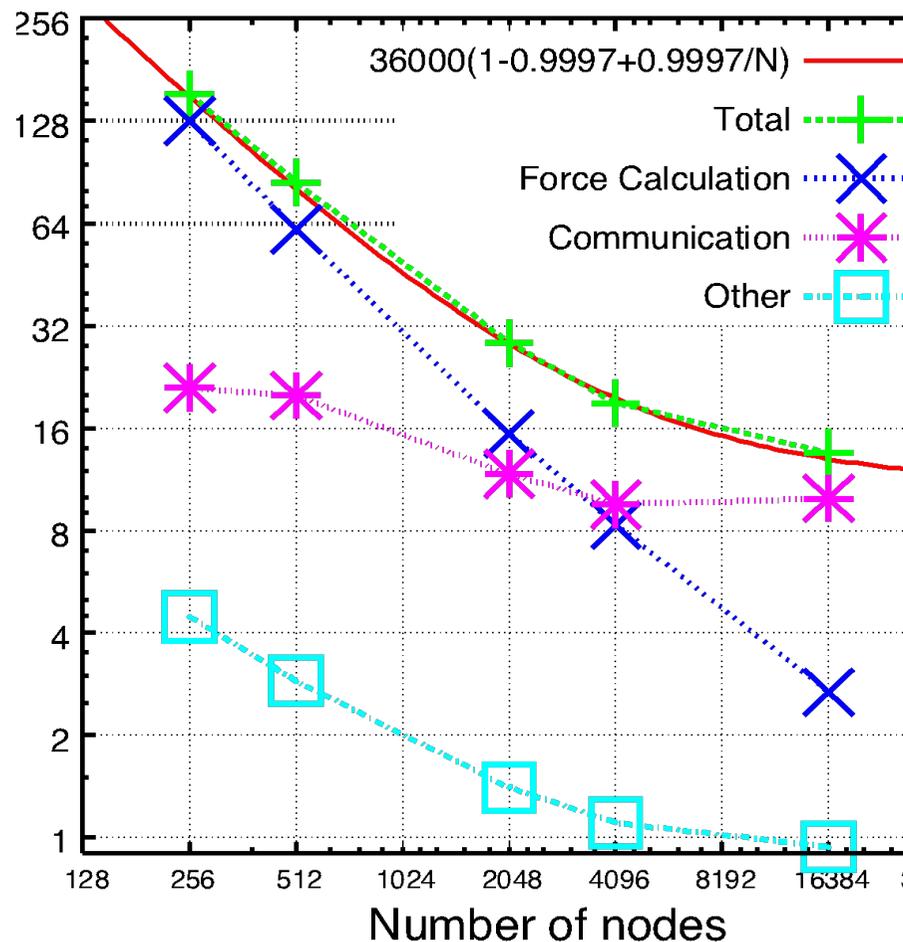
Color indicates compression force. 縮力を表す

Visualized by Fujitsu



Occlusion (blockade)

Strong scaling shown by cppmd



Model	432 <i>in vitro</i>
Number of atoms	180,881,424
Cutoff radius	28 Å + 2 Å margin
Number of pairs per atom	8,835(+ 2,031 in margin)
FLOP counts for 1,000 steps	202,851,990,144 MFLOP
Topology of computation node	24 × 24 × 48
Number of nodes	27,648
Number of cores	221,184
Theoretical peak performance	3.539 PFLOPS
Calculation time for 1,000 step	154.29 sec
Sustained performance	1.315 PFLOPS
Efficiency	0.3716

This computation was performed under special operation to accelerate grand challenge projects in both nano and life sciences

Measured in March, 2011

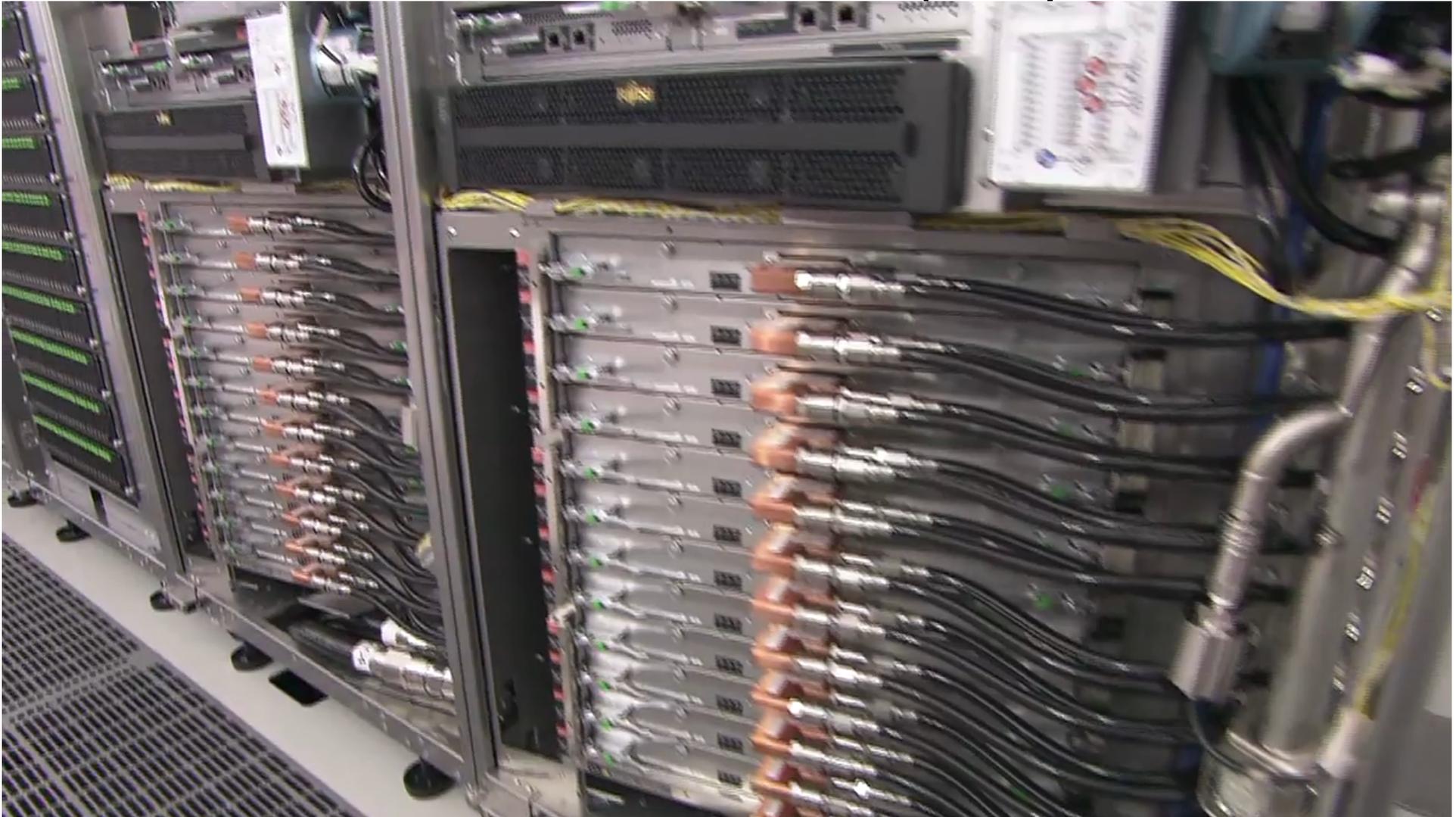


Molecular Dynamics Simulation Code: cppmd



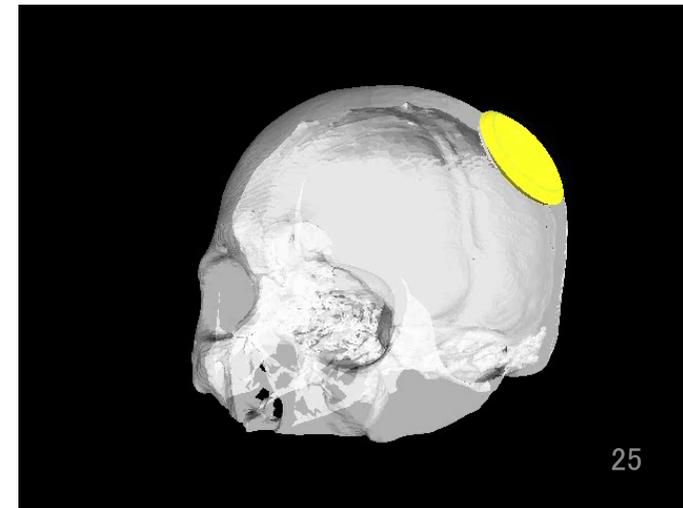
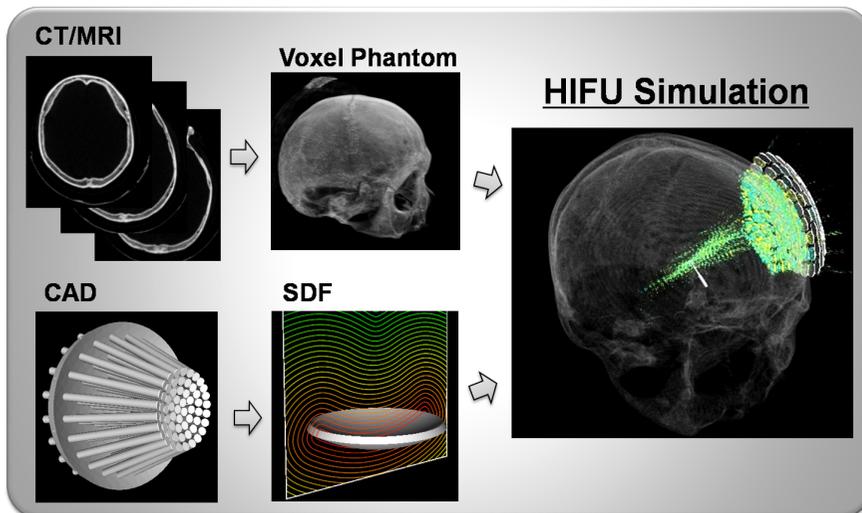
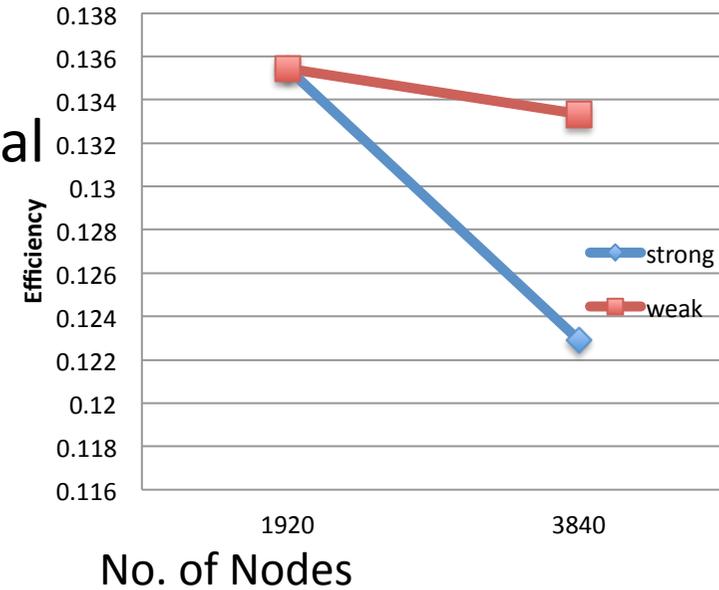
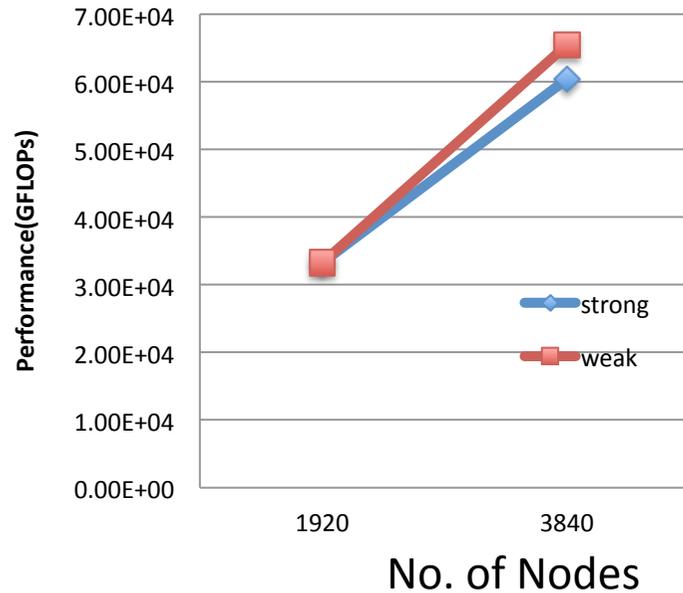
- Designed for K computer

- Achieved about 50% of theoretical peak performance



Scalability of ZZ-HIFU

0.3Pflops using
12,288 nodes
21% of theoretical
peak

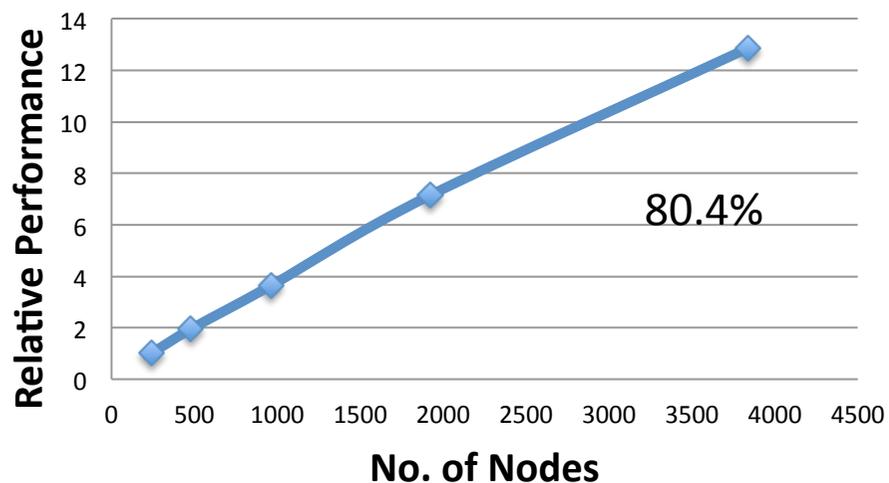




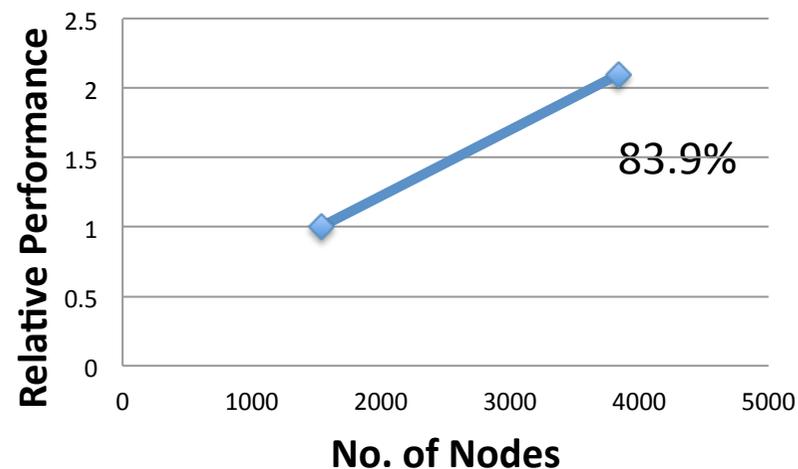
Scalability of some codes on K



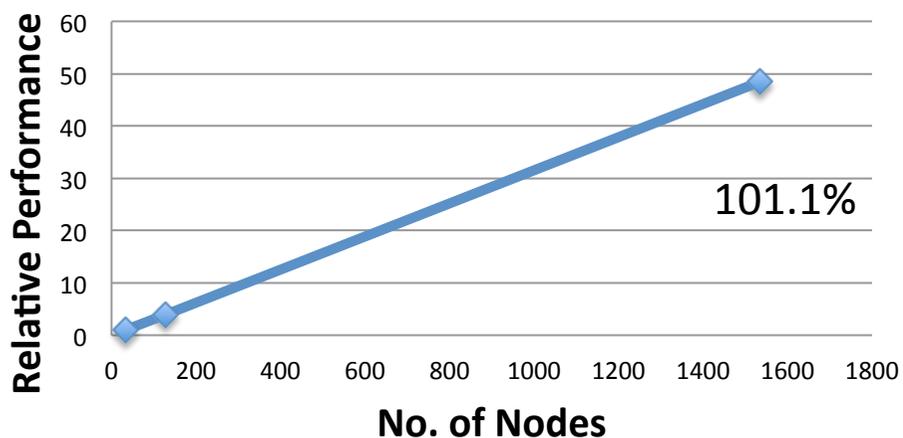
cppmd



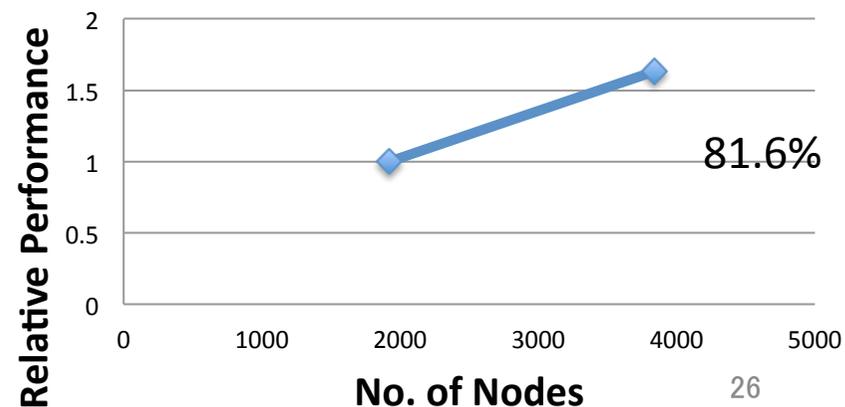
SiGN-BN



LiSDAS



IOSSIM





Some difficulties at this moment



- Several important software has been not supported yet
 - This makes porting difficult in some cases
- SIMD optimization in case of C/C++ code is less strong than that in case of FORTRAN
- Remote access is not available

gradually improving...



Summary



- K has been very stable and powerful although it was a new design and at the very early stage.
- Several codes have already shown very high effective performance on K.
- Scalability on K shows very good.
 - Effective neighboring network TOFU and ICC.
- c/c++ compiler needs more improvement (SIMD optimization)
- Need more libraries to be supported and optimized on K computer
- Computation time of application is getting longer and longer to get better scalability on peta-scale system. This may make design of Exa-scale system more difficult.
- All results on K computer have been measured as trial use and K is still on developing and testing stage.