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shaping tomorrow with you

Applications for PRIMEHPC FX1000/FX700

November 17, 2020

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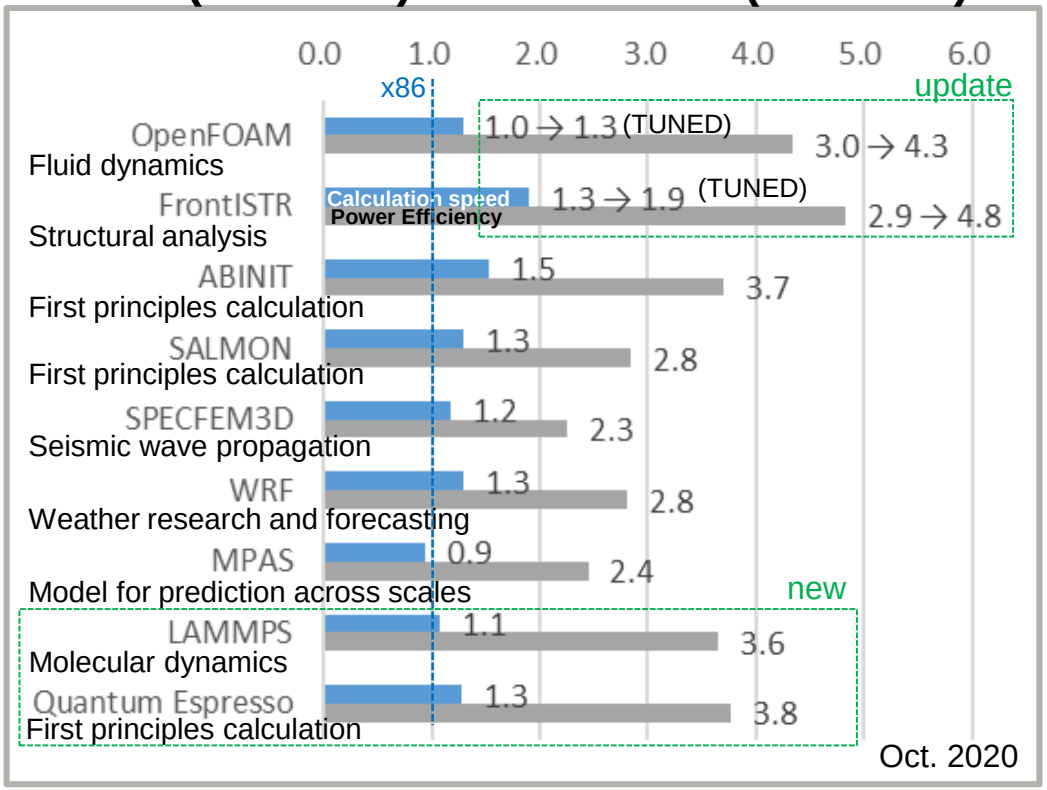
FX1000 (48 cores) vs x86 server (48 cores)*



LAMMPS performance is preliminary result which is by Fujitsu compiler to be released in 2021/1Q.

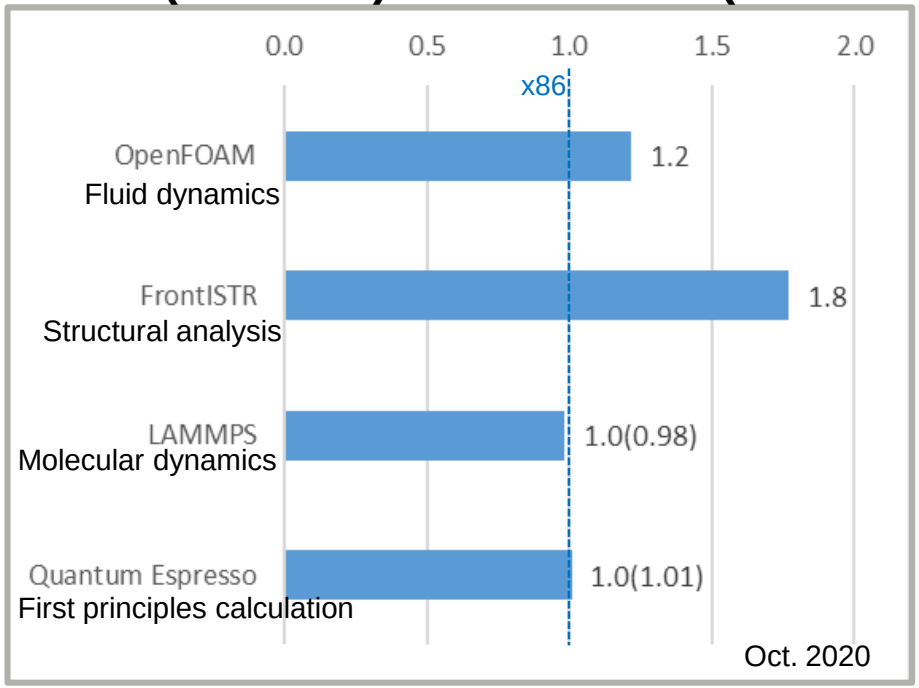
- Xeon and A64FX with the same number of cores*
  - Up to 1.9 times faster
  - Up to 4.8 times lower energy

*A64FX on FX1000: 48 cores ×1 CPU (2.2 GHz)
Xeon Platinum 8268: 24 cores ×2 CPU (2.9 GHz)

- Performance improved by
  - Enhanced microarchitecture (SVE and HBM)
  - Energy-saving design & implementation
- LAMMPS and QE performance are newly added.
- OpenFOAM and FrontISTR performance are improved by tuning and compiler enhancement in SIMD instructions.

OSS Application Performance Results on FX700

FX700 (48 cores) vs x86 server (48 cores)*



LAMMPS performance is preliminary result which is by Fujitsu compiler to be released in 2021/1Q.

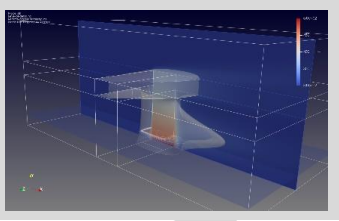
FX700

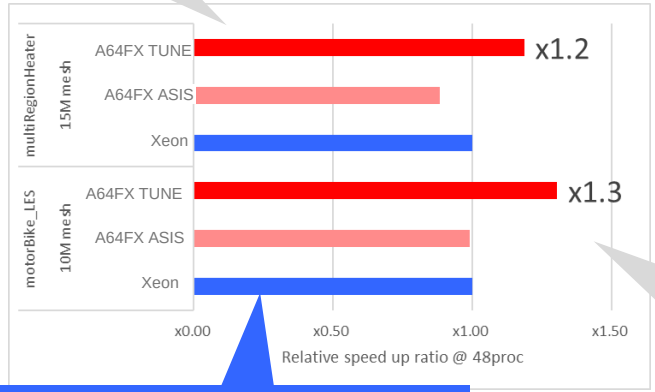
- FX700: rack mount type and air-cooling machine
- We evaluate the application performance of four OSS applications used for manufacturing and material science.
- FX700 has reasonable performance of these applications in comparison with that of FX1000.

*A64FX(FX700) : 48 cores ×1 CPU (2.0GHz)
x86 server : Xeon Platinum 8268(24 cores,2.9GHz) × 2CPU

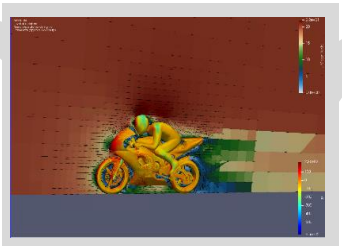
OpenFOAM

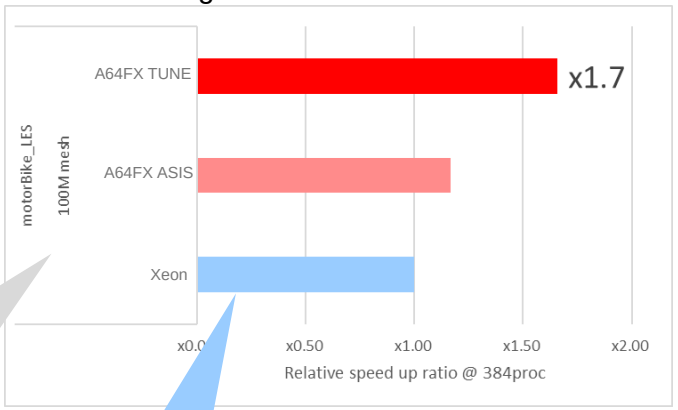
- Open-source CFD software which can execute various fluid dynamics simulation, including thermal conduction and turbulence analysis
- Conditions in the performance measurement
  - Version: OpenFOAM-V1812
  - multiRegionHeater :15M mesh, thermal transport through multiple solid and fluid
  - motorBike LES :10M mesh, flux around running motorbike
  - motorBike LES(Large model) :100M mesh, flux around running motorbike





Intel(R) Xeon(R) Platinum 8268 CPU @ 2.90GHz





Intel(R) Xeon(R) Platinum 8260M CPU @ 2.40GHz

- A64FX has similar performance to Xeon with asis code. Better performance is obtained by tuning.
- Similar performance between thermal-fluid and aero-dynamics are obtained.

Even if the model size is large, A64FX keeps performance better than Xeon.

LAMMPS

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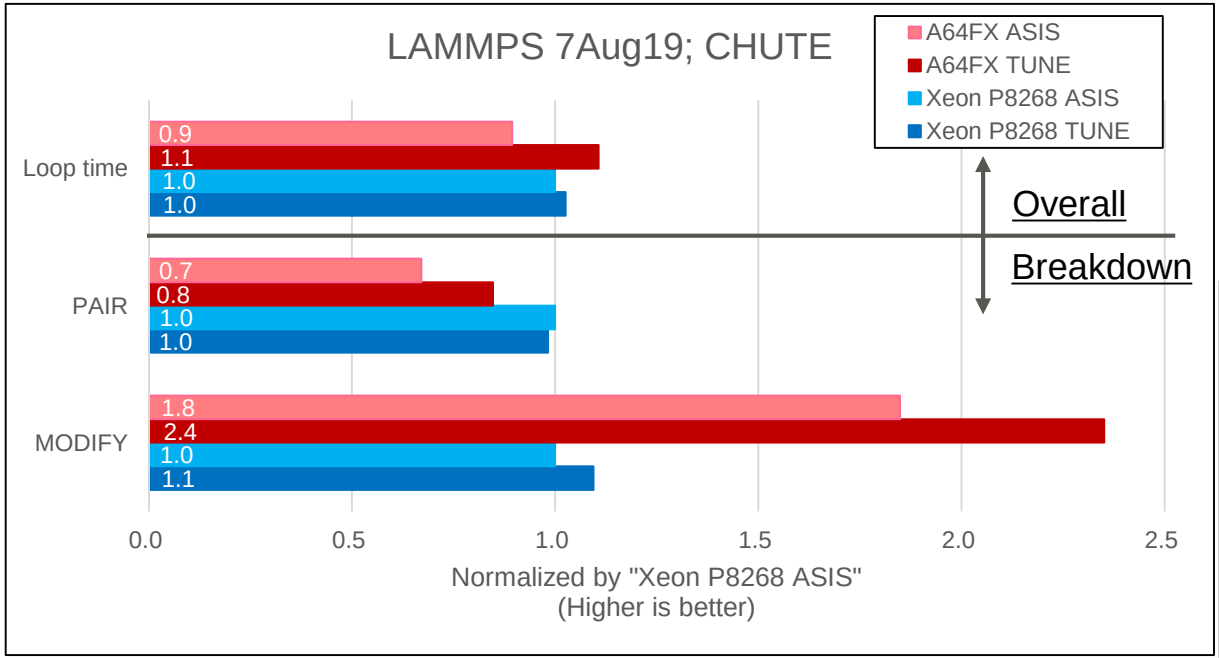
- A64FX performance for LAMMPS
  - By tuning two sections, "PAIR" and "MODIFY“, which account for 90% of *Loop time*, the performance on A64FX has been achieved 1.1x faster than Xeon P8268.



- LAMMPS 7Aug19 (USER-OMP)
- Problem system for this performance measurement:
  - Granular chute flow with frictional history potential
  - 12,800,000 atoms for 100 timesteps
  - NVE time integration

Performance Tuning:

- Best compiler options
- SIMD optimization
  - Compiler pragma, Change data layout
- Efficient data access
  - Prefetch, Data alignment

SIMD and large memory bandwidth enhance the tuning effect on A64FX.

LAMMPS performance is preliminary result which is by Fujitsu compiler to be released in 2021/1Q.

Quantum ESPRESSO

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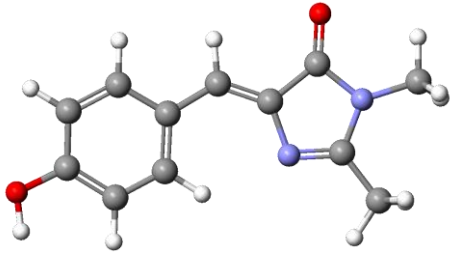
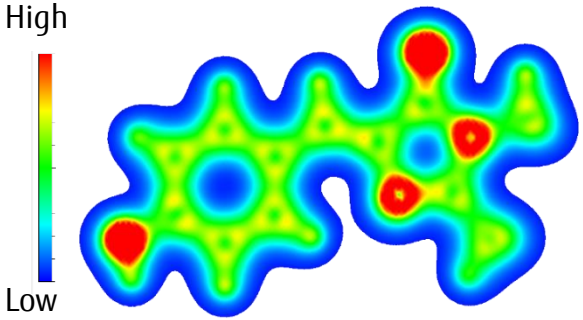
- A64FX performance measurement for Quantum ESPRESSO 6.4.1
  - First Principles Calculation

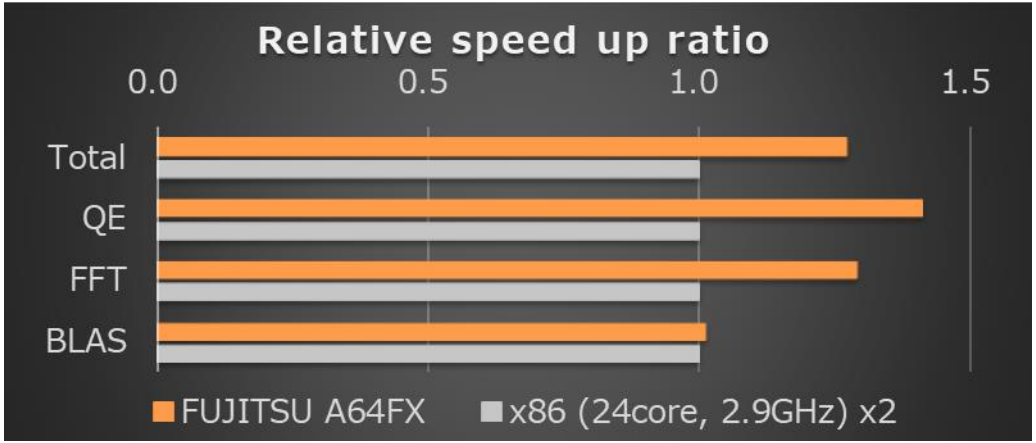


Molecular Geometry



Calculation of Electron Density

- A64FX has 1.3x faster over the latest x86 processor (24 core, 2.9GHz) x2 in structural optimization simulation
  - QE[*1] :1.4x faster by high memory b/w and using SIMD instructions
  - FFT[*2] :1.3x faster by long data-length and using SIMD instructions
  - BLAS[*3]: Equivalent performance by using cache and SIMD instructions

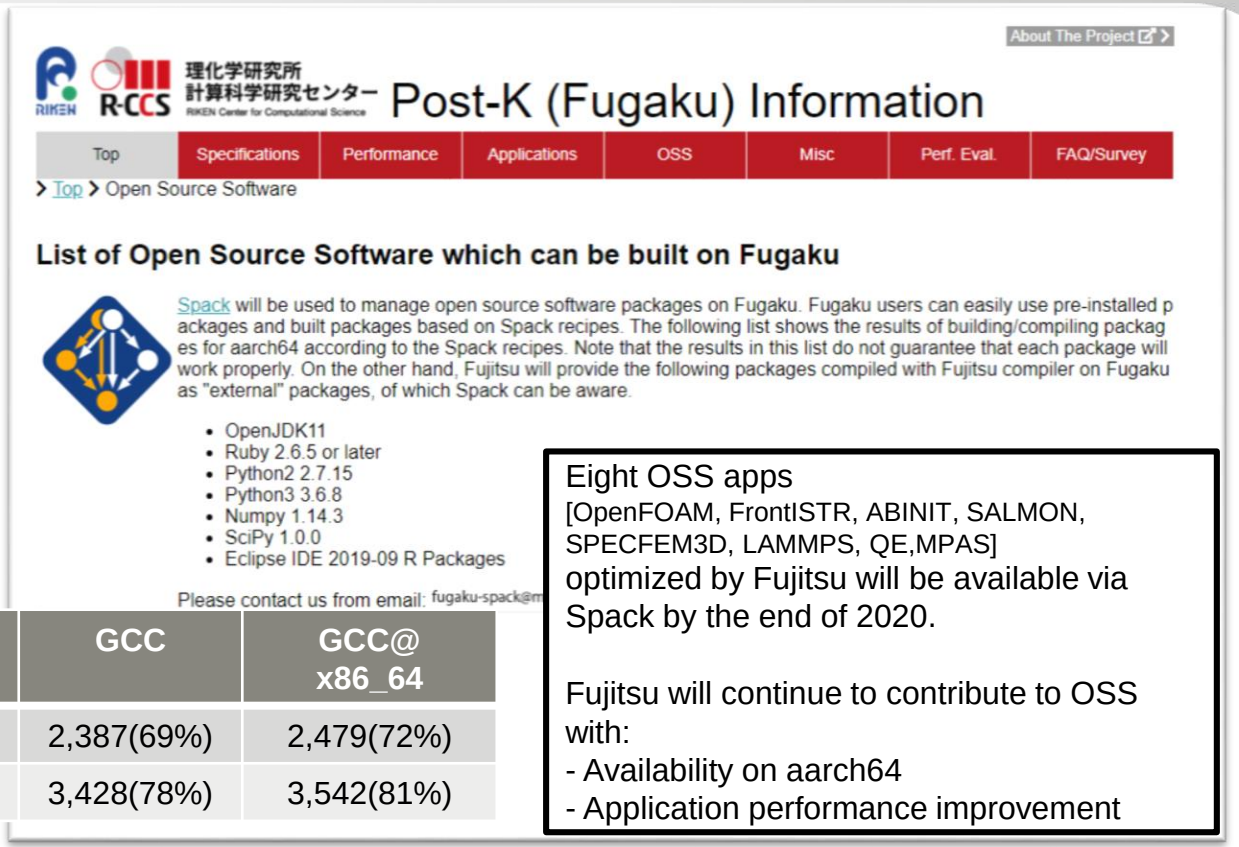


*Input-data: Structural Optimization Simulation (SCF calculation),
Based on QEF/benchmarks/small-benchmarks/test_1.in, 224 atoms

*1:ELPA used for deriving eigenvalue *2: FFTW3 Library tuned by FUJITSU *3: FUJITSU SSL Ⅱ Library

Line-up of OSS on aarch64 with Spack

- RIKEN and Fujitsu are maintaining OSS packages to be built / compiled for *aarch64.*
- Over 3000 OSS are built successfully for A64FX and close to x86.



Time	Reg. packages	Fujitsu compiler	GCC	GCC@ x86_64
SC19	3,451	2,072(60%)	2,387(69%)	2,479(72%)
SC20	4,335	3,194(73%)	3,428(78%)	3,542(81%)

Eight OSS apps
[OpenFOAM, FrontISTR, ABINIT, SALMON, SPECFEM3D, LAMMPS, QE,MPAS]
optimized by Fujitsu will be available via Spack by the end of 2020.

Fujitsu will continue to contribute to OSS with:
- Availability on aarch64
- Application performance improvement

OSS packages include applications, middlewares, libraries.

https://postk-web.r-ccs.riken.jp/oss/public/ captured on Oct. 8th, 2020

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Commercial Applications

Commercial Applications

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- Fujitsu works with vendors to make commercial apps available for FX1000, also for FX700 and Fugaku with binary compatibility.

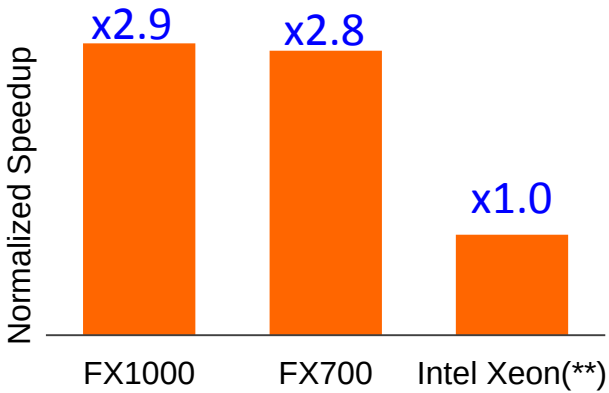
Available	In a research & development phase (as of November 2020)
Engineering (Structural analysis, Fluid dynamics and Electronics)	
Available in Q4 '20: LS-DYNA (by Ansys)	ADVENTURECluster (by Allied Engineering Co.)
	Altair Radioss™ (by Altair Engineering, Inc.)
	Ansys Fluent (by Ansys)
Now available: Poynting (by Fujitsu Limited)	CONVERGE CFD SOFTWARE (by Convergent Science)
	HELYX® (by ENGYS Ltd. & VINAS Co., Ltd.)
	JMAG® Simulation Technology for Electromechanical Design (by JSOL Corporation)
Chemistry*	
Now available for FX1000: Amber	Marc (by HEXAGON, MSC Software)
Gaussian16 (by Gaussian, Inc.)	scFLOW (by HEXAGON, Cradle)
	Simcenter STAR-CCM+ (by Siemens Industry Software Inc.)
	VASP
	VPS (PAM-CRASH) (by ESI Group)

*Collaboration with Australian National University

**All application names used in this slide are trademarks or registered trademarks of their respective venders.

Poynting

- ***Poynting*** is electromagnetic wave analysis software based on FDTD* method developed by Fujitsu.
- ***Poynting*** is extremely advantageous electromagnetic wave analysis software on ***FX1000*** and ***FX700***, because the FDTD* method provides massive parallel efficiency while requires memory bandwidth.
- Poynting is available for ***FX1000*** and ***FX700***, and will be evaluated on ***Fugaku*** in this fiscal year.



Poynting solver performance on one node
(Dipole antenna model, 125 million cells)

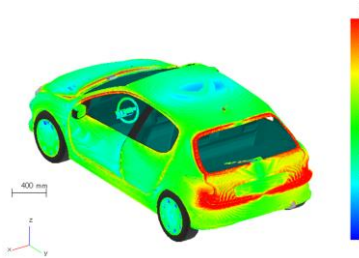
* FDTD : finite difference time domain
** Intel Xeon Platinum 8268 (2.9GHz, 24core) x 2sockets

Challenge on ***Fugaku***

Ensuring safety at intersections with autonomous driving via simulation:
- ✓ Performance prediction of vehicle to vehicle(V2V) and vehicle to infrastructure(V2I) communications.
- ✓ Electro-magnetic compatibility(EMC) evaluations for V2V and/or V2I communication systems.

Current leading-edge Customer:
- ✓ Analysis of a single vehicle.
- ✓ Billions cells / Thousands parallels.

Fugaku:
- ✓ Analysis of real road situation.
- ✓ 10 **Trillions** cells / Several millions parallels.



Result form a single vehicle simulation.

Scale up
With Fugaku

We will start with a feasibility study.

Computational Domain: 120m x120m x 12m
Estimated Calculation time: **a Few Hours *on Fugaku***

CONVERGE

About ***CONVERGE***

- ✓ CFD software featuring truly autonomous meshing.
- ✓ Geometries are allowed to move complexly or even interactively with fluid.
- ✓ More information : https://convergecfd.com
  https://www.idaj.co.jp/product/converge/ (in Japanese)

Current Status of Porting ***CONVERGE*** on ***FX1000***

- ✓ Working on ***FX1000.***
- ✓ Max 6 million cell model & max 1536 parallel running was evaluated.
- ✓ Verified all features of ***CONVERGE***

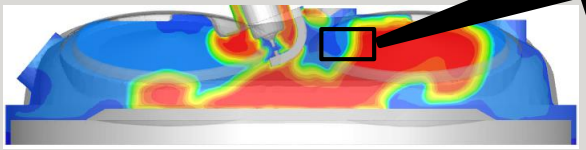
Challenges on ***Fugaku***

We started evaluation of ***CONVERGE*** on ***Fugaku*** this November.
We will run a high-fidelity large eddy simulation of in-cylinder combustion, against which customers can validate the results of reduced-complexity simulations.

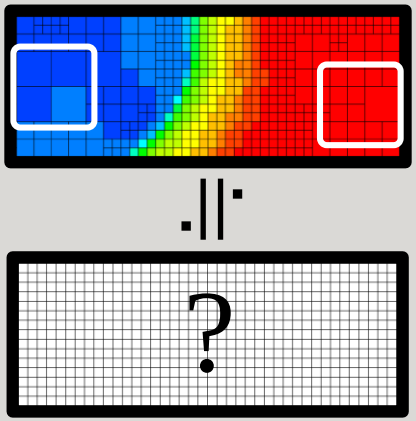
[Evaluation plan up to March 2021]

Target	In-cylinder combustion
Mesh number	> 2 Billion
Turbulence model	LES
Combustion model	Detailed Chemistry
Walltime per cycle	12 hours (Estimated)
# of Parallel	25,000

CONVERGE includes models and options (e.g., AMR) to reduce complexity.



How can we evaluate the effect of these options on simulation results?



About *JMAG*

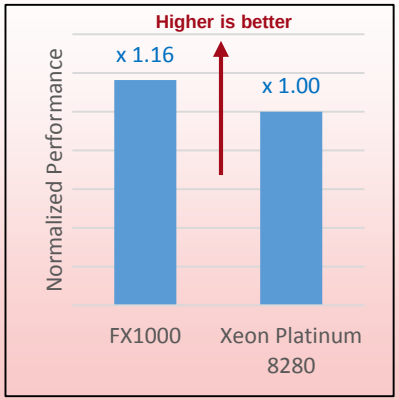
- ✓ Commercial software for electric device design and development. Developed & provided by **JSOL Corporation**.
- ✓ Used in various industries (automotive, electric appliances, digital equipment, electric power equipment, factory automation, etc.)
- ✓ More information : https://www.jmag-international.com/

Current status of porting *JMAG* on *FX1000*

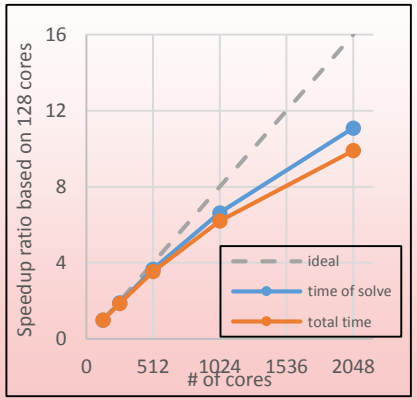
- ✓ Max 20 million element model & max 2,048 hybrid parallel was evaluated.
- ✓ Verified all major features of ***JMAG HPC solver***

Preliminary results of ***JMAG*** on ***FX1000***

- ✓***JMAG*** performance on ***FX1000*** is 1.16 x faster than Xeon Platinum 8280 2.7GHz
- ✓***JMAG***'s scaling up to 2,048 parallel was measured on ***FX1000***



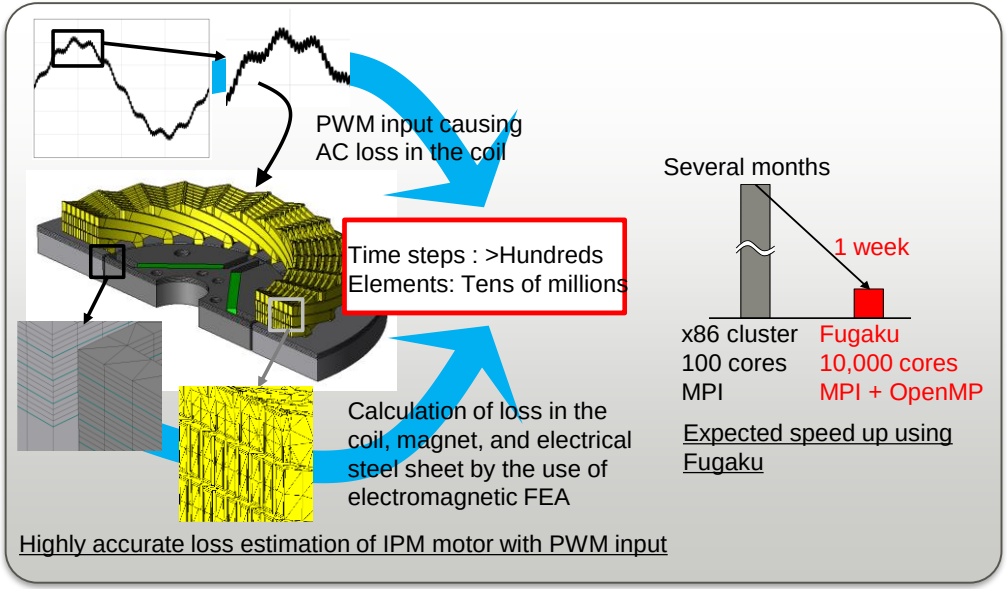
Performance of JMAG (IPM motor with sinusoidal wave input, 10 million elements, 50 steps, 128 hybrid parallel)



Scalability of JMAG on FX1000 (IPM motor with sinusoidal wave input, 10 million elements, 50 steps)

Challenges on *Fugaku*

- ✓ To validate highly accurate loss estimation of IPM motor with PWM input in practical time, we started evaluation of ***JMAG*** on ***Fugaku*** from this November.



scFLOW

About ***scFLOW***

- ✓ **Commercial CFD** software with **Multiphysics** and **General Purpose** Capabilities
- ✓ Used in Various **Industries** (aerospace, automotive, construction, electronics, heavy manufacturing, medical and pharmaceutical, etc.)
- ✓ More information : https://www.mscsoftware.com/product/scflow

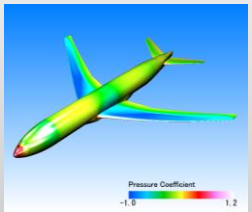
Purpose of using HPC

Accuracy :
- ✓ Advanced analysis of turbulence (LES, DNS)
- ✓ High resolution of shape
- ✓ Transient analysis

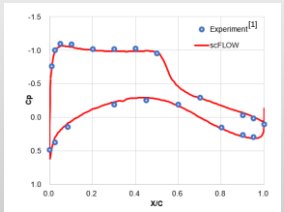
Complex physical phenomenon :
- ✓ Aero-acoustic
- ✓ Cavitation
- ✓ Fluid-Structure Interaction(FSI)
- ✓ etc.

Current status of porting **scFLOW** on **FX1000**

Results on ***FX1000***:



Surface pressure coefficient distribution



Cp distribution on the wing

Aerodynamics of Transonic Flow around Aircraft
- ✓ Model : NASA-CRM (Common Research Model)
- ✓ Mach number : 0.847
- ✓ Attack angle : 2.94 [deg]

[1] Third Aerodynamics Prediction Challenge (APC-III), JAXA-SP-17-001.

Achievement :
- ✓ Working on ***FX1000***
- ✓ Max 80 million elements
- ✓ Max 1536 parallel
- ✓ Verified all physical features of ***scFLOW***

Goal in Q4 '20 on ***Fugaku***:
- ✓ NASA-CRM
- ✓ 200 million elements
- ✓ 20,000 parallels
- ✓ Hundreds nodes
- ✓ 10,000 elements/core

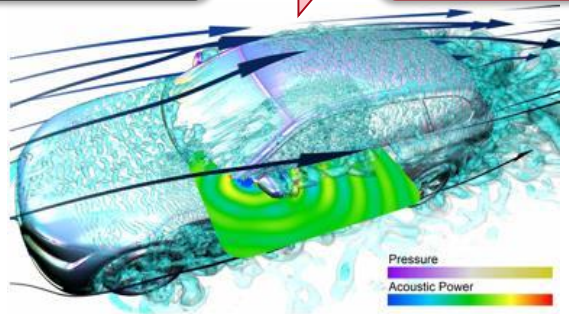
Challenges on ***Fugaku***

- ✓ We started evaluation of **scFLOW** on ***Fugaku*** from this November.

Currently (Major Customer) :
- ✓ Tens of millions elements
- ✓ Hundreds parallels
- ✓ Only CFD

Scale up
× 100
Multiphysics

On ***Fugaku***:
- ✓ Over 1 **Billion** elements
- ✓ Over 100,000 parallels
- ✓ FSI coupling with ***Marc***



CFD by LES and AeroAcoustic analysis

Target Application:
- ✓ Automotive : Aerodynamics / Thermal management of Engine / Wind noise
- ✓ Aerospace : Aeroelasticity using FSI / Aerodynamics for off-design condition
- ✓ Construction : Ventilation in buildings / Wind design around buildings

Apps for Automotive Industry

- Japan Automobile Manufacturers Association (JAMA) starts from second half of FY2020 to try and evaluate leading-edge computer aided engineering for automobile on supercomputer Fugaku with Fujitsu's supports.
- LS-DYNA and VPS, which are used for car crash simulation by automobile companies, will be evaluated on Fugaku

LS-DYNA

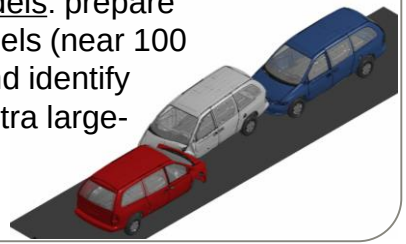
- ✓ LS-DYNA is a general-purpose finite element program capable of simulating complex real world problems.
- ✓ Major features are already validated, and it will be released until Dec. '20 for FX1000 and FX700.

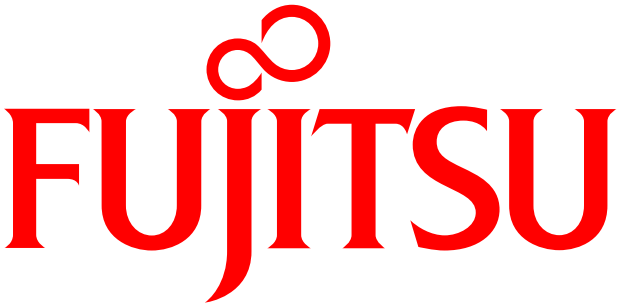
VPS

- ✓ VPS is the world first car crash simulation software and later expanded to the other structural simulations by leveraging its Single Core Modeling concept.
- ✓ Features used in car crash simulation are built and validated on FX1000.

JAMA's plan of using Fugaku (Nov. '20 – Mar. '21)

- ✓ As preparation for the full-fledged use of Fugaku from FY2021, JAMA will evaluate car crash simulation using 100s – 1,000 nodes of Fugaku.
  1. Actual car crash models: evaluate with actual car crash models used by companies participating JAMA and/or large-scale models (more than 10 millions elements)
  2. Ultra large-scale models: prepare ultra large-scale models (near 100 millions elements) and identify issues with solving ultra large-scale models





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