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shaping tomorrow with you

Applications for PRIMEHPC FX1000/FX700

June 24, 2021

Fujitsu Limited

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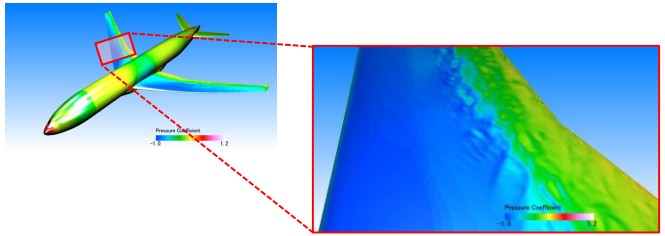

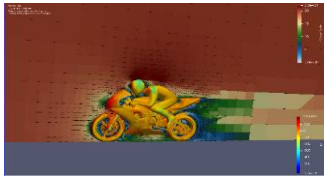

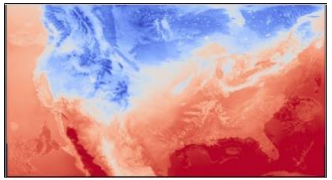

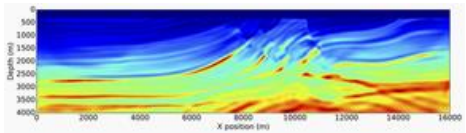

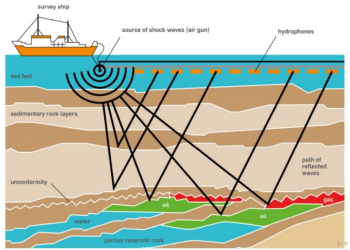

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Commercial Applications

Commercial Applications

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Chemistry

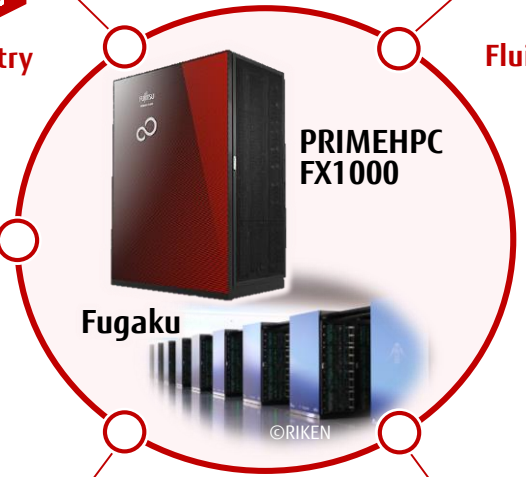
- Amber (by University of California, San Francisco.)
- Gaussian16 (by Gaussian, Inc.)

Fluid dynamics

- CONVERGE CFD SOFTWARE (by Convergent Science)
- Cradle CFD | scFLOW (by HEXAGON / Cradle)
- Fluent (Ansys)
- HELYX (by ENGYS Ltd.)
- Simcenter STAR-CCM+ (by Siemens Digital Industry Software Inc.)

Electromagnetics

- JMAG (by JSOL Corporation)
- Poynting (by Fujitsu Limited)



Structural analysis

- ESI Virtual Performance Solution (VPS) (by ESI Group)
- LS-DYNA (Ansys)

Others

- NAG Fortran Compiler (by nag)

= Already Available
= Available in July' 21 or later
F = Verified on ***Fugaku***
(as of June 2021)

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

Commercial Applications List

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- Availability of commercial applications for FX1000.
  Several applications were already verified on Fugaku.

Categories	Applications	Vendors	Availability	Notes
Engineering (Fluid dynamics)	CONVERGE	Convergent Science (East Asia distributor : IDAJ Co., LTD.)	Available in 3Q '21	Solver components only Verified on Fugaku
	Cradle CFD | scFLOW	Software Cradle Co., Ltd.	Beta ver. in 3Q '21	Verified on Fugaku
	Fluent	Ansys, Inc.	Alpha ver. in July '21	Solver components only
	HELYX	ENGYS Ltd.	Plan to be available *	
	Simcenter STAR-CCM+	Siemens Digital Industries Software, Inc.	Plan to be available *	
Engineering (Structural analysis)	ESI Virtual Performance Solution(VPS)	ESI Group	Available in 3Q '21	Explicit features only Verified on Fugaku
	LS-DYNA	Ansys, Inc.	**Available**	Verified on Fugaku
Engineering (Electromagnetics)	JMAG	JSOL Corporation	Plan to be available *	Verified on Fugaku
	Poynting	Fujitsu Limited	**Available**	Verified on Fugaku
Chemistry	Amber	University of California, San Francisco	**Available**	Collaboration with Australian National University
	Gaussian16	Gaussian, Inc.	**Available**	
Others	NAG Fortran Compiler	Numerical Algorithms Group Ltd	Available for FX700	Will be verified for FX1000 on customer request

*Release date will be announced later. **All application names used in this slide are trademarks or registered trademarks of their respective venders.

CONVERGE

About ***CONVERGE***

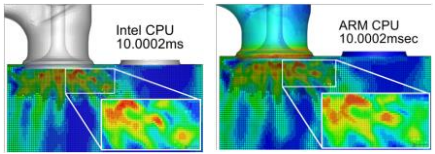
- ✓ CFD software featuring truly autonomous meshing.
- ✓ Geometries are allowed to move complexly or even interactively with fluid.
- ✓ More information : https://convergecfd.com
  https://www.idaj.co.jp/product/converge/ (in Japanese)

Verification and Performance evaluation

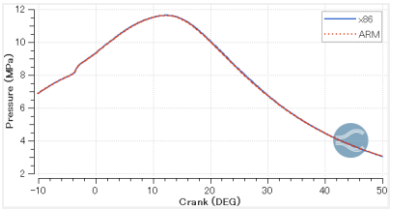
- ✓ Version 3.0.21, or later(Plan)
- ✓ Verified all features of ***CONVERGE*** on ***FX1000***
- ✓ Confirmed parallel scalability over 300 cores on ***Fugaku***
- ✓ Will be available on ***Fugaku/FX1000*** in 3Q, 2021

Challenges on ***Fugaku****

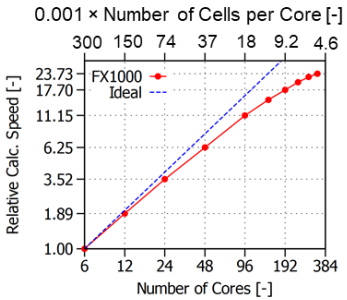
- ✓ Confirmed that the main features and main physical models work normally as well as on x86.
- ✓ Good parallel scalability even in moving surface case and Large-scale calculation enables detailed simulation(LES, detailed chemistry, fine mesh) in short walltime.
- ✓ In-cylinder combustion simulation of Internal Combustion Engine(ICE) aims to evaluate heat release rate, emissions, knocking, etc., and eventually engine performance.
- ✓ It is expected that the knocking prediction becomes more accurate by considering the intermediate species distribution of the knocking reaction caused by detail spatial varieties of temperature and fuel and considering wrinkled flame propagation by LES with fine mesh in whole domain.



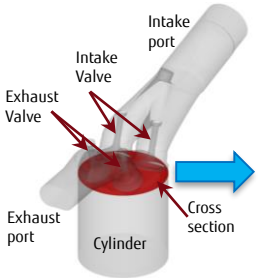
Steady port flow(almost the same results)



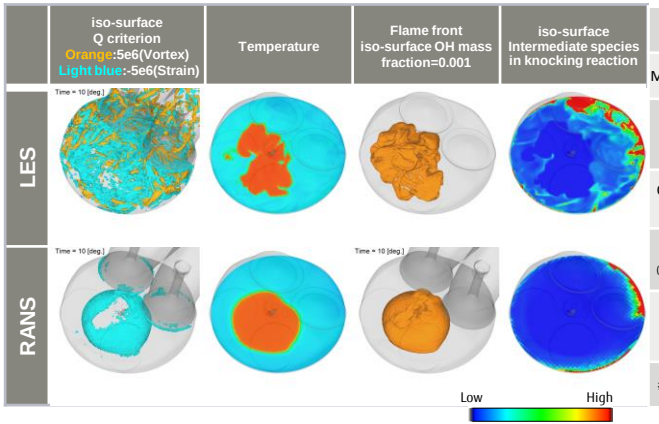
In-cylinder pressure(ICE combustion)



Parallel scalability
(ICE combustion with moving surface)



ICE model

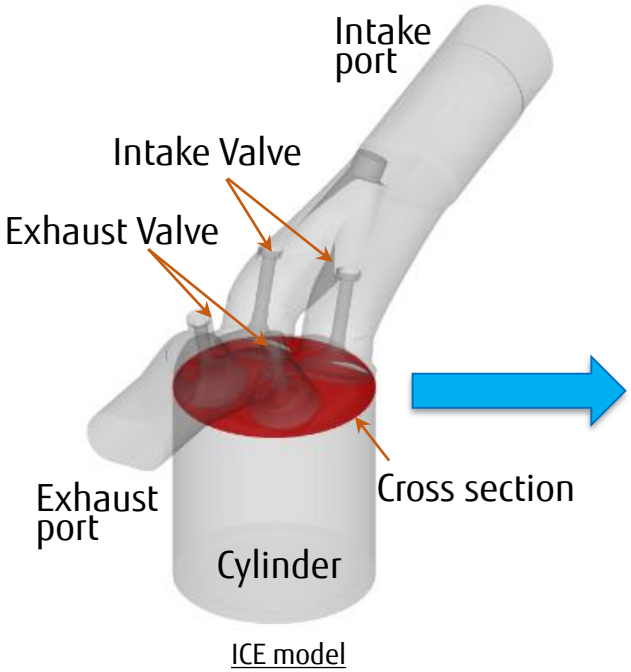


Application	ICE combustion
Mesh number	7 million (max)
Turbulence model	LES
Combustion model	Detailed Chemistry
Walltime (combustion only)	2 hours
Mesh size	0.5[mm] (whole domain)
# of Parallel	4096(max)

ICE combustion results at 10deg. of crank angle

* This work used computational resources of the supercomputer Fugaku provided by RIKEN through the HPCI System Research Project (Project ID: hp200209).

CONVERGE



ICE model

	iso-surface Q criterion Orange:5e6(Vortex) Light blue:-5e6(Strain)	Temperature	Flame front iso-surface OH mass fraction=0.001	iso-surface Intermediate species in knocking reaction
LES				
RANS				

Low High

ICE combustion results from -20 to 140 degrees of crank angle

Cradle CFD | scFLOW

About *Cradle CFD | 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
- ✓ ***Cradle CFD | scFLOW*** beta version will be available for ***Fugaku*** and FX1000 in 3Q '21.

Verification and Performance evaluation

- ✓ Verified all physical features of ***scFLOW.***
- ✓ Improved performance of ***scFLOW*** with a view to large-scale execution in A64FX.

◆ Improved performance of the linear solver of system equation.

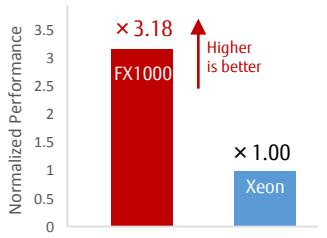


Fig.1 Performance comparison in scFLOW (FX1000 vs Xeon Platinum 8260)

Computational Model :
Aerodynamics of flow around Car. (108 million cells)

◆ Improved parallel performance by implementation of thread parallelization.

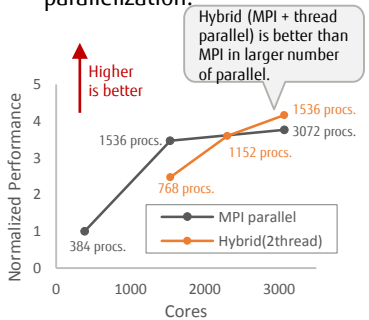


Fig.2 Scalability comparison (MPI vs Hybrid)

Computational Model :
Aerodynamics of transonic-flow around Aircraft. (73 million cells)

Challenges on ***Fugaku****

scFLOW and ***Fugaku*** enable **running a lot of large-scale simulations in a feasible time frame**.

- ✓ 0.2 billion cells of Large-scale LES for unsteady flow around an aircraft
  - ◆ Large-scale LES is important for the evaluation of stability and safety of aircrafts operations by a numerical simulation, especially for off-design conditions.
  - ◆ **Max. 192,000 hybrid parallel / 4,000 nodes** was evaluated.
  - ◆ **The simulation result shows unsteady vortex generation** on the upper surface of wing (Fig.3). The computation for 0.05 seconds in real time was **completed in about 10 hours**.
- ✓ 70 million cells of RANS for steady flow around a car
  - ◆ Steady flow around a car is evaluated to improve energy efficiency when designing cars.
  - ◆ The simulation was **completed in about 1 hour** by 40 nodes (result is Fig.4). It allows that car designers simulate a lot of cases in a feasible time frame.

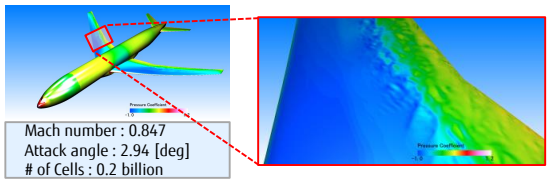


Fig.3 Surface pressure coefficient of aircraft (LES, 12,000procs. x 4threads/1,000nodes, 50,000steps)

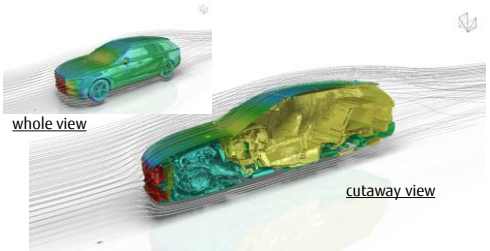
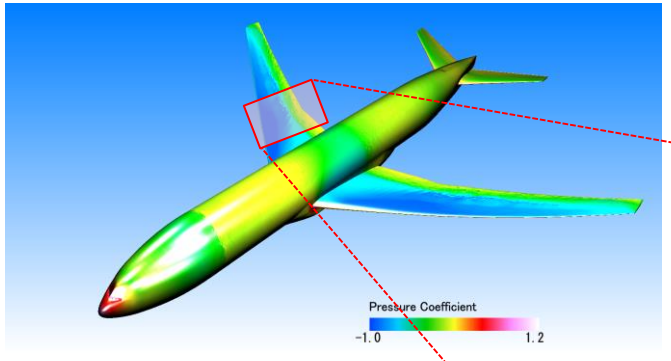
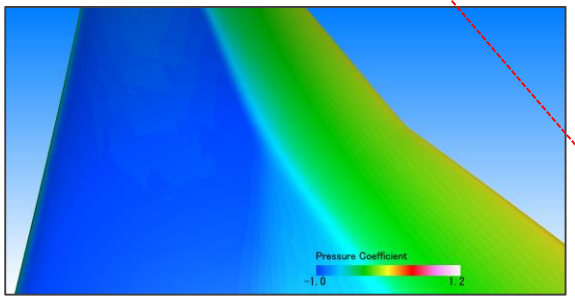


Fig.4 Steady flow around a car (RANS, 960procs./40nodes, 1,000steps)

*This work used computational resources of the supercomputer ***Fugaku*** provided by RIKEN through the HPCI System Research Project (Project ID: hp200209, hp200302).





Aircraft surface pressure coefficient in steady flow for comparison with video on the right
(RANS, 4,800procs. x 1thread / 150nodes, 1,387steps)

Pressure vibration due to fine vortexes, which couldn't be seen in the RANS result, is obtained on the surface of the wing in video on the right.

Aircraft surface pressure coefficient in unsteady flow
(LES, 12,000procs. x 4threads /1,000nodes, 50,000steps)

About *JMAG*

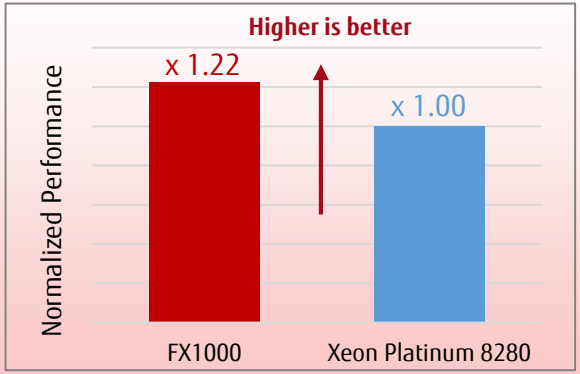
- ✓ Commercial software for electric device design and development. Developed & provided by ***JSOL Corporation***.
- ✓ Used in various industries (automotive, electric appliances, digital equipment, electric power equipment, factory automation, etc.)
- ✓ More information : https://www.jmag-international.com/
- ✓ Plan to be available on ***Fugaku/FX1000***. Release date will be announced later.

Verification and Performance evaluation

- ✓ Max 20 million element model & max 8,192 hybrid parallel was evaluated.
- ✓ Verified all major features of ***JMAG HPC solver***.

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

✓***JMAG*** performance on ***FX1000*** is 1.22 x faster than Xeon Platinum 8280 2.7GHz

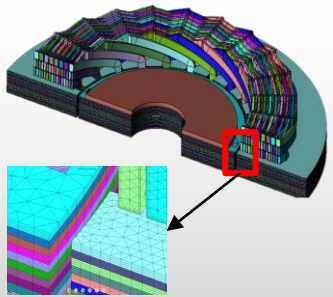


Performance of JMAG (IPM motor with sinusoidal wave input, 10 million elements, 50 steps, 128 hybrid parallel)

Challenges on ***Fugaku****

- ✓ To validate highly accurate loss estimation of IPM motor with PWM input in practical time, we have evaluated ***JMAG*** on ***Fugaku***.

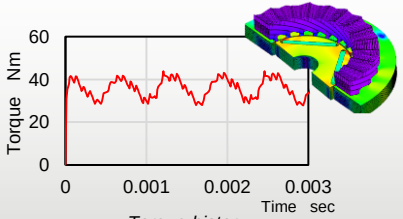
Model



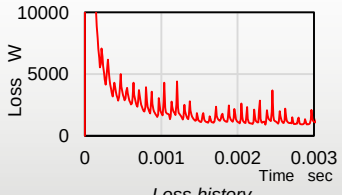
IPM motor with laminated steel sheet modeled one by one, 15 million elements

Results

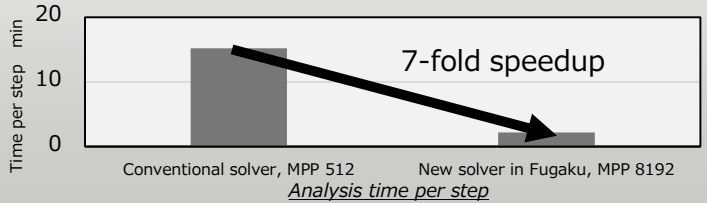
✓Using new hybrid solver in Fugaku, we succeeded in analyzing 332 steps in 8192 parallel, which was 7 times faster than the conventional solver in 512 parallel.



Torque history



Loss history



Analysis time per step

*This work used computational resources of the supercomputer Fugaku provided by RIKEN through the HPCI System Research Project (Project ID: hp200209).

Poynting

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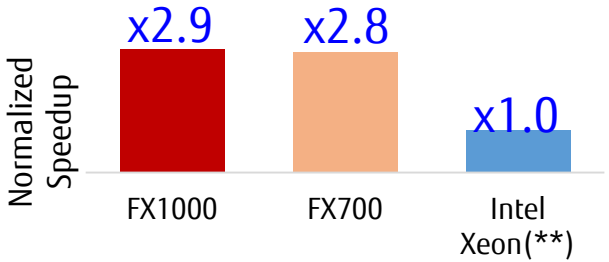
About ***Poynting***

- ✓ ***Poynting*** is an electromagnetic wave analysis software based on FDTD* method developed by Fujitsu.
- ✓ ***Poynting*** is an extremely advantageous electromagnetic wave analysis software on ***FX1000*** and ***FX700***, because the FDTD* method provides massive parallel efficiency while requires memory bandwidth.

Verification and Performance evaluation

- ✓ Verified major features of Poynting solver
- ✓ Verified parallel scalability up to 1,728 cores
- ✓ Poynting shows high-performance on A64FX because of high memory bandwidth as below



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

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

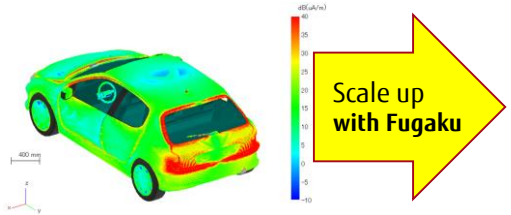
Challenge on ***Fugaku***

Study of a high-performance and easy-to-use computing environment:

- ✓ Study for business model and usability of a high-performance cloud service on Fugaku
- ✓ Verification for a large-scale electromagnetic wave simulation with Poynting on Fugaku
- ✓ Target: More than 1 trillion cells model of 5G "Vehicle to Vehicle" and "Vehicle to Infrastructure" communications at cross-section in a few hours

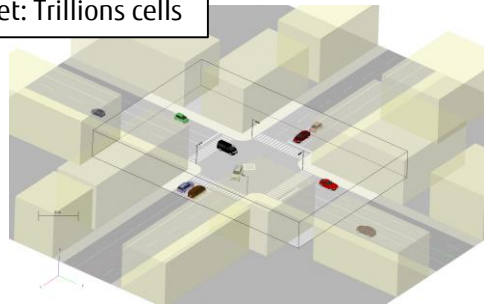
Fujitsu works to demonstrate large-scale simulations of Poynting and enable it on ***Fugaku.***

Current: Billions cells



Result form a single vehicle simulation.

Target: Trillions cells



Computational Domain: 120m x120m x 12m

Apps for Automotive Industry

- **Japan Automobile Manufacturers Association** (**JAMA**) has started since FY2020 evaluating leading-edge computer aided engineering for automobile on supercomputer **Fugaku** with **Fujitsu**'s supports.
- In FY2020, car crash models of 4 – 16 millions elements were evaluated, using **LS-DYNA** and **VPS** on Fugaku*.
- In FY2021, to develop technologies improving the accuracy of crash performance prediction, JAMA will conduct 20,000 cases of crash simulation utilizing Fugaku. Fluid dynamics using **Simcenter STAR-CCM+** will also be evaluated on Fugaku.

LS-DYNA
✓ LS-DYNA is a multiphysics simulation software capable of solving complex real world problems.

ESI Virtual Performance Solution (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.

Simcenter STAR-CCM+
✓ Simcenter STAR-CCM+ is a multiphysics computational fluid dynamics (CFD) software for the simulation of products operating under real-world conditions.

*This work used computational resources of the supercomputer Fugaku provided by RIKEN through the HPCI System Research Project (Project ID: hp200228).

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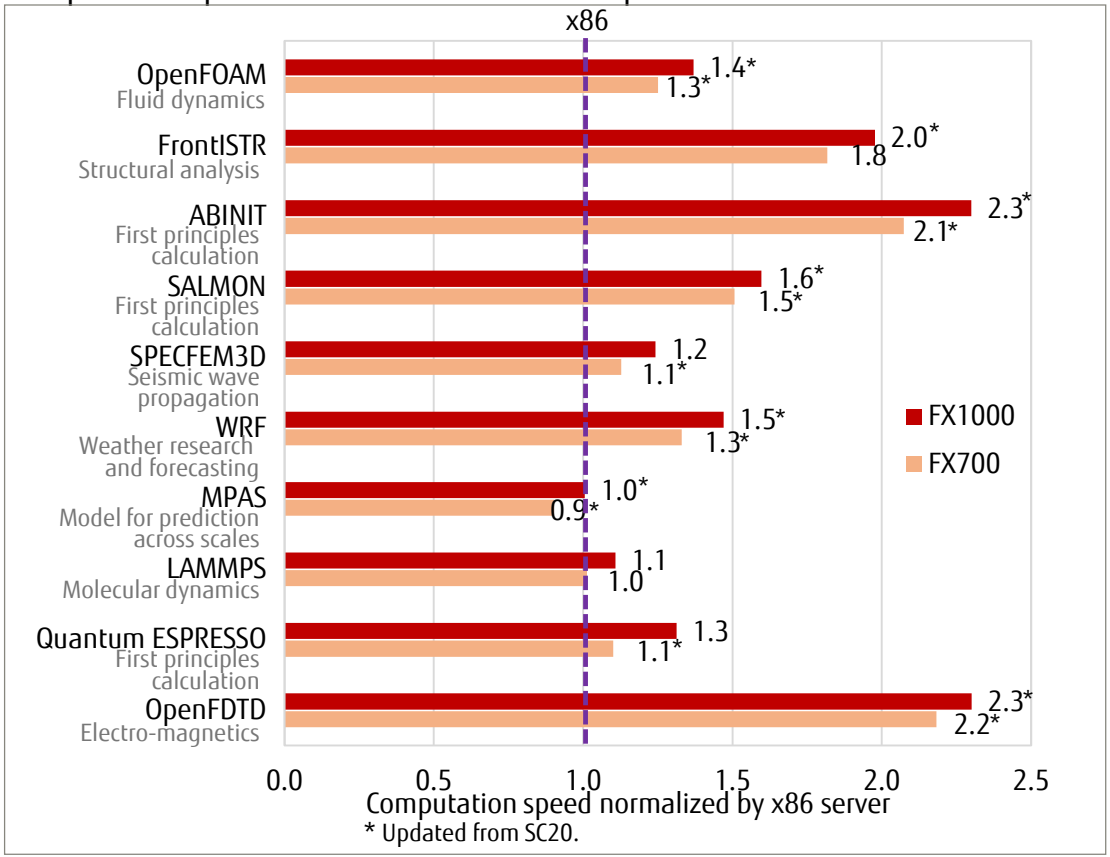
Open-Source Software (OSS) Applications

OSS Application Performance on FX1000/FX700

Computation Speed of FX1000 and FX700 compared with x86 server



- Computation speed of FX1000 and FX700 is faster than x86 server up to 2.3 times with these OSS.
- Performance is improved by
  - Enhanced microarchitecture (SVE)
  - High bandwidth memory(HBM)
- Several software are improved by code tuning and enhancement of compiler and libraries.

FX1000

FX700

Benchmark Platform

FX1000: A64FX (2.2GHz x 48cores)
FX700: A64FX (2.0GHz x 48cores)
x86 server: Xeon 8268 (2.9GHz x 24cores) x2

OSS Application Power Efficiency on FX1000

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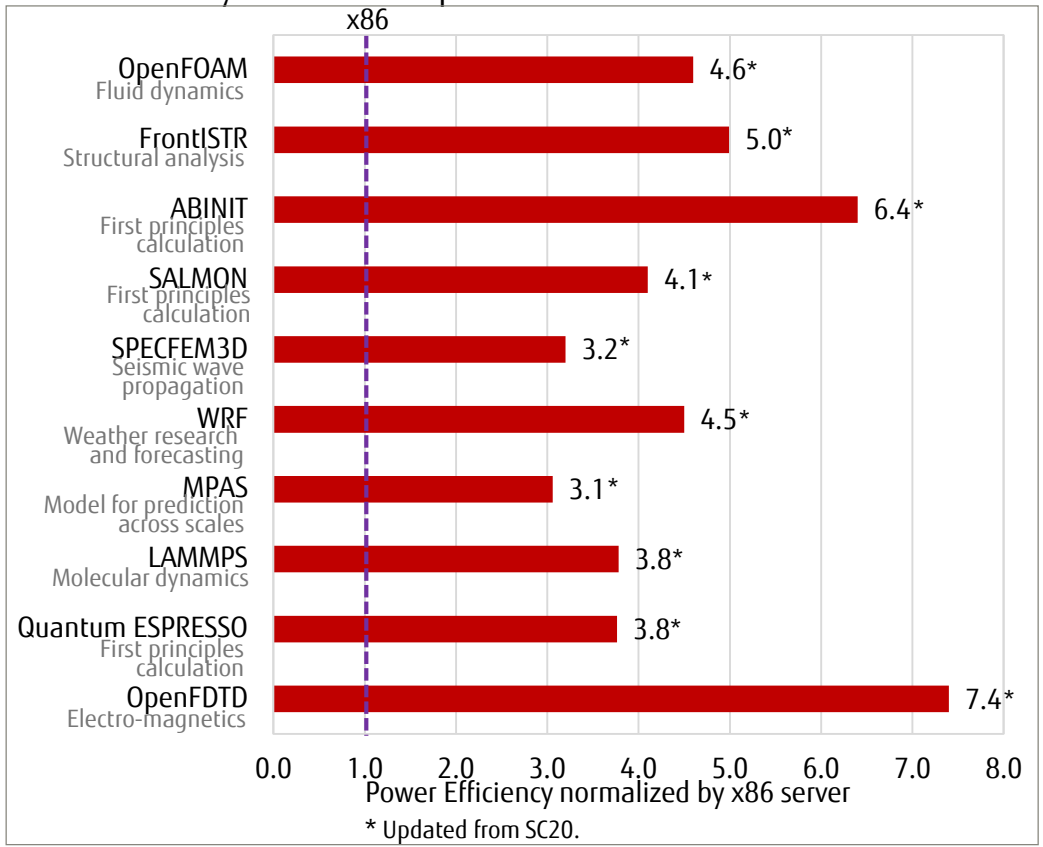
Power Efficiency of FX1000 compared with x86 server



* Updated from SC20.

- FX1000 has significant advantage of power efficiency in comparison with x86 server.
- The energy-saving technology developed for Fugaku which won the top of Green500 is applied to FX1000. This technology provides exceptional performance/power rates in large-scale systems.

FX1000

Benchmark Platform

FX1000: A64FX (2.2GHz x 48cores)
x86 server: Xeon 8268 (2.9GHz x 24cores) x2
Power consumption of a system board in single node was measured.

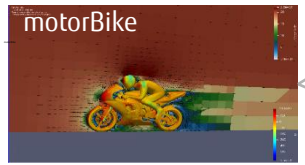
OpenFOAM

About *OpenFOAM*

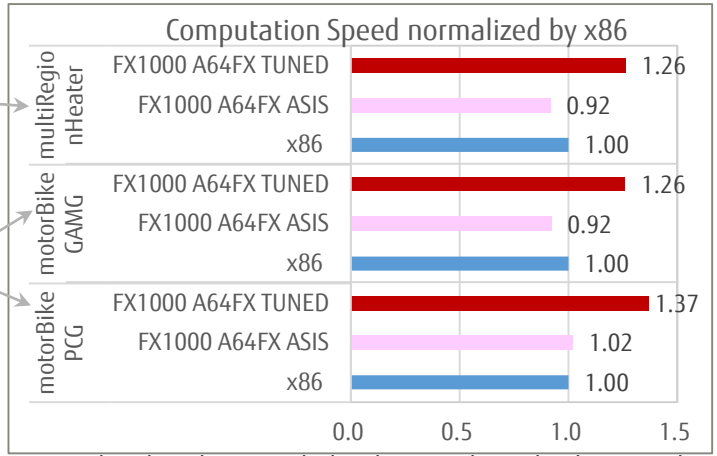
- ✓ **Open source Field Operation And Manipulation (OpenFOAM)** is Open-source CFD software which has various functionality of fluid dynamics simulation, including thermal conduction and turbulence analysis (https://www.openfoam.com/).

Performance Data

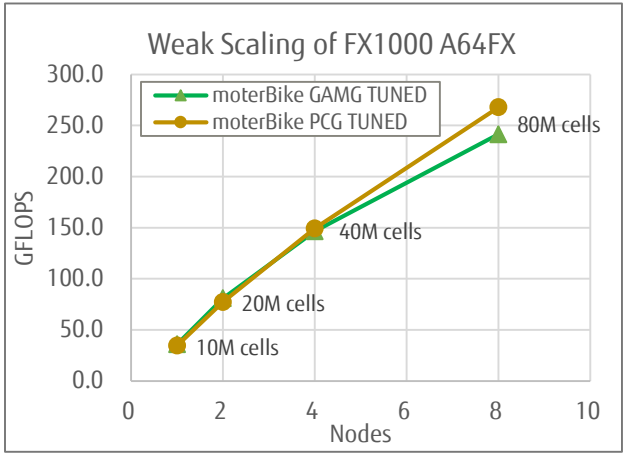
- ✓ Computation speed is better than x86 in almost cases. It is much enhanced by code tunning. The optimization of loop structure to enhance vectorization (more efficient use of SIMD) in code tunning has significant effect with Computation speed for A64FX.
- ✓ Two benchmark models were calculated. One is aero-dynamics of motorBike (LES) and another is thermal fluid of multiRegionHeater (RANS). Two matrix solvers PCG and GAMG are applied to Computation of motorBike model.



- **OpenFOAM**: v1812
- **Benchmark Platform**
  FX1000 A64FX (2.2GHz x 48cores)
  x86: Xeon 8268 (2.9GHz x 24cores) x2
- **Input data**: multiRegionHeater and motorBike



Two benchmarks were calculated. Asis and tuned code are used in FX1000. High Computation speed is obtained compared with x86. (multiRegionHeater: 15M cells, motorBike:10M cells)



Weak scaling is shown. The size of input data is changed with the number of cores. FX1000 has good weak scalability and Computation scale increase with the number of nodes.

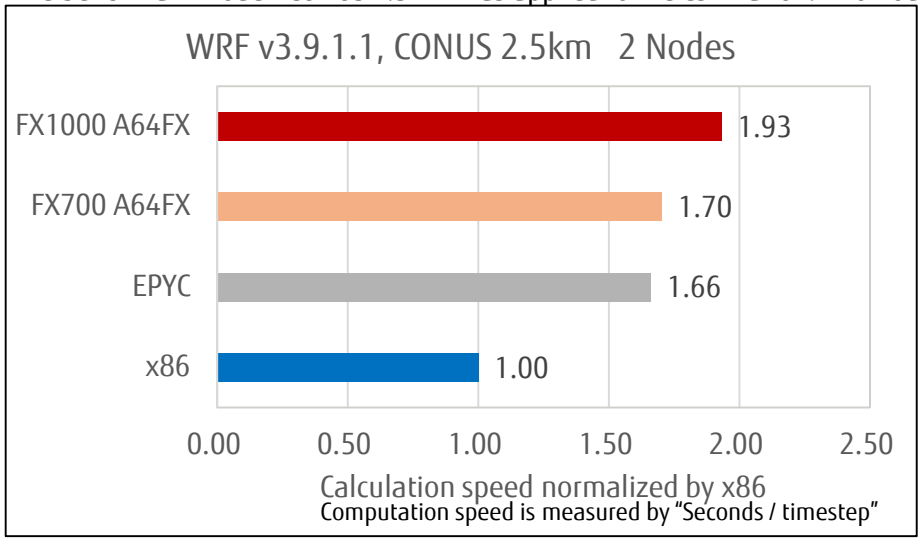
WRF

About *WRF*

- ✓ **The Weather Research and Forecasting (WRF) Model** is a next-generation mesoscale numerical weather prediction system designed for both atmospheric research and operational forecasting applications. It features two dynamical cores, a data assimilation system, and a software architecture supporting parallel computation and system extensibility. (https://www.mmm.ucar.edu/weather-research-and-forecasting-model)

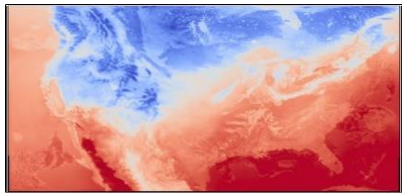
Performance Data

- ✓ The performance of WRF on A64FX systems shows better performance than other platforms because of high memory bandwidth.
- ✓ The benchmark model "CONUS 2.5km" was applied to the estimation. Two node are used to calculate this benchmark model.



Testing environment

- **WRF: version 3.9.1.1 (Tuned code)**
- **Benchmark platform**
  - FX1000 A64FX (2.2GHz x 48cores)
  - FX700 A64FX (2.0GHz x 48cores)
  - x86: Xeon P8260M (2.4GHz x 24cores) x2
  - EPYC : 7742 (2.25GHz x 64cores) x2
- **Input data**
  - CONUS 2.5km
    - 1501x1201x35
    - 3 hours forecasting



(https://www2.mmm.ucar.edu/wrf/bench/benchdata_v3911.html)

LAMMPS

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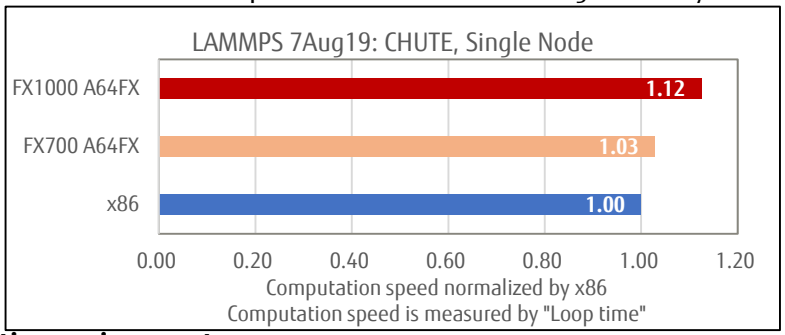
About ***LAMMPS***

- ✓ **Large-scale Atomic / Molecular Massively Parallel Simulator (LAMMPS)** is a classical molecular dynamics simulation code with a focus on materials modeling.
  It was designed to run efficiently on parallel computers. (https://www.lammps.org/)

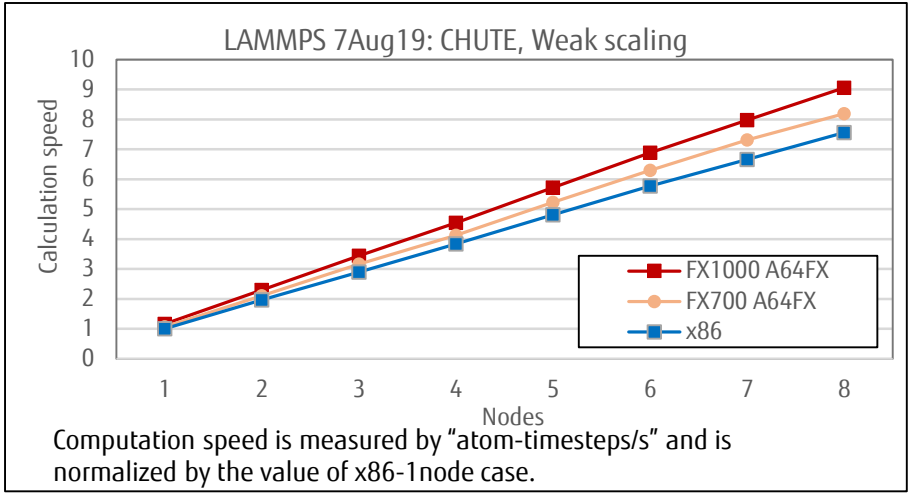
Performance Data

- ✓ The performance on FX1000 was achieved 1.12x faster than x86. SIMD and efficient data access enhance performance of FX1000 and FX700.
- ✓ The benchmark model CHUTE was applied to this estimation. Two sections "PAIR" and "MODIFY" which account for 90% of loop time with CHUTE were tuned to obtain fine performance of SIMD and high memory bandwidth.



Testing environment

- **LAMMPS: version 7Aug19 (Tuned code)**
- **Benchmark platform**
  - FX1000 A64FX (2.2GHz x 48cores)
  - FX700A64FX (2.0GHz x 48cores)
  - x86: Xeon P8260M (2.4GHz x 24cores) x2
- **Input data: "CHUTE"** Granular chute flow
  - 12,800,000 atoms (/node) for 100 timesteps



Computation speed is measured by "atom-timesteps/s" and is normalized by the value of x86-1node case.

Ideal scalability is shown on FX1000 and FX700

Quantum ESPRESSO

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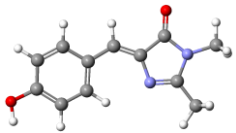
About ***Quantum ESPRESSO***

✓ ***Quantum ESPRESSO*** is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (https://www.quantum-espresso.org/).

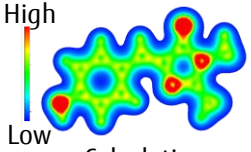
Performance Data

✓A64FX performance measurement for Quantum ESPRESSO 6.4.1

- First Principles Calculation

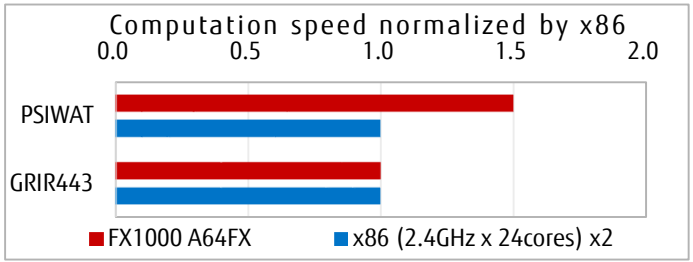


Molecular Geometry



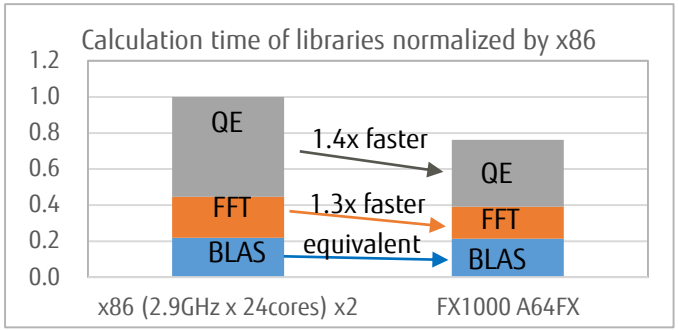
Calculation of Electron Density

- FX1000 A64FX has 1.5x faster over the x86 (2.4GHz x 24cores) x2 in QEF benchmark



*PSIWAT: QEF/benchmarks/PSIWAT/psiwat.in, 8 node
*GRIR443: QEF/benchmarks/GRIR443/grir443.in, 8 node

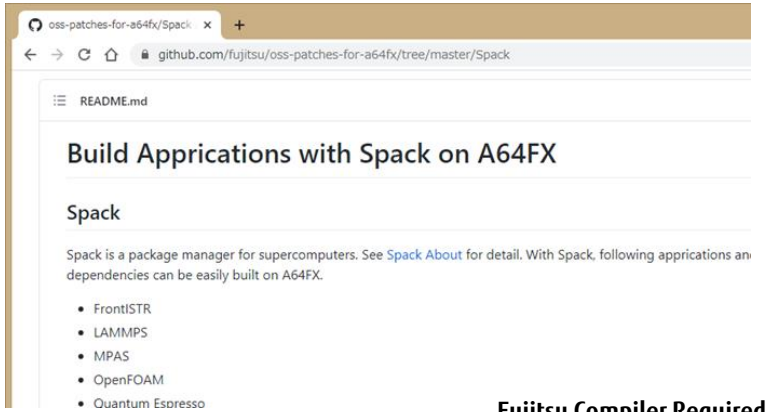
- A64FX has 1.3x faster over the x86 processor (2.9GHz x 24cores) x2 in structural optimization simulation
  - QE[*1] :1.4x faster by high memory b/w and using SIMD instructions
  - FFT[*2] :1.3x faster by long data-length and using SIMD instructions
  - BLAS[*3]: Equivalent performance by using cache 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 (https://github.com/fujitsu/elpa)
*2: FFTW3 Library tuned by FUJITSU (https://github.com/fujitsu/fftw3)
*3: FUJITSU SSL Ⅱ Library

Information and Tools for OSS

Installation guides and build scripts using Spack



Fujitsu Compiler Required

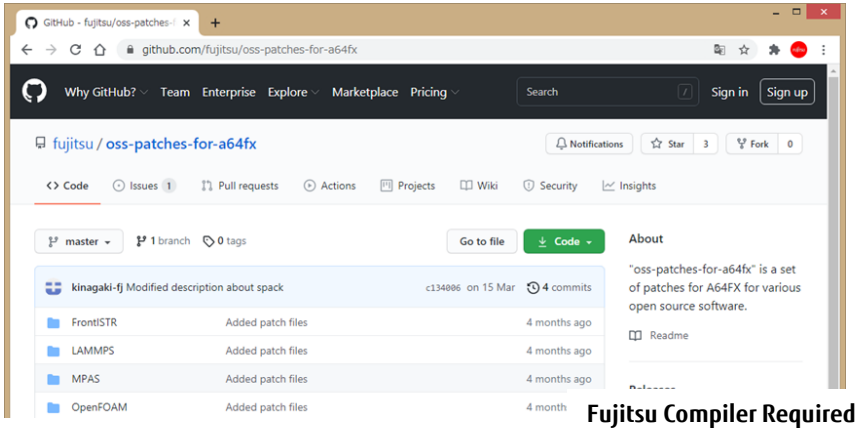
■ Target OSS

OpenFOAM | FrontISTR | ABINIT | SALMON | SPECFEM3D | MPAS | LAMMPS | QUANTUM ESPRESSO

■ Information site (Provided by Spack*)

https://github.com/fujitsu/oss-patches-for-a64fx/tree/master/Spack

Performance tuning information and patches



Fujitsu Compiler Required

■ Target OSS

OpenFOAM | FrontISTR | SPECFEM3D | QUANTUM ESPRESSO | MPAS | LAMMPS

*OpenFOAM and LAMMPS is going to be updated in the 2nd quarter of FY2021.

■ Information site (Fujitsu official Github)

https://github.com/fujitsu/oss-patches-for-a64fx

*Spack： An OSS package manager developed at Lawrence Livermore National Laboratory. For various computing environments and applications, a build script called a recipe is prepared, and the tool can build the application including the dependent library with one command. https://spack.readthedocs.io/en/latest/

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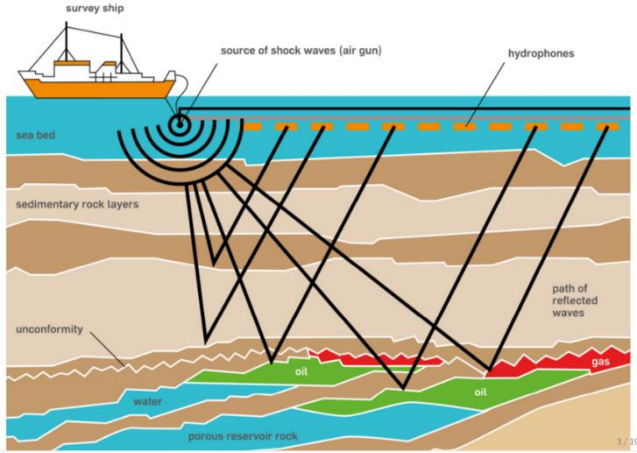
Open Source Oil & Gas Applications evaluated with Arm ecosystem collaborators

A64FX advantage in Oil & Gas applications

- Seismic simulation = important technology for Oil & Gas vendors
- Requires a huge amount of 3D data calculation to identify the geological structure
- Can benefit from High Bandwidth Memory and Scalable Vector Extension of A64FX

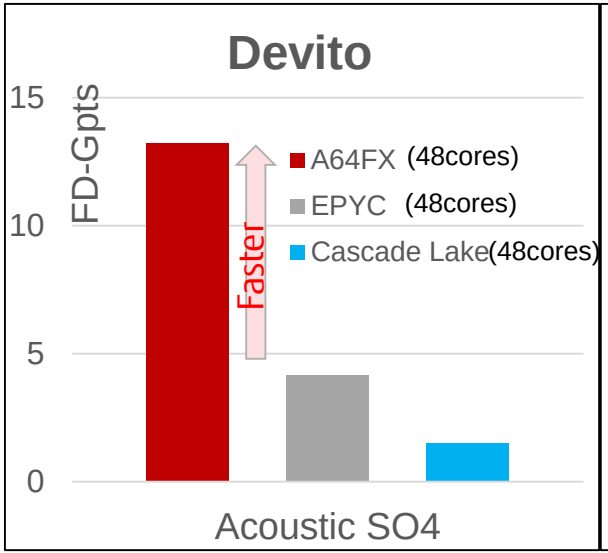
➢ Seismic Simulation image

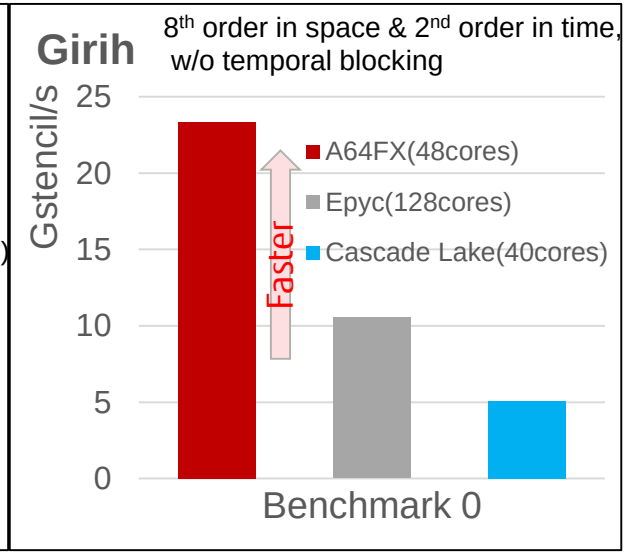


https://www.devitoproject.org/

https://github.com/ecrc/girih

➢ Example of Seismic Simulation Performance on A64FX





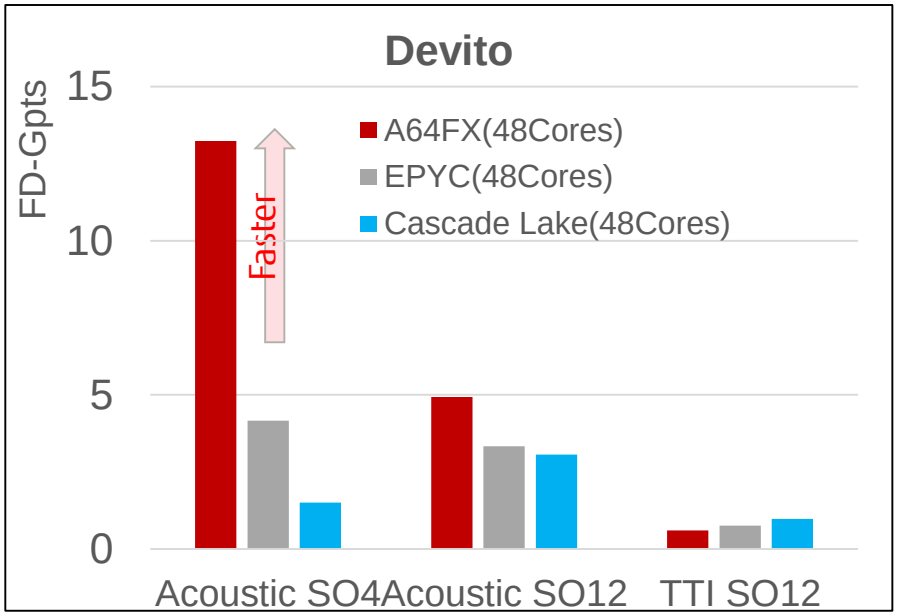
Devito

- About ***Devito***
  - ✓ Domain-specific Language (DSL) and code generation framework for the design of highly optimized finite difference kernels for use in inversion methods. Developed by Imperial college London https://www.devitoproject.org/

- Performance Data
  - ✓ A64FX shows remarkable performance over other CPUs especially acoustic model of 4th space order (SO4)
  - ✓ HBM (High Bandwidth Memory) and SVE (Scalable Vector Extension) contributes this advantage.
  - ✓ Reference: https://www.youtube.com/watch?v=--2LrXL6Y2g&list=PLcsG4X8Zn_UAdbYQODr5PQLCcdCo_sovO&index=36&t=61s

arm FUJITSU

- A64FX: 2.2GHz 48cores 32GB HBM2
  12 threads x 4 MPI process to fit A64FX Core Memory Group
- Xeon 9275CL: 2.4GHz 24cores x 2 sockets
- EPYC 7R32: 3.3GHz 48cores



GIRIH

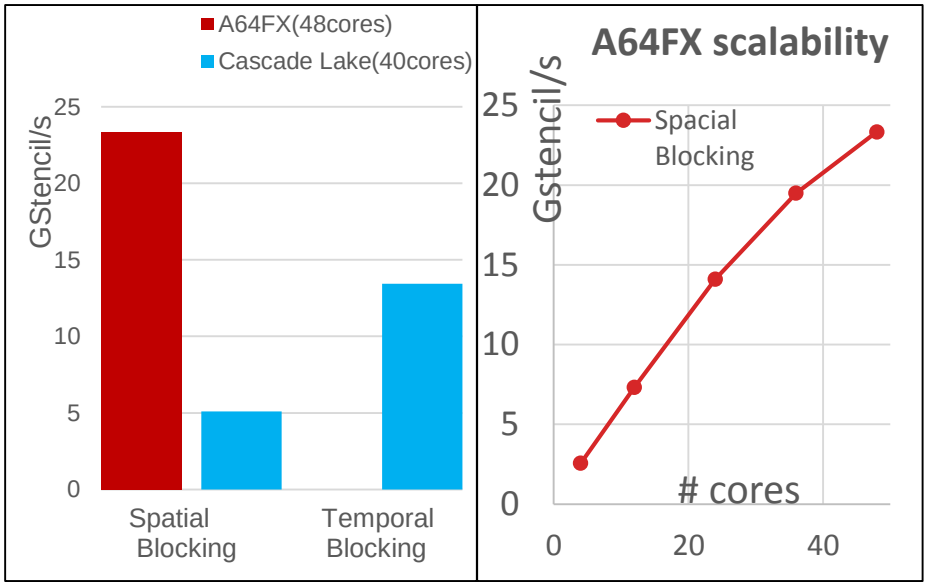
FUJITSU

About ***GIRIH***

- ✓A high-performance stencil framework using multicore wave front diamond tiling. Developed by Extreme Computing Research Center at KAUST *
- ✓ Spatial and temporal blocking techniques are implemented

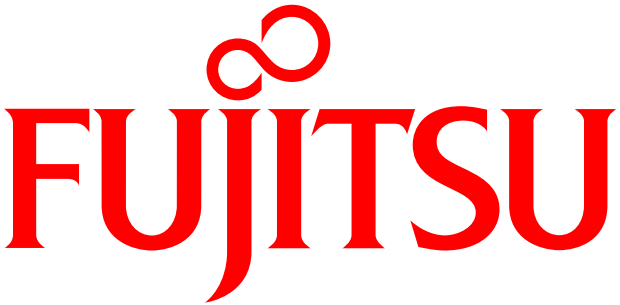
Performance Data

- ✓ A64FX shows remarkable performance and scalability with spatial blocking, compared with spatial/temporal blocking performance on Cascade Lake.
- ✓ HBM (High Bandwidth Memory) and SVE (Scalable Vector Extension) contributes this advantage.



- 8th order, domain size 1024x1024x512, Single precision (benchmark 0)
- A64FX: 2.2GHz 48cores 32GB HBM2 (Tuned code) 1/3/6/9/12 threads x 4 MPI process to fit A64FX CMG (CMG=Core Memory Group)
- Cascade Lake performance are quoted from github https://github.com/ecrc/girih and provided by KAUST.

* KAUST: King Abdullah University of Science and Technology



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