

Integration of Simulation/Data/Learning and Beyond

Kengo Nakajima
Information Technology Center
The University of Tokyo



**Wisteria
BDEC-01**



Hierarchical, Hybrid, Heterogeneous
h3-Open-BDEC
Big Data & Extreme Computing



International Workshop on “Integration of Simulation/Data/Learning and Beyond”
45th ASE Seminar (Advanced Supercomputing Environment)
November 29, 2023, Kashiwa, Japan & Online

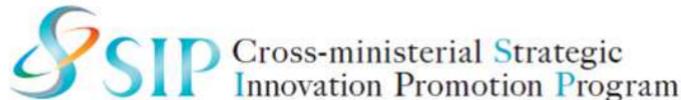
Acknowledgements



- JSPS Grant-in-Aid for Scientific Research (S) (19H05662)
- New Energy & Industrial Technology Development Organization (NEDO): Cross-ministerial Strategic Innovation Promotion Program (SIP): Big-Data and AI-Enabled Cyberspace Technologies
- Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures (JHPCN)
– jh210022-MDH, jh220029, jh230017, jh230018
- Information Technology Center, The University of Tokyo



新エネルギー・産業技術総合開発機構
New Energy and Industrial Technology Development Organization



- Integration of (Simulation/Data/Learning)
 - Wisteria/BDEC-01
 - h3-Open-BDEC
- Applications on Wisteria/BDEC-01 with h3-Open-BDEC
 - Seismic Wave Propagation
 - Global Atmosphere
 - International/Domestic Collaborations
- Integration of (Simulation/Data/Learning) and Beyond
- Summary

2001-2005

2006-2010

2011-2015

2016-2020

2021-2025

2026-2030

Hitachi SR8000
1,024 GF

Hitachi SR11000
J1, J2
5.35 TF, 18.8 TF

Hitachi SR16K/M1
Yayoi
54.9 TF

Hitachi
SR2201
307.2GF

Hitachi
SR8000/MPP
2,073.6 GF

OBCX
(Fujitsu)
6.61 PF

Hitachi HA8000
T2K Today
140 TF

Oakforest-
PACS (Fujitsu)
25.0 PF

OFP-II
75+ PF

Fujitsu FX10
Oakleaf-FX
1.13 PF

Wisteria
BDEC-01 Fujitsu
33.1 PF

BDEC-
02
250+ PF

Supercomputers @ITC/U.Tokyo

2,600+ Users

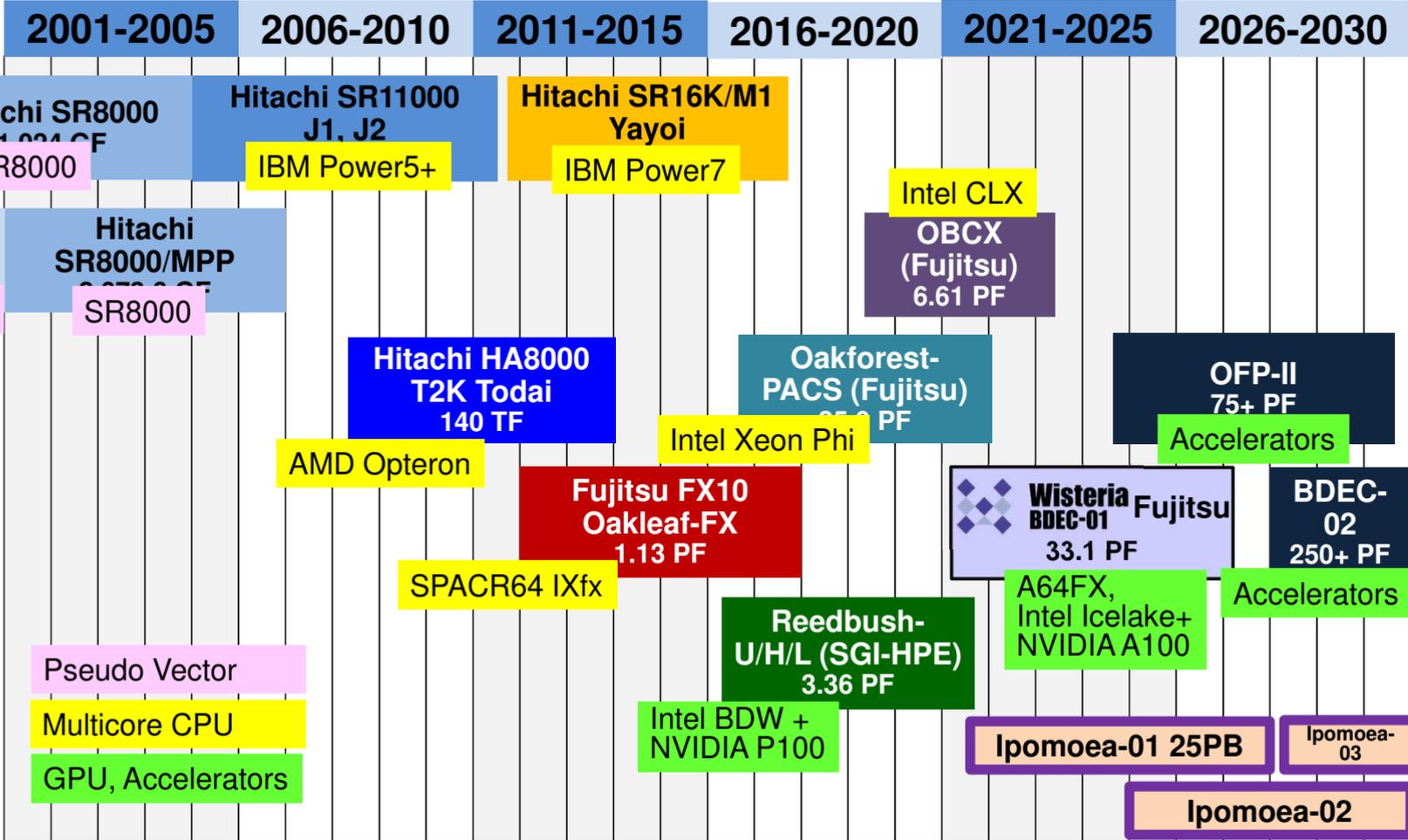
55+% outside of U.Tokyo

Reedbush-
U/H/L (SGI-HPE)
3.36 PF

Ipomoea-01 25PB

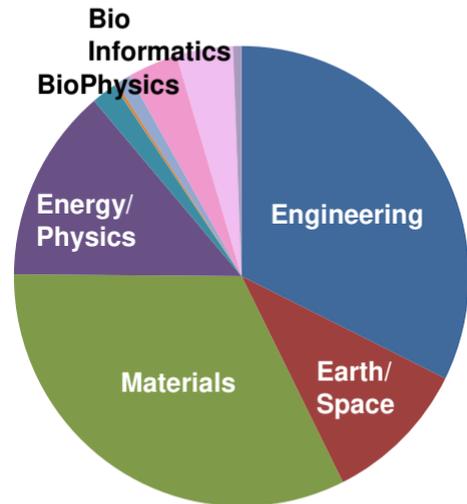
Ipomoea-
03

Ipomoea-02

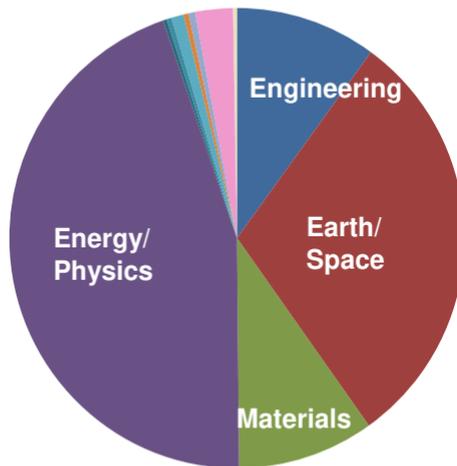


Research Area based on Machine Hours (FY.2022)

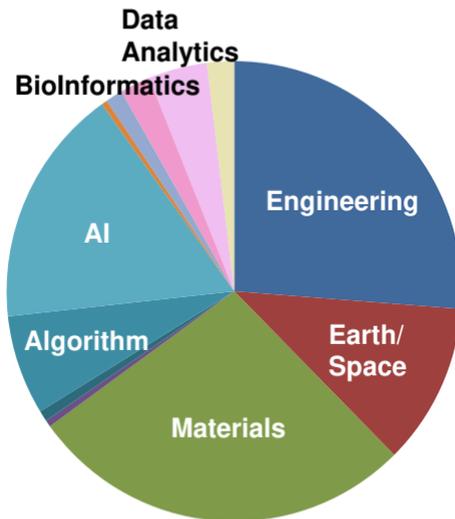
■ CPU, ■ GPU



**OBCX
CascadeLake**



**Odyssey
A64FX**



**Aquarius
A100**

- Engineering
- Earth/Space
- Material
- Energy/Physics
- Info. Sci. : System
- Info. Sci. : Algorithms
- Info. Sci. : AI
- Education
- Industry
- Bio
- Bioinformatics
- Social Sci. & Economics
- Data

Supercomputing is changing

- Various Types of Workloads
 - Computational Science & Engineering: Simulations
 - Big Data Analytics
 - AI, Machine Learning ...

Integration of (Simulation+Data+ Learning) (S+D+L) is important towards Society 5.0, Human-Centered Society proposed by Japanese Gov.

– By Integration of Cyber & Physical Space

BDEC (Big Data & Extreme Computing)

- Platform for Integration of (S+D+L)
- Focusing on S (Simulation)
 - AI for HPC, AI for Science
- Planning started in 2015



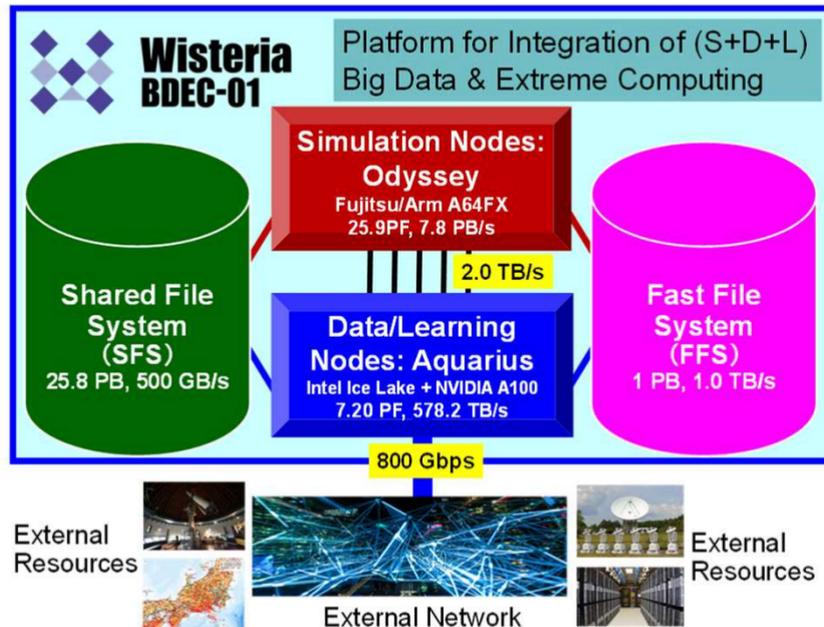
BDEC (Big Data & Extreme Computing)

S + D + L

Wisteria/BDEC-01

- Operation starts on May 14, 2021
- 33.1 PF, 8.38 PB/sec by **Fujitsu**
 - ~4.5 MVA with Cooling, ~360m²
- 2 Types of Node Groups
 - Hierarchical, Hybrid, Heterogeneous (h3)
 - Simulation Nodes: Odyssey
 - Fujitsu PRIMEHPC FX1000 (A64FX), 25.9 PF
 - 7,680 nodes (368,640 cores), Tofu-D
 - General Purpose CPU + HBM
 - Commercial Version of “Fugaku”
 - Data/Learning Nodes: Aquarius
 - Data Analytics & AI/Machine Learning
 - Intel Xeon Ice Lake + NVIDIA A100, 7.2PF
 - 45 nodes (90x Ice Lake, 360x A100), IB-HDR
 - Some of the DL nodes are connected to external resources directly
- File Systems: SFS (Shared/Large) + FFS (Fast/Small)

The 1st BDEC System (Big Data & Extreme Computing) Platform for Integration of (S+D+L)



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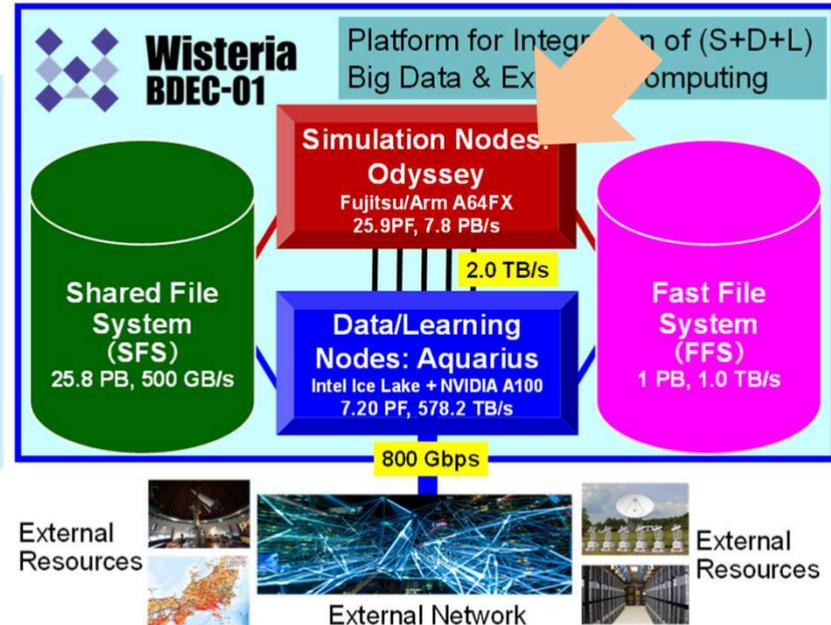
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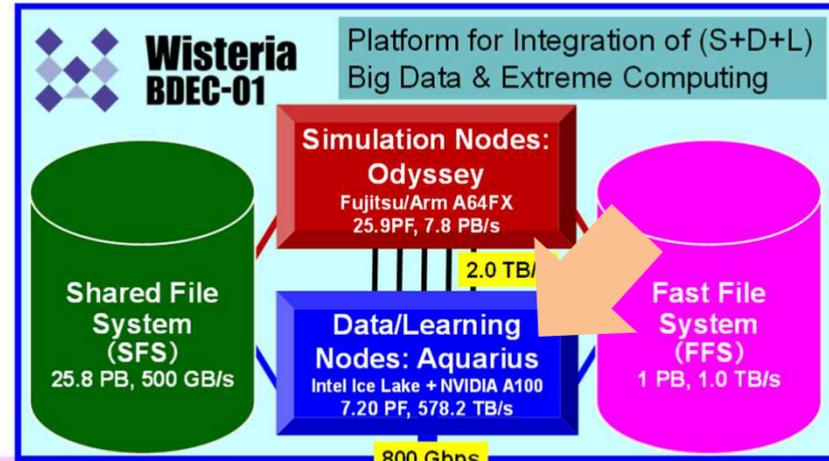
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External Resources



External Network



External Resources

Simulation Nodes Odyssey

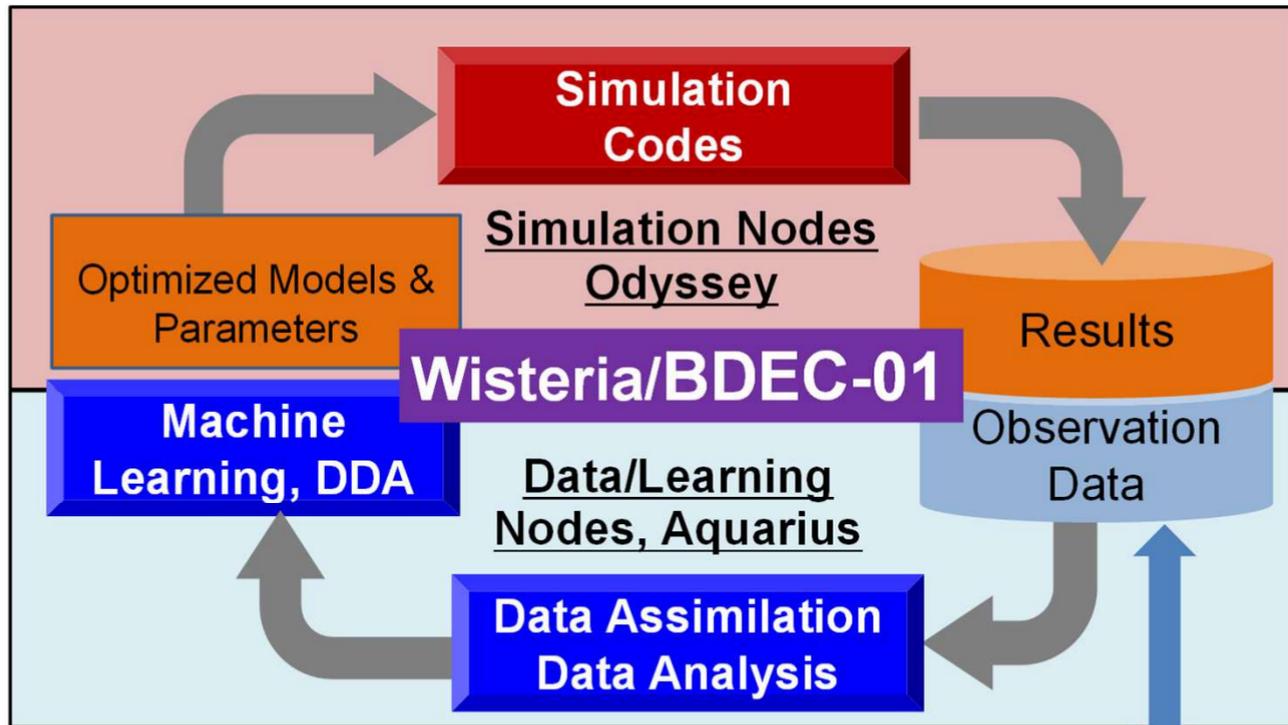
25.9 PF, 7.8 PB/s

Fast File
System
(FFS)
1.0 PB,
1.0 TB/s

Shared File
System
(SFS)
25.8 PB,
0.50 TB/s

Data/Learning Nodes Aquarius

7.20 PF, 578.2 TB/s



Server,
Storage,
DB,
Sensors,
etc.



External Network



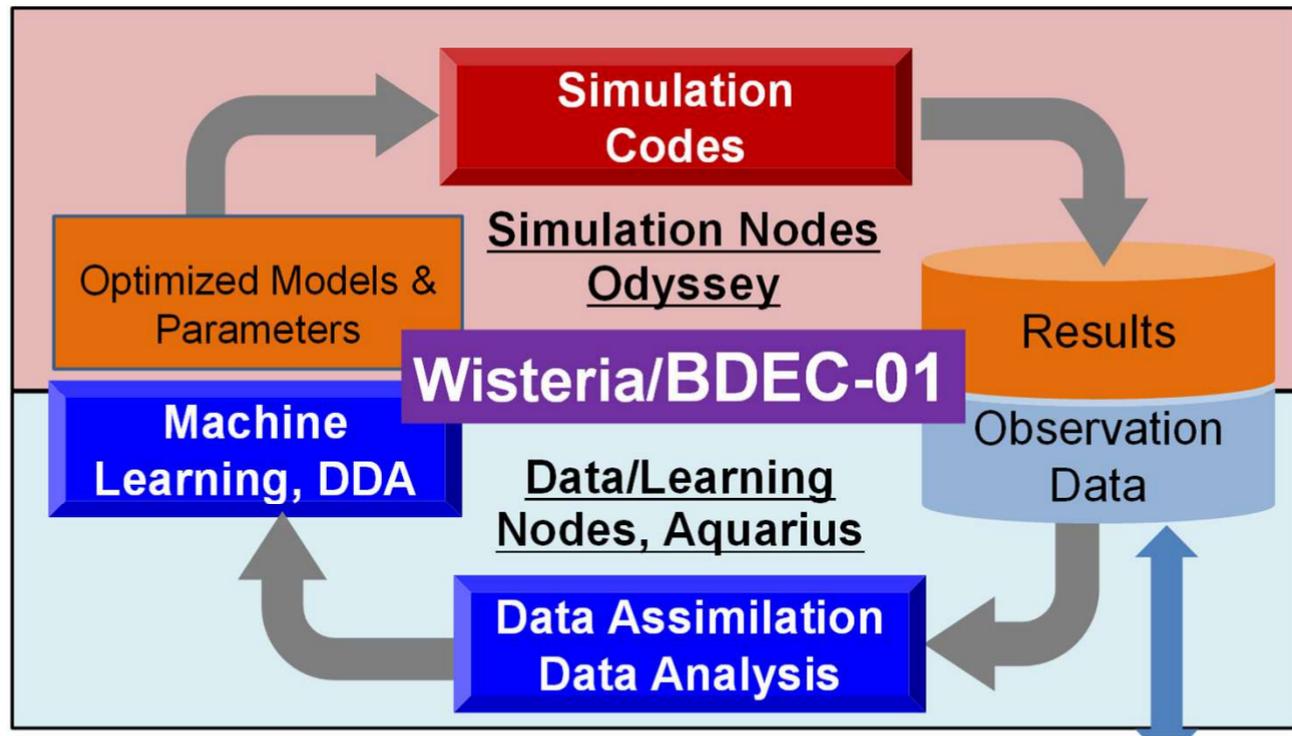
External
Resources

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Odyssey**
25.9 PF, 7.8 PB/s

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1.0 PB,
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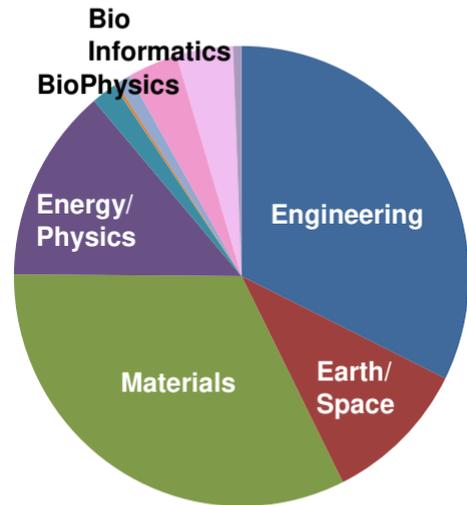
**Data/Learning Nodes
Aquarius**
7.20 PF, 578.2 TB/s



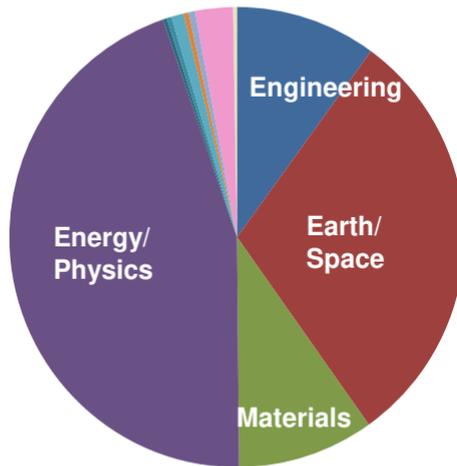
Optimization of Models/Parameters for Simulations by Data Analytics & Machine Learning (S+D+L)

Research Area based on Machine Hours (FY.2022)

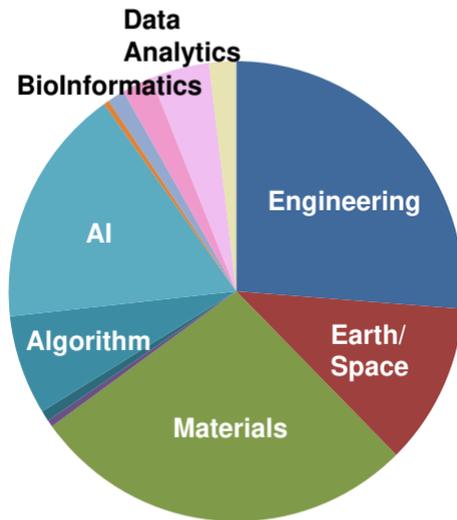
■ CPU, ■ GPU



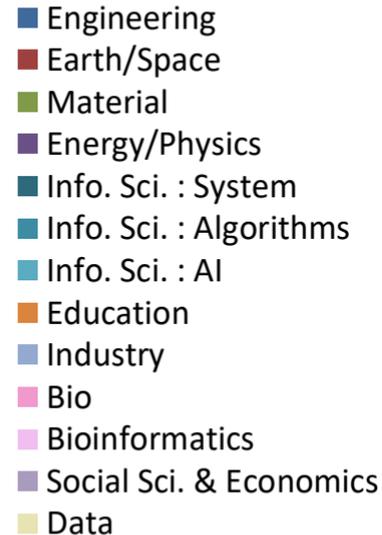
OBCX



Odyssey

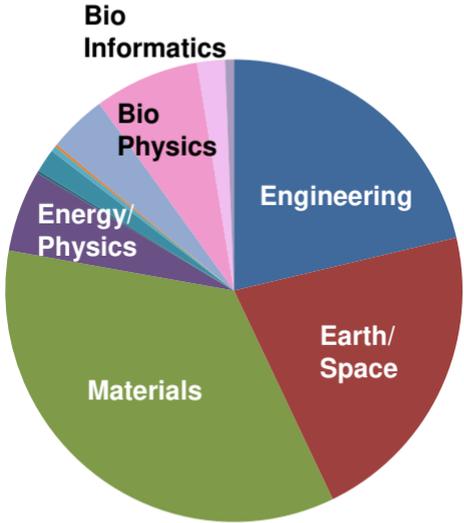


Aquarius

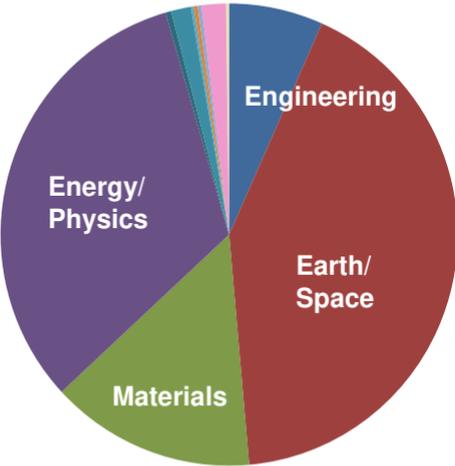


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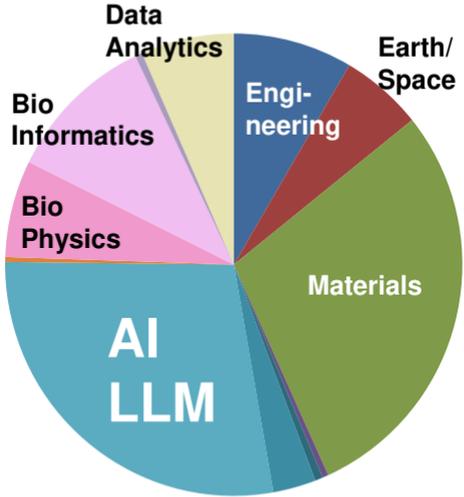
■ CPU, ■ GPU (April-September)



OBCX
Retired in
September 2023



Odyssey



Aquarius

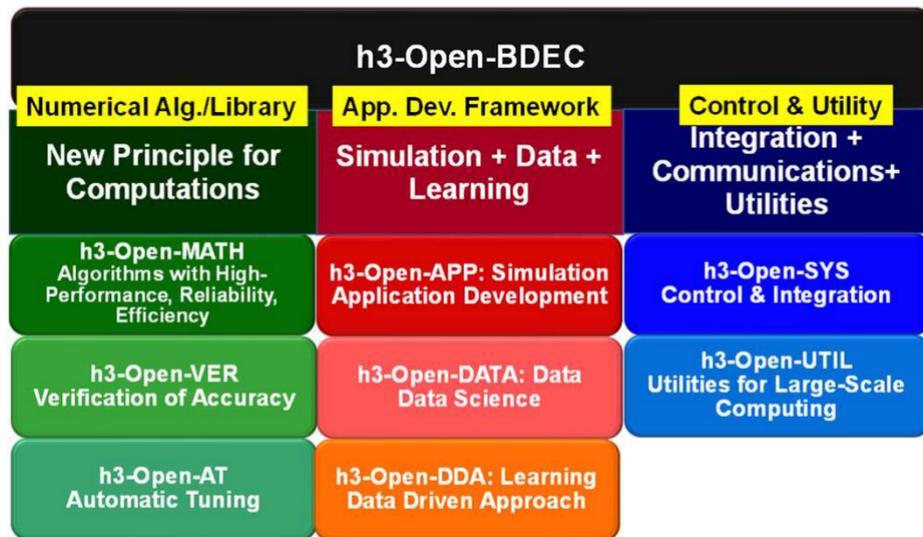
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h3-Open-BDEC Innovative Software Platform for Integration of (S+D+L) on the BDEC System, such as Wisteria/BDEC-01



- 5-year project supported by Japanese Government (JSPS) since 2019
 - FY.2023 is the final year
 - Today is the WS of this Project
- Leading-PI: Kengo Nakajima (The University of Tokyo)
- Total Budget: 1.41M USD



Members (Co-PI's) of h3-Open-BDEC Project

Computer Science, Computational Science, Numerical Algorithms,
Data Science, Machine Learning

- Kengo Nakajima (ITC/U.Tokyo, RIKEN), Leading-PI
- Takeshi Iwashita (Hokkaido U), Co-PI, Algorithms
- Hisashi Yashiro (NIES), Co-PI, Coupling, Utility
- Hiromichi Nagao (ERI/U.Tokyo), Co-PI, Data Assimilation
- Takashi Shimokawabe (ITC/U.Tokyo), Co-PI, ML/hDDA
- Takeshi Ogita (Waseda U.), Co-PI, Accuracy Verification
- Takahiro Katagiri (Nagoya U), Co-PI, Appropriate Computing
- Hiroya Matsuba (ITC/U.Tokyo, Hitachi), Co-PI, Container



HITACHI



Former Pos-Doc's



- Masatoshi Kawai (ITC/U.Tokyo -> Nagoya U.)
- Hayato Shiba (ITC/U.Tokyo -> U.Hyogo)



Contributors/Collaborators

- **Information Technology Center, The University of Tokyo**
 - **S. Sumimoto, T. Arakawa**
 - T. Suzumura, M. Hanai
 - T. Hanawa
- **Earthquake Research Institute, The University of Tokyo**
 - T. Furumura, H. Tsuruoka
 - T. Ichimura, K. Fujita, S. Ito
- **Tokyo Institute of Technology**
 - R. Yokota, R. Sakamoto
- **Hokkaido University**
 - T. Fukaya
- **Nagoya University**
 - T. Hoshino
- **Kyushu University**
 - S. Oshima, K. Inoue
- **RIKEN R-CCS**
 - M. Nakao, T. Imamura
- **Fujitsu**
 - Y. Sakaguchi, Y. Kasai, D. Obinata
- **My Former Students**
 - Y.C. Chen (KIT), R. Yoda (BWU)
 - A.T. Magro (Aitia)



北海道大学
HOKKAIDO UNIVERSITY



名古屋大学
NAGOYA UNIVERSITY



九州大学
KYUSHU UNIVERSITY



東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO



東京大学
THE UNIVERSITY OF TOKYO



東京工業大学
Tokyo Institute of Technology



(Part of) International Collaborators

- Osni Marques (Lawrence Berkeley National Laboratory, USA)
- **Richard Vuduc (Georgia Institute of Technology, USA)**
- Edmond Chow (Georgia Institute of Technology, USA)
- Weichung Wang (National Taiwan University, Taiwan)
- Feng-Nan Hwang (National Central University, Taiwan)
- Gerhard Wellein (FAU Erlangen & Nuremberg, Germany)
- Mathias Bolten (University of Wuppertal, Germany)
- Serge Petiton (University of Liles/CNRS, France)
- **Xing Cai (Simula Research Laboratory, Norway)**
- Estela Suarez (Jülich Supercomputing Center/Univ. Bonn, Germany)
- France Boillod-Cerneux (CEA, France)

h3-Open-BDEC Innovative Software Platform for Integration of (S+D+L) on the BDEC System, such as Wisteria/BDEC-01

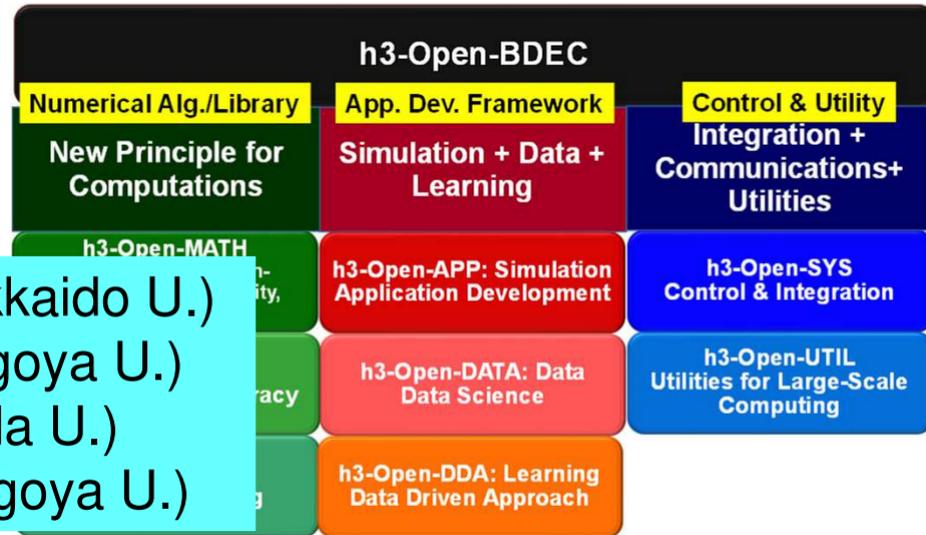


- “Three” Innovations

- New Principles for Numerical Analysis by Adaptive Precision, Automatic Tuning & Accuracy Verification

13:30-13:45 Takeshi Iwashita (Hokkaido U.)
 13:45-14:00 Takahiro Katagiri (Nagoya U.)
 15:35-15:50 Takeshi Ogita (Waseda U.)
 15:50-16:05 Masatoshi Kawai (Nagoya U.)

Wisteria/BDEC-01



Approximate Computing with Low/Adaptive/Trans Precision

- Mostly, scientific computing has been conducted using FP64 (double precision, DP)
 - Sometimes, problems can be solved by FP32 (single precision, SP) or lower precision
- **Lower precision may save time, energy and memory**

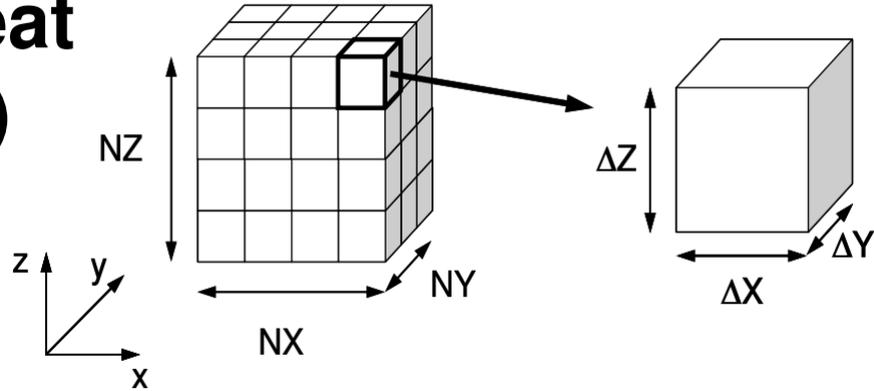
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 - Sometimes, problems can be solved by FP32 (single precision, SP) or lower precision
- **Lower precision may save time, energy and memory**
- **Approximate Computing**
 - Originally for image recognition etc. where accuracy is not necessarily required
 - Also applied to numerical computations
- **Computations by lower precision and by mixed precision may provide results with less accuracy**

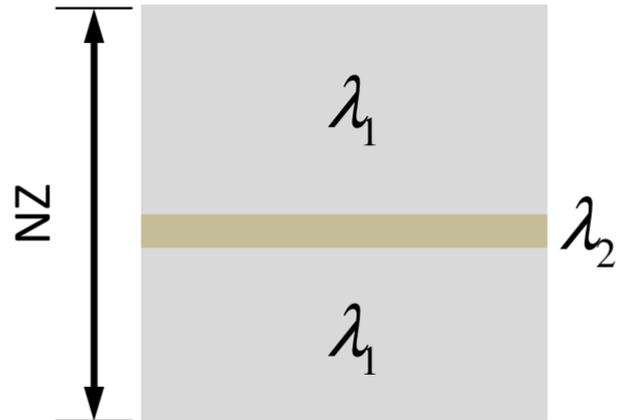
P3D: Steady State 3D Heat Conduction by FVM (1/2)

$$\nabla \cdot (\lambda \nabla \phi) + f = 0$$

- 7-point Stencil
- Heterogenous Material Property



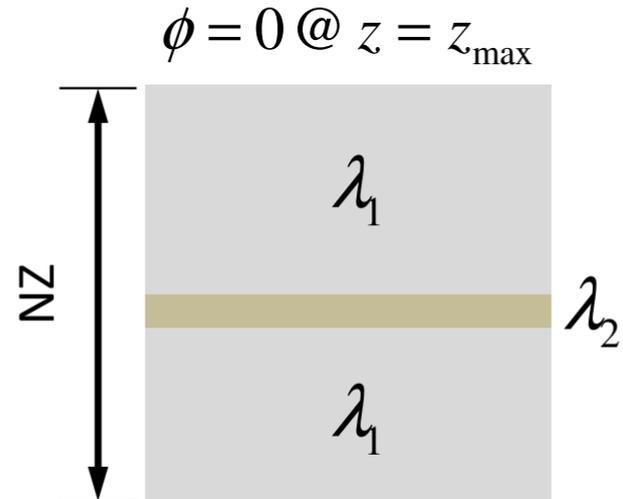
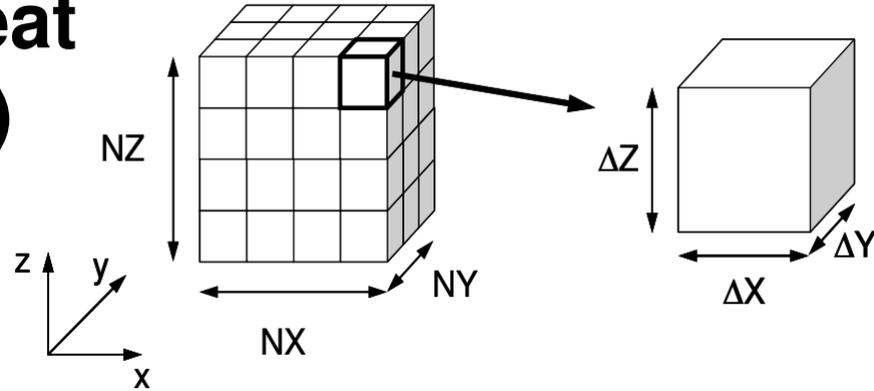
$$\phi = 0 @ z = z_{\max}$$



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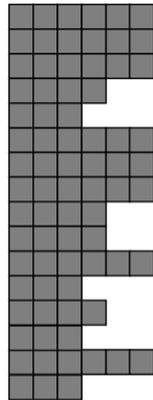
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- 7-point Stencil
- **Heterogenous Material Property**
 - λ_1/λ_2 is proportional to the condition number of coefficient matrices
- **Coefficient Matrix**
 - Sparse, SPD
- **ICCG Solver**
- **Fortran 90 + OpenMP**
- **CM-RCM Reordering**

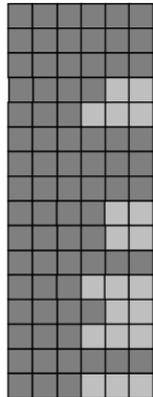


P3D: Steady State 3D Heat Conduction by FVM (2/2)

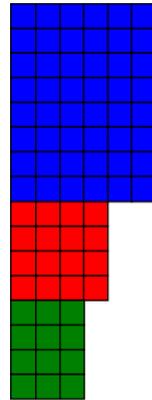
- Various Configurations
 - FP64 (Double), FP32 (Single), FP16 (Half) (just for preconditioning)
 - Matrix Storage Format (CRS, ELL, SELL-C- σ etc.)



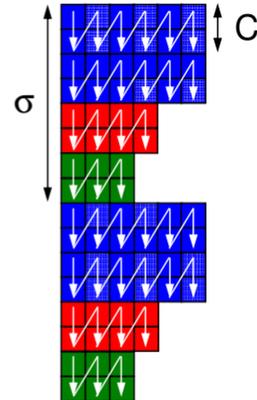
CRS



ELL



Sliced ELL



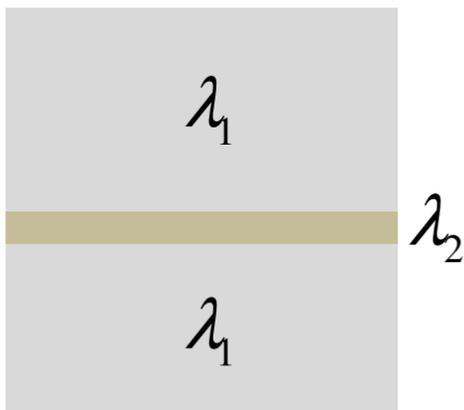
SELL-C- σ

Ratio of FP32(SP)/FP64(DP): CRS

Iterations ● & Time Δ for ICCG

λ_1/λ_2 , 128^3 DOF, CRS

Ratio < 1 \Rightarrow FP32 is faster

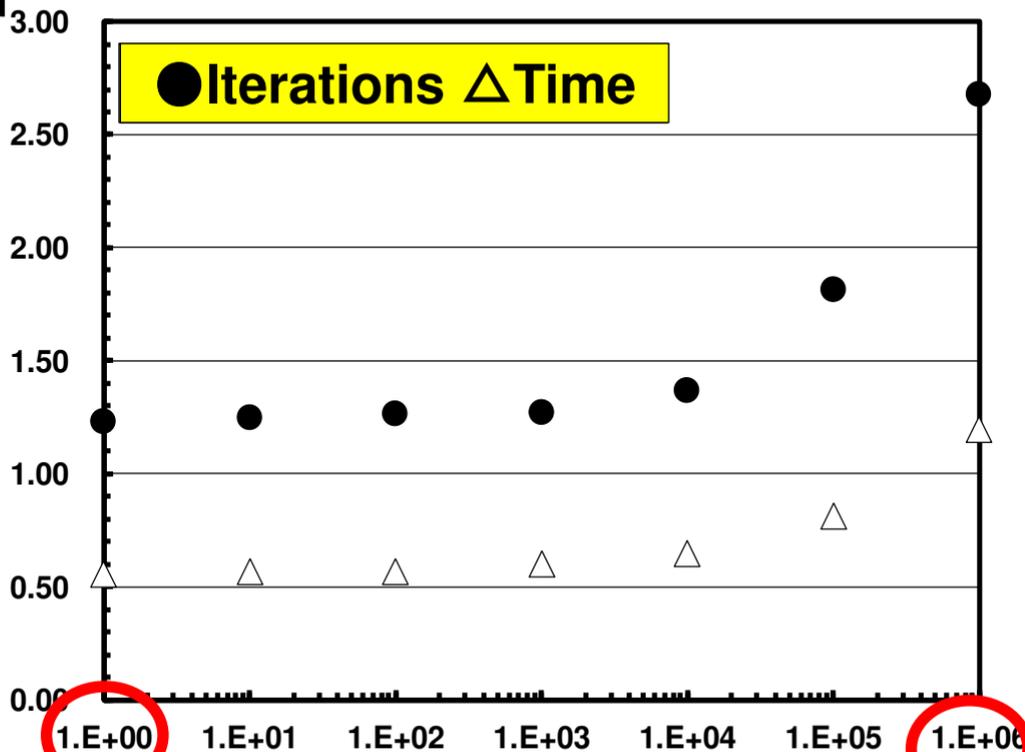


$$\nabla \cdot (\lambda \nabla \phi) + f = 0$$

Intel Xeon BDW

1 Node: 18 cores x 2 soc's

Ratio of FP32/FP64



Ratio of λ_1/λ_2

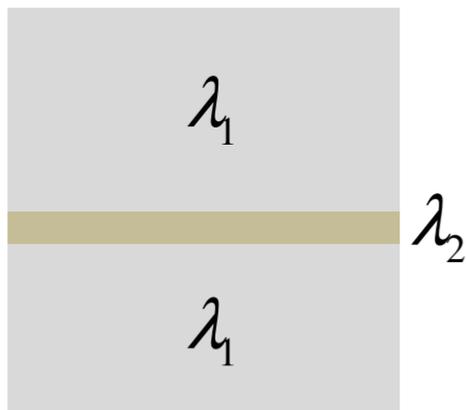
[KN et al. 2018]

Ratio of FP32(SP)/FP64(DP) : CRS

Iterations● & Time△ for ICCG_{3.00}

λ_1/λ_2 , 128³ DOF, CRS

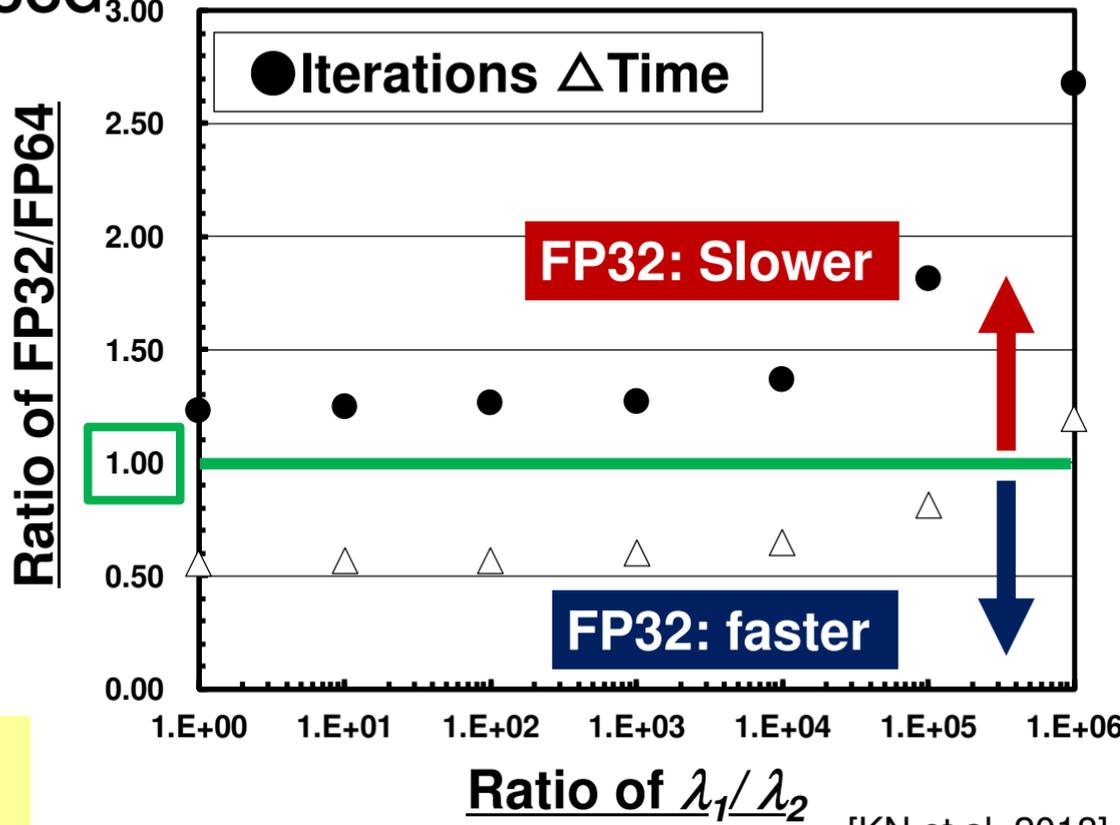
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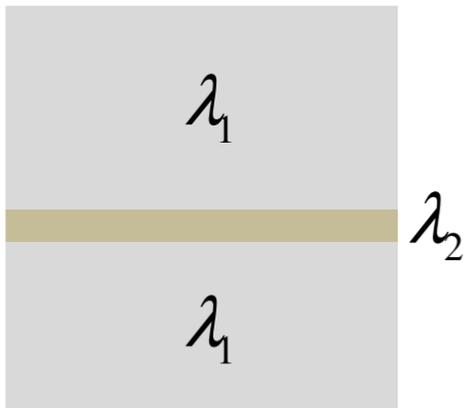


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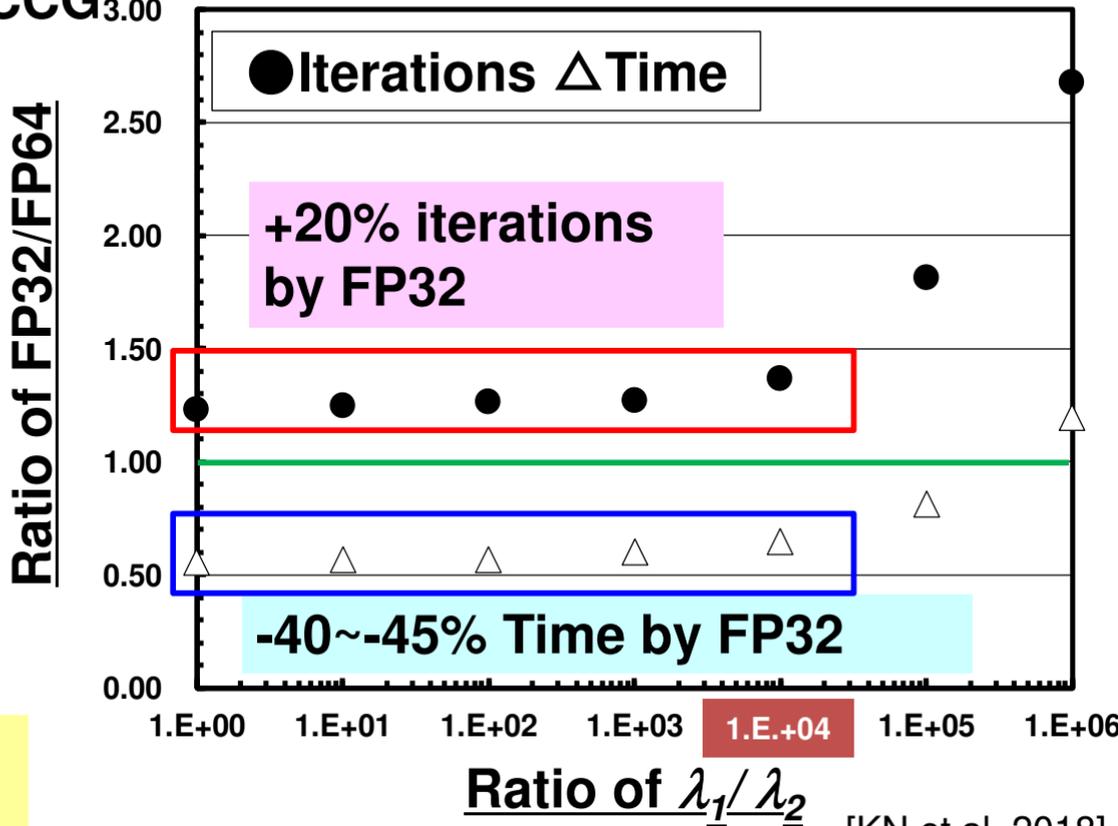
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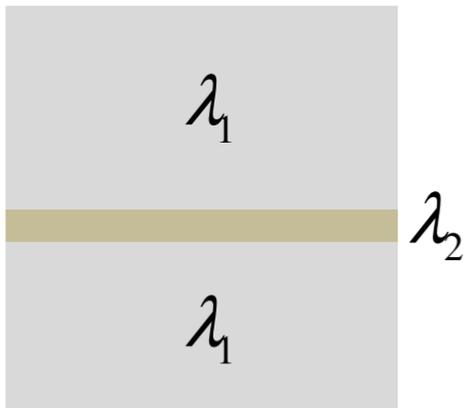


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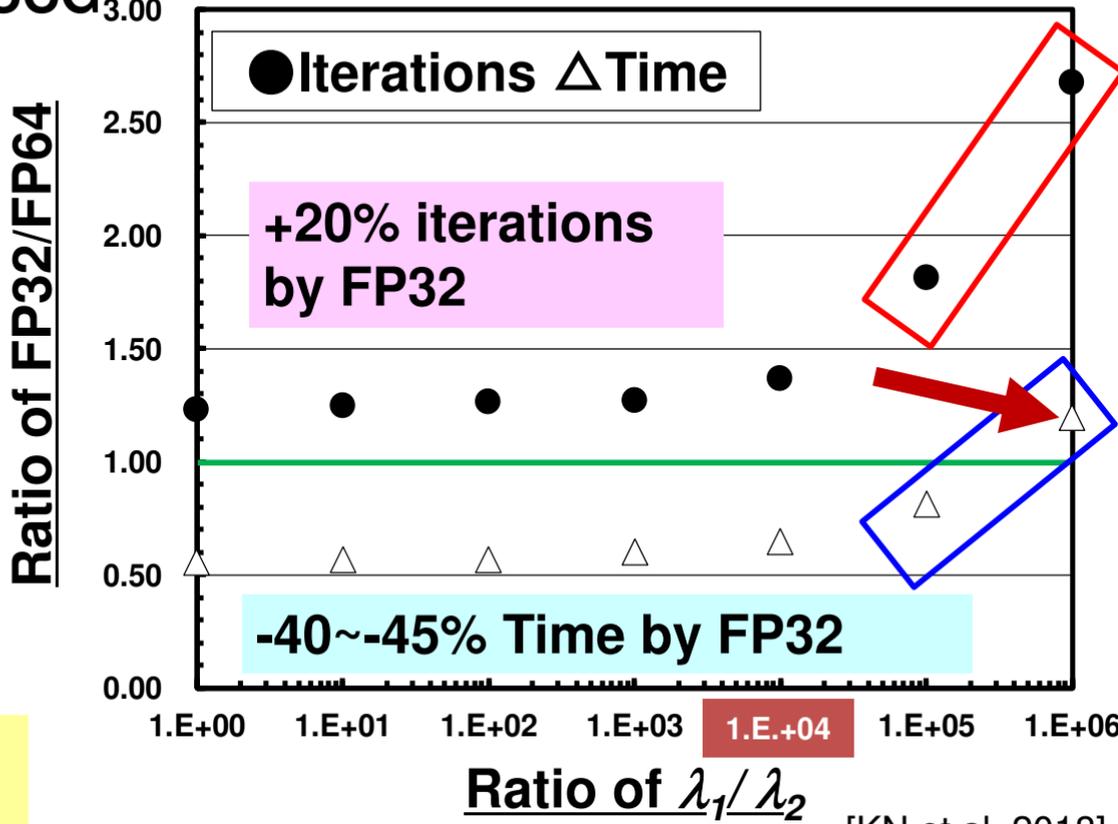
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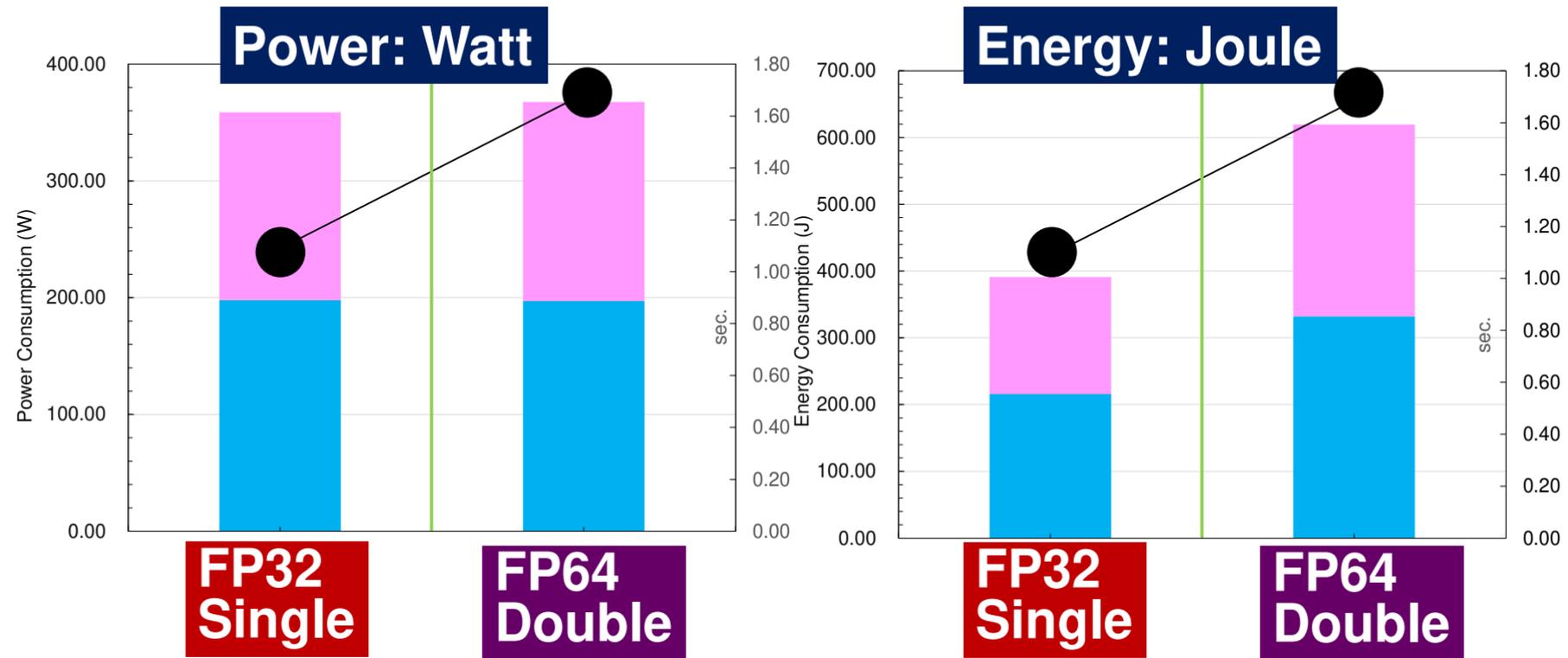
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Results on Intel Xeon BDW $\lambda_1 = \lambda_2$

[Sakamoto et al. 2020]

$N=128^3$, ■: CPU, ■: Memory, ●: Time



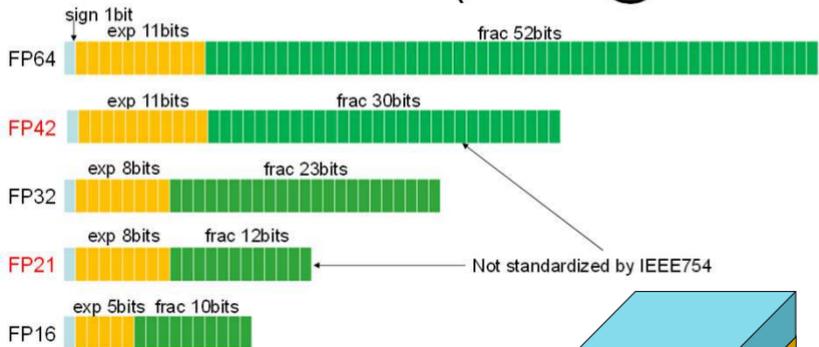
Approximate Computing with Low/Adaptive/Trans Precision

- Accuracy verification is important, especially for computation with lower/mixed precision.
- A lot of methods for accuracy verification have been developed for problems with dense matrices
 - But very few examples for
- Generally speaking, process expensive
 - Sophisticated Method needed
 - Automatic Selection of Optimum Precision by Technology of AT (Auto Tuning)
- [Accuracy Verification of Sparse Linear Solvers \[Ogita, Nakajima 2019\]](#)

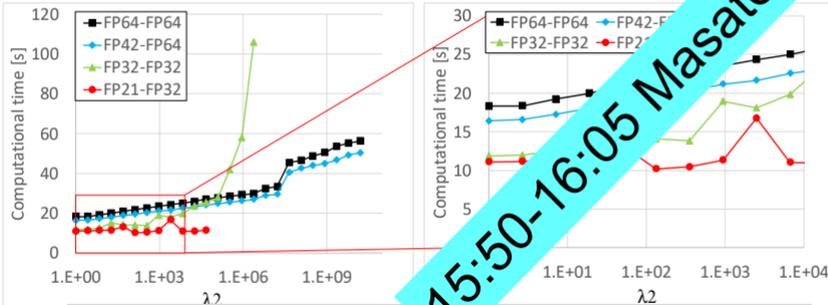
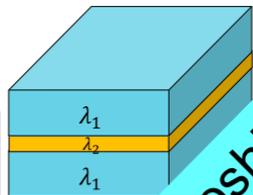
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Adaptive Precision Computing with FP21/FP42

Masatoshi Kawai (kawai@cc.u-tokyo.ac.jp)



Heat Conduction with Heterogeneous Material Property



Computation Time for ICCG Solver
Various Types of Precisions on Intel Xeon Cascadelake

In recent years, the usefulness of low-precision floating-point representation has been realized in various fields such as machine learning. Low accuracy can be expected to have effects such as shortening calculation time and reducing power consumption. For example, in applications with a memory bandwidth bottleneck, the effect of shortening the calculation time by reducing the amount of memory transfer is significant. However, in fields such as iterative methods, it is common to use FP64 because the calculation accuracy greatly affects the convergence, and there are few application examples of low-precision arithmetic. This study investigates the applicability of low-precision representation to the Krylov subspace and stationary iterative methods. In this research, we focus on the FP32, FP16, and FP42, FP21, which are not standardized by IEEE754. Developed method has been evaluated for ICCG solver, which solves linear equations derived from 3D FVM code for steady-state head conduction with heterogeneous material property ($\lambda_1=10^0$, $\lambda_2=10^0\sim 10^9$). Generally, computation with lower precision (e.g. FP32-FP32, FP21-FP32) becomes unstable, if condition number of the coefficient matrix is larger (λ_2 is larger), FP21-FP32 provides the best performance if λ_2 is up to 10^4 . (“FP21-FP32” means “matrices are in FP21, and vectors are in FP32”).

15:50-16:05 Masatoshi Kawai (Nagoya U.)

h3-Open-BDEC Innovative Software Platform for Integration of (S+D+L) on the BDEC System, such as Wisteria/BDEC-01



- “Three” Innovations

- New Principles for Numerical Analysis by Adaptive Precision Automatic Tuning & Accuracy Verification

- Integration of (S+D+L) by Hierarchical Data Driven Approach (*hDDA*)

- Software & Utilities for Heterogeneous Environment, such as Wisteria/BDEC-01

14:00-14:15 Hiromichi Nagao (U.Tokyo)

14:15-14:30 Takashi Shimokawabe (U.Tokyo)

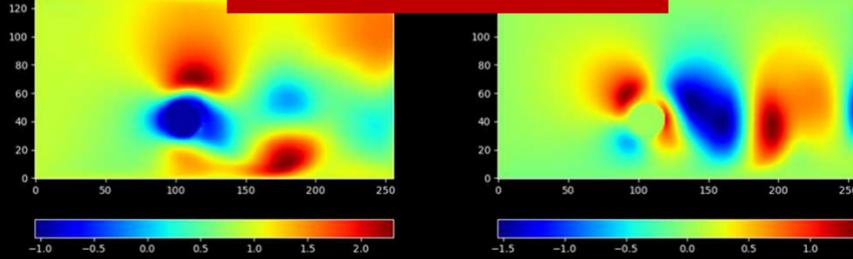
16:35-16:50 Hayato Shiba (U.Hyogo)

New Principle for Computations	Simulation + Data Learning	Communications+ Utilities
h3-Open-MATH Algorithms with High-Performance, Reliability, Efficiency	h3-Open-APP: Simulation Application Development	h3-Open-SYS Control & Integration
h3-Open-VER Verification of Accuracy	h3-Open-DATA: Data Data Science	h3-Open-UTIL Utilities for Large-Scale Computing
h3-Open-AT Automatic Tuning	h3-Open-DDA: Learning Data Driven Approach	

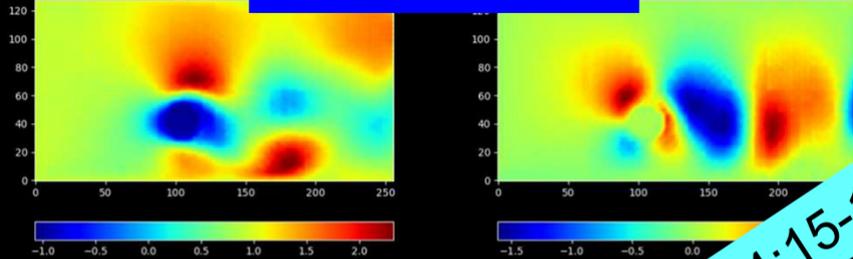
Prediction of CFD Simulation by ML/CNN

Takashi Shimokawabe (shimokawabe@cc.u-tokyo.ac.jp)

Simulations: LBM



CNN Predictions



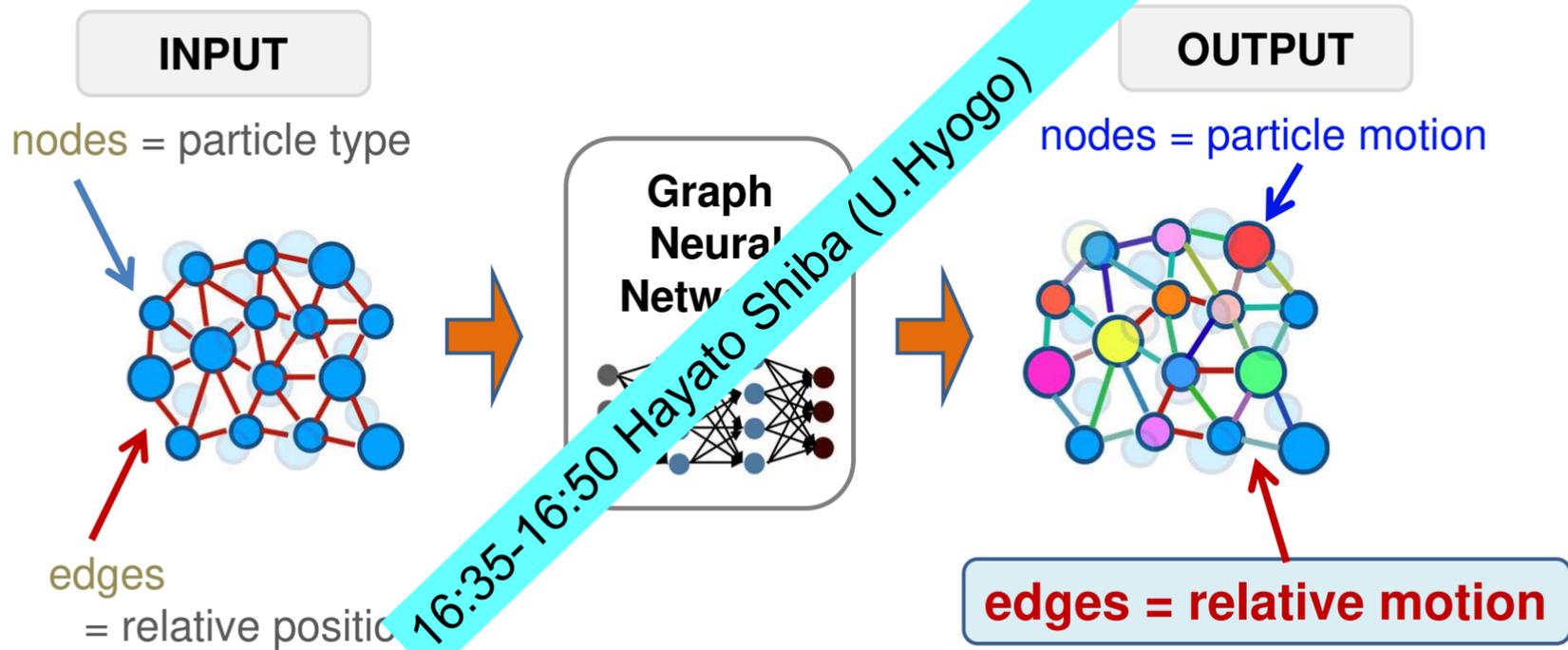
Computational fluid dynamics (CFD) is widely used in science and engineering. However, since CFD simulations requires a large number of grid points and particles for these calculations, these kinds of simulations demand a large amount of computational resources such as supercomputers. Recently, deep learning has attracted attention as a surrogate method for obtaining simulation results by CFD simulation approximately at half the cost. We are working on a project to develop a parallelized method to make it possible to apply the surrogate method to the deep learning to large scale geometry. Unlike the conventional parallel computing, the method we are currently developing divides large-scale steady flow simulation results by dividing the input geometry into multiple parts and applying a small neural network to each part in parallel. This method is developed based on considering the characteristics of CFD simulation and the consistency of the boundary condition of each subdomain. By using the physical values on the adjacent subdomains as boundary conditions, applying deep learning to each subdomain can predict simulation results consistently in the entire computational domain. It is possible to predict the simulation results in about 36.9 seconds by the developed method, compared to about 286.4 seconds by the conventional numerical method. In addition to this, we are also attempting to develop a method for fast prediction of time evolution calculations using deep learning.

14:15-14:30 Takashi Shimokawabe (U.Tokyo)

Comparison of the flow velocity results obtained by the conventional simulation (upper) and the prediction of these results by deep learning (lower)

Machine learning slow molecular dynamics

Our proposal — **B**Ond Targeting Network (BONN)

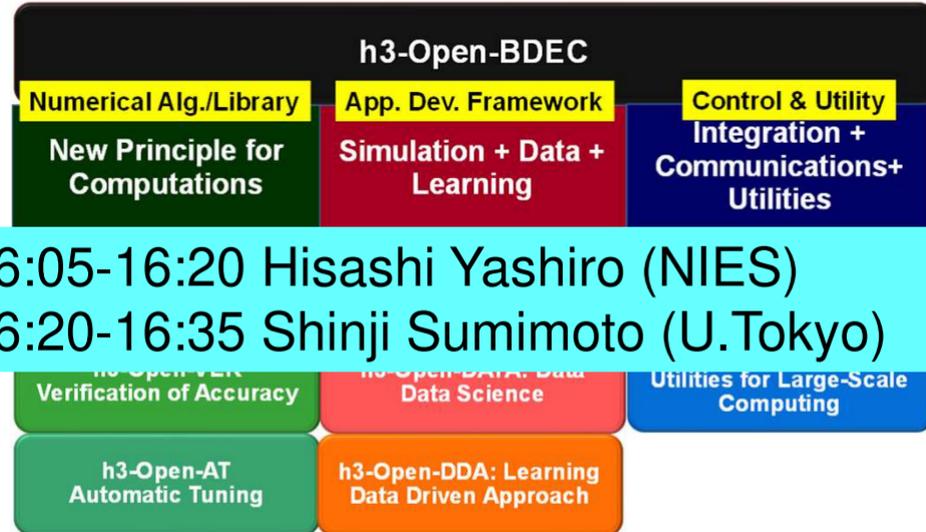


h3-Open-BDEC Innovative Software Platform for Integration of (S+D+L) on the BDEC System, such as Wisteria/BDEC-01

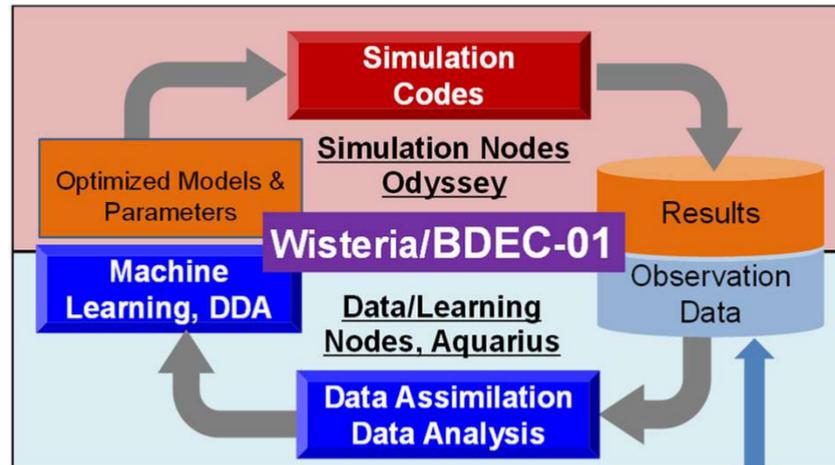
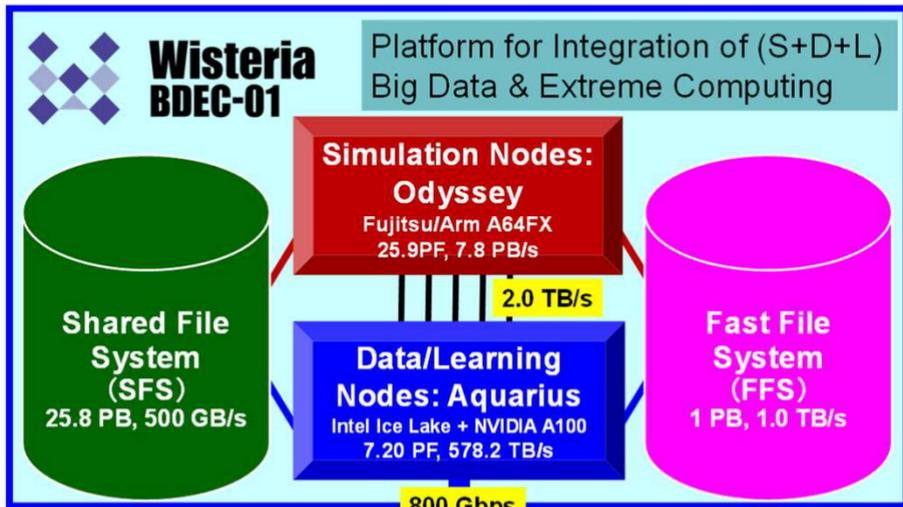


- “Three” Innovations

- New Principles for Numerical Analysis by Adaptive Precision, Automatic Tuning & Accuracy Verification
- Integration of (S+D+L) by Hierarchical Data Driven Approach (*hDDA*)
- Software & Utilities for Heterogenous Environment, such as Wisteria/BDEC-01



Wisteria/BDEC-01: The First “Really Heterogenous” System in the World



External Resources



External Network



External Resources

Server,
Storage,
DB,
Sensors,
etc.



External Network

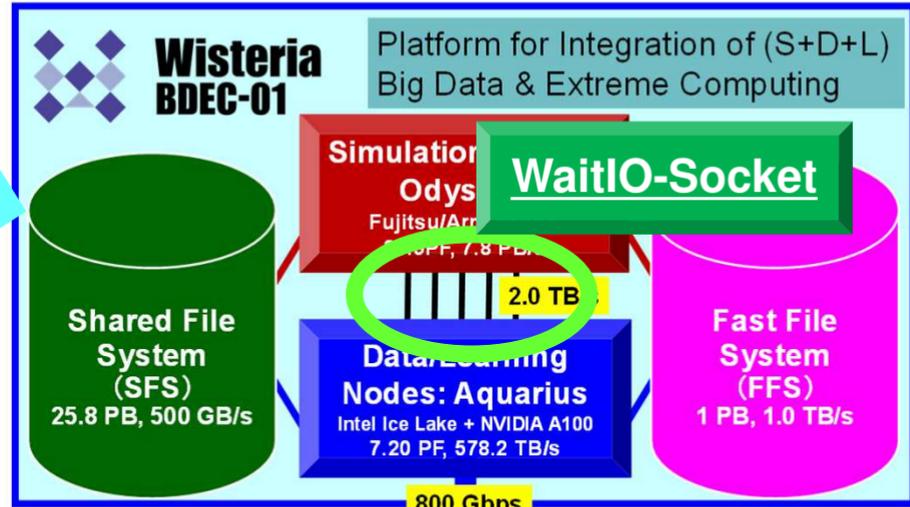


External Resources

h3-Open-SYS/WaiIO-Socket

- Wisteria/BDEC-01
 - Aquarius (GPU: NVIDIA A100)
 - Odyssey (CPU: A64FX)
- Combining Odyssey-Aquarius
 - Single MPI Job over O-A is impossible
- **Connection between Odyssey-Aquarius**
 - IB-EDR 2TB/sec.
 - Fast File System
- **h3-Open-SYS/WaiIO-Socket**
 - Library for Inter-Process Communication through IB-EDR with MPI-like interface

16:20-16:35 Shinji Sumimoto (U.Tokyo)



External Resources

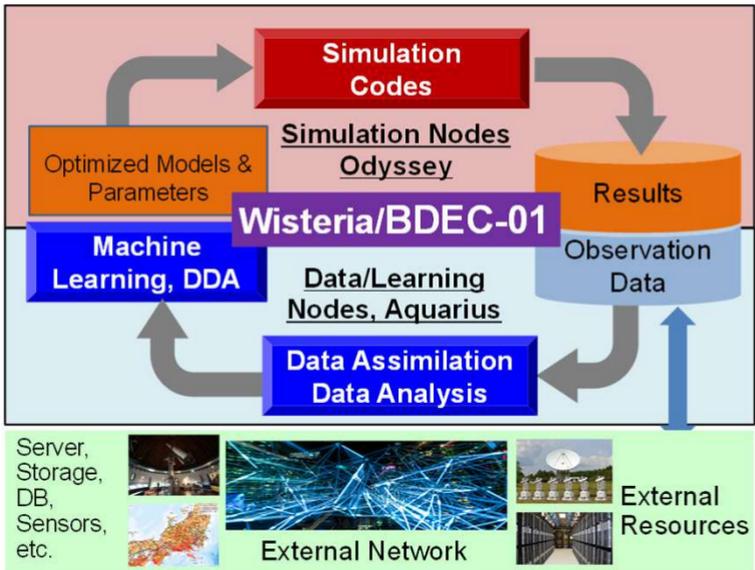


External Network

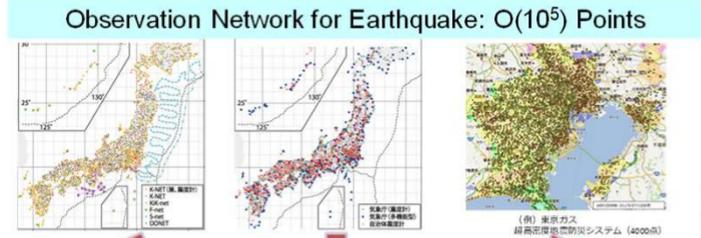


External Resources

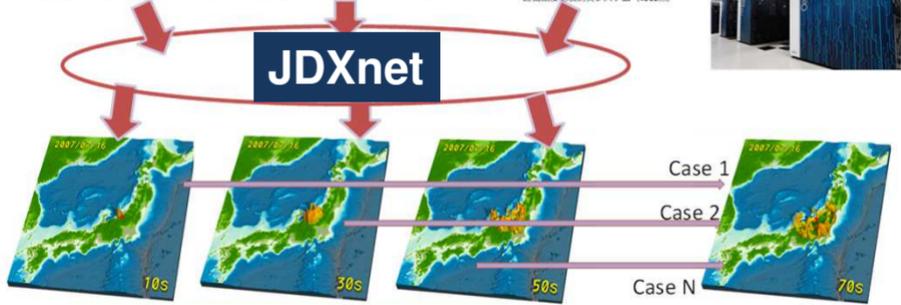
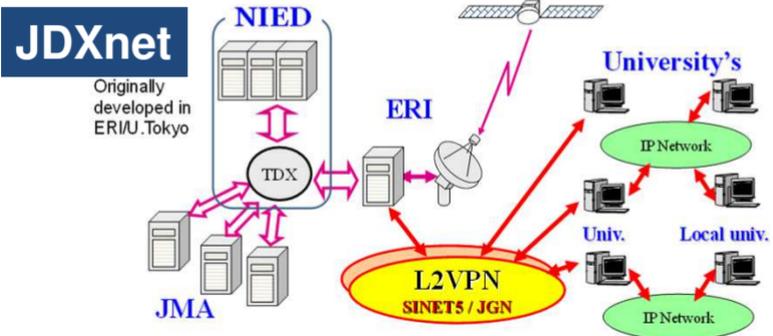
- Integration of (Simulation/Data/Learning)
 - Wisteria/BDEC-01
 - h3-Open-BDEC
- **Applications on Wisteria/BDEC-01 with h3-Open-BDEC**
 - **Seismic Wave Propagation**
 - Global Atmosphere
 - International/Domestic Collaborations
- Integration of (Simulation/Data/Learning) and Beyond
- Summary



3D Earthquake Simulation with Real-Time Data Observation/Assimilation Simulation of Strong Motion (Wave Propagation) by 3D FDM



[c/o Furumura]

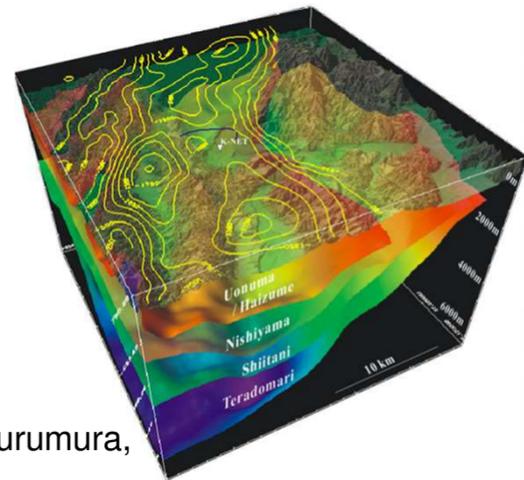
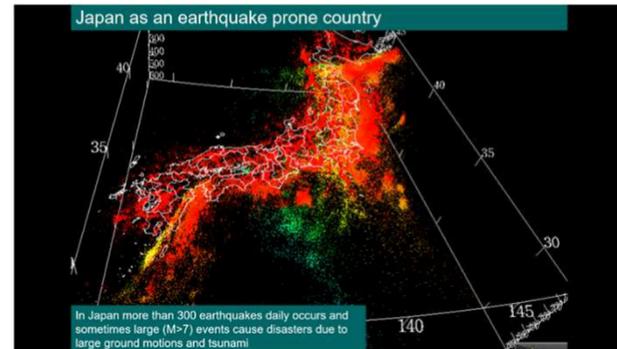


Real-Time Data/Simulation Assimilation
Real-Time Update of Underground Model

[c/o Prof. T.Furumura (ERI/U.Tokyo)]

Earthquake simulation is always with uncertainty

- Subsurface/Underground Structure
 - Heterogenous, Random, Stochastic
 - Fluctuations
- Traditional Simulations
 - Forward Simulations
- **Integration of Simulation/Observation is essential**
- **New Types of Methods for Simulations combined with Data Assimilation/Real-Time Observation is under development**
 - Forecast by Simulations, Correction by Data Assimilation



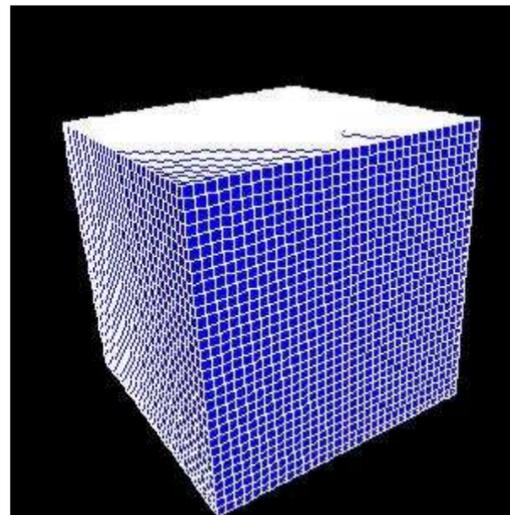
[c/o Prof. T. Furumura,
ERI/U.Tokyo]

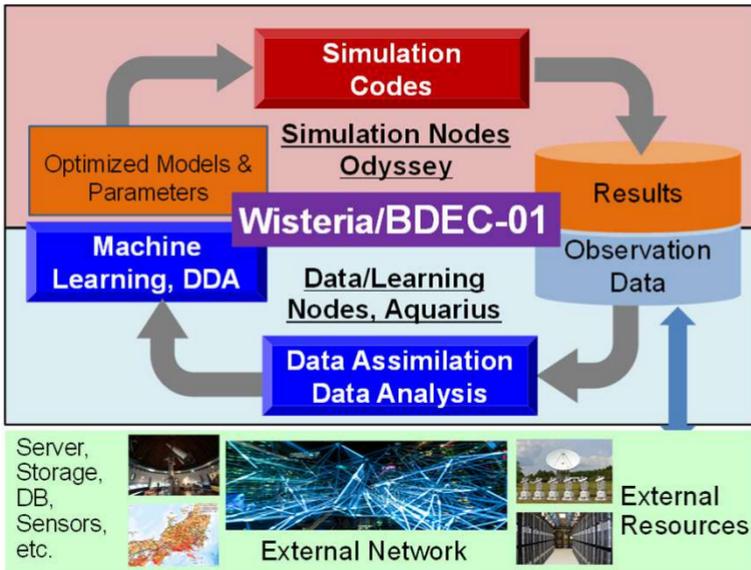
Simulations of Long-Period Ground Motion [Furumura et al.]

- 3D Equation of Motions solved by FDM (Finite-Difference Method)

$$v_p^n = v_p^{n-1} + \frac{1}{\rho} \left(\frac{\partial \sigma_{xp}^{n-1/2}}{\partial x} + \frac{\partial \sigma_{yp}^{n-1/2}}{\partial y} + \frac{\partial \sigma_{zp}^{n-1/2}}{\partial z} \right) \Delta t \quad (p = x, y, z)$$

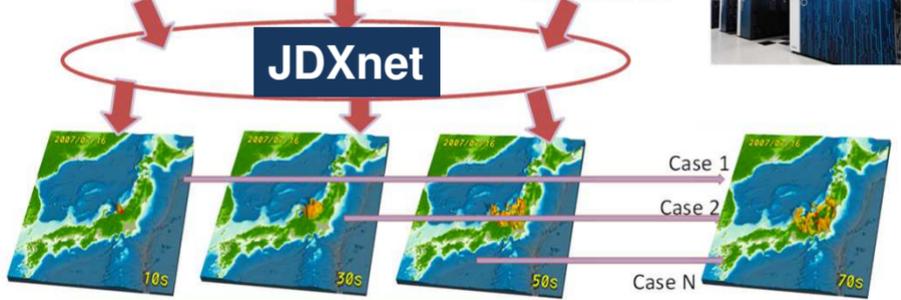
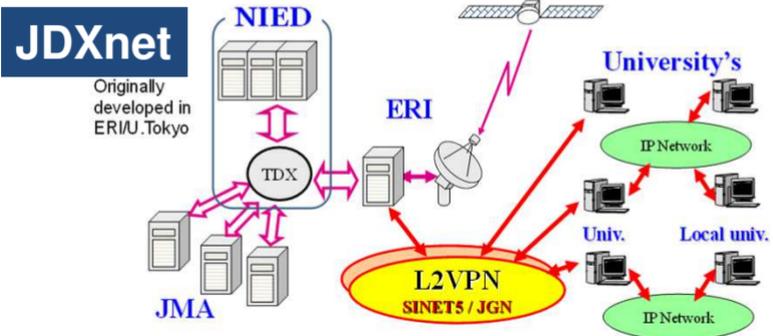
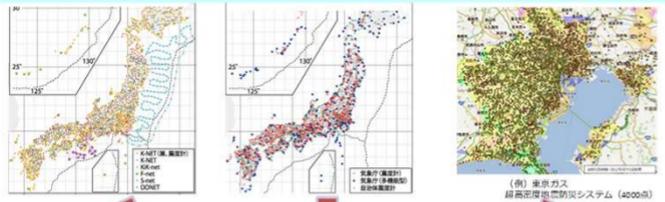
- Seism3D
 - Staggered Discretization in Space/Time
 - 4th order in Space
 - 2nd order in Time (Explicit Time Marching)
 - OpenMP + MPI, Fortran





3D Earthquake Simulation with Real-Time Data Observation/Assimilation Simulation of Strong Motion (Wave Propagation) by 3D FDM

Observation Network for Earthquake: $O(10^5)$ Points



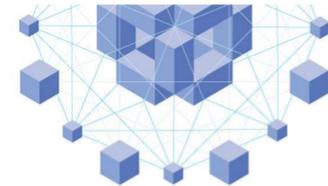
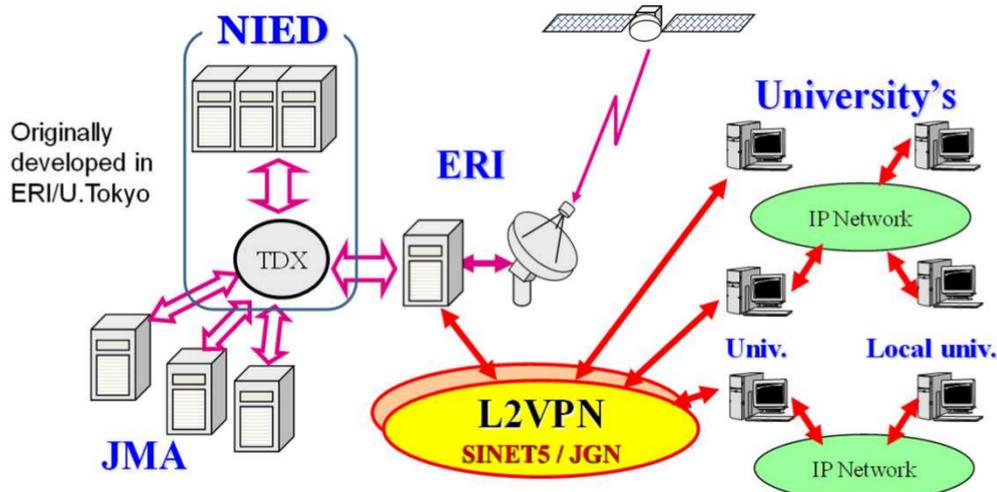
Real-Time Data/Simulation Assimilation
Real-Time Update of Underground Model

[c/o Prof. T.Furumura (ERI/U.Tokyo)]

Real-Time Sharing of Seismic Observation is possible in Japan by JDXnet with SINET

Japan Data eXchange network

- Seismic Observation Data (100Hz/3-dir's/O(10³) observation points) by JDXnet is available through SINET in Real Time
 - O(10²) GB/day: available at Website of NIED
 - O(10⁵) pts in future including stations operated by industry



[c/o Prof. H.Tsuruoka
(ERI/U.Tokyo)]

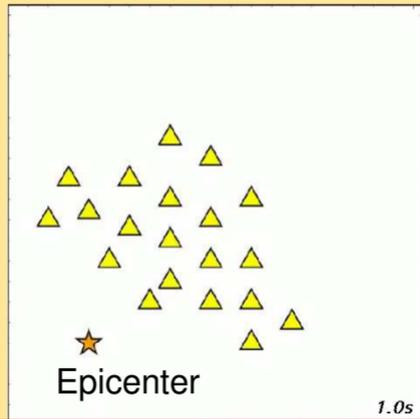
Real-Time Assimilation of “Observation+Computation” in Seismic Wave Propagation [c/o Oba & Furumura]

- Data Assimilation of Wave Propagation by “Optimal Interpolation Technique”

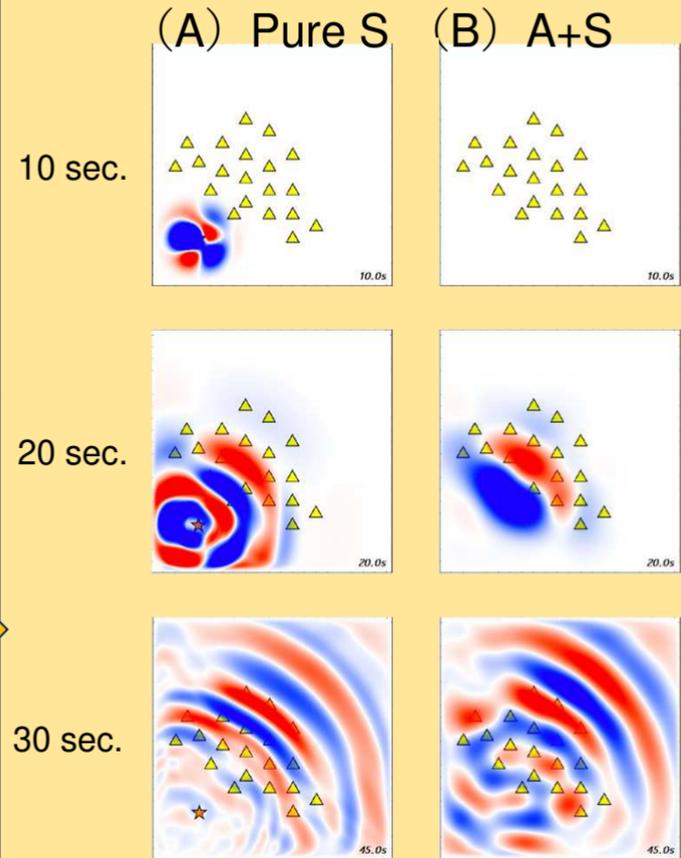
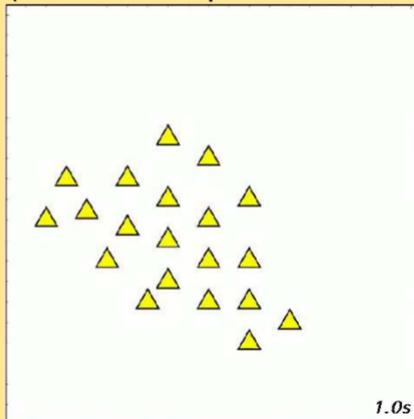
$$\begin{array}{c}
 \text{Assim.} \quad \text{Comp.} \quad \text{Residual} \quad \text{Comp.} \quad n: \text{Time Step} \\
 \mathbf{x}_n^a = \mathbf{x}_n^f + \mathbf{W}(\mathbf{y}_n - \mathbf{H}\mathbf{x}_n^f) \quad \mathbf{W}: \text{Weighting Matrix} \\
 \text{Comp.} \quad \text{Assim.} \quad \text{F: Wave Propagation} \\
 \mathbf{x}_{n+1}^f = \mathbf{F}\mathbf{x}_n^a \quad \text{simulation}
 \end{array}$$

(A) Pure Simulation

▲ : Obs. Pts.



(B) Assimilation+Sim. (No info for Epicenter needed)



Real-Time Assimilation of “Observation+Computation” in Seismic Wave Propagation [c/o Oba & Furumura]

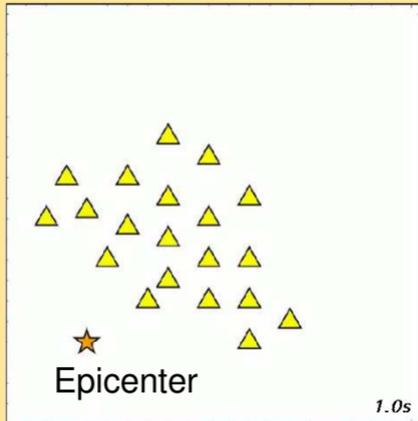
- Data Assimilation of Wave Propagation by “Optimal Interpolation Technique”

$$\begin{array}{c}
 \text{Assim.} \quad \text{Comp.} \\
 \mathbf{x}_n^a = \mathbf{x}_n^f + \mathbf{W}(\mathbf{y}_n - \mathbf{H}\mathbf{x}_n^f) \\
 \text{Comp.} \quad \text{Assim.} \\
 \mathbf{x}_{n+1}^f = \mathbf{F}\mathbf{x}_n^a
 \end{array}$$

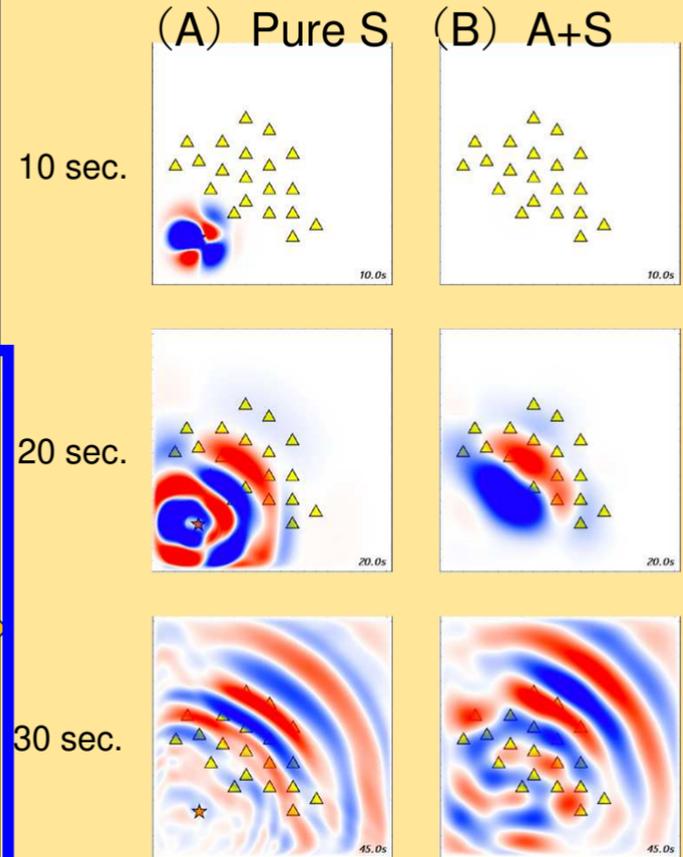
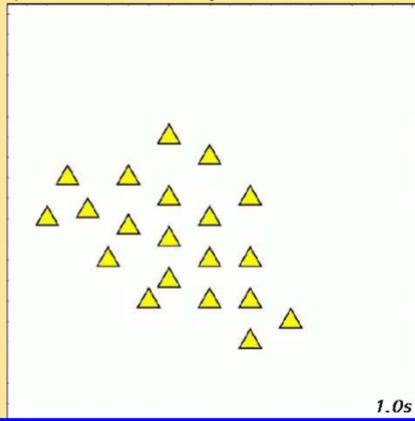
\mathbf{y}_n : Residual Obs. \mathbf{H} : Residual Comp. n : Time Step
 \mathbf{W} : Weighting Matrix
 \mathbf{F} : Wave Propagation simulation

(A) Pure Simulation

▲ : Obs. Pts



(B) Assimilation+Sim. (No info for Epicenter needed)



Starting from (A+S: Assim+Sim.) to (Pure S: Pure Simulation)

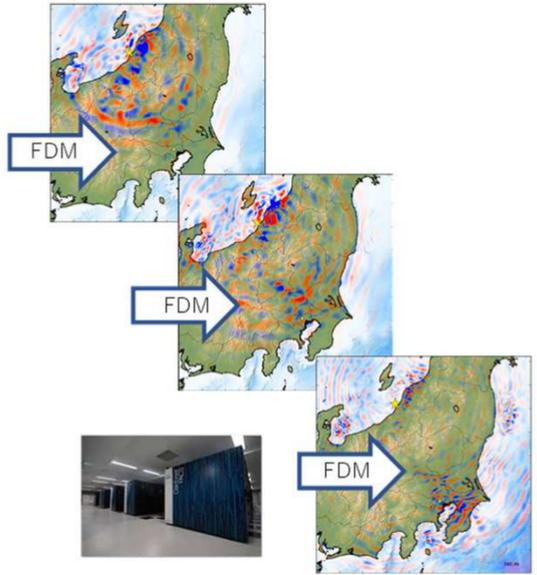
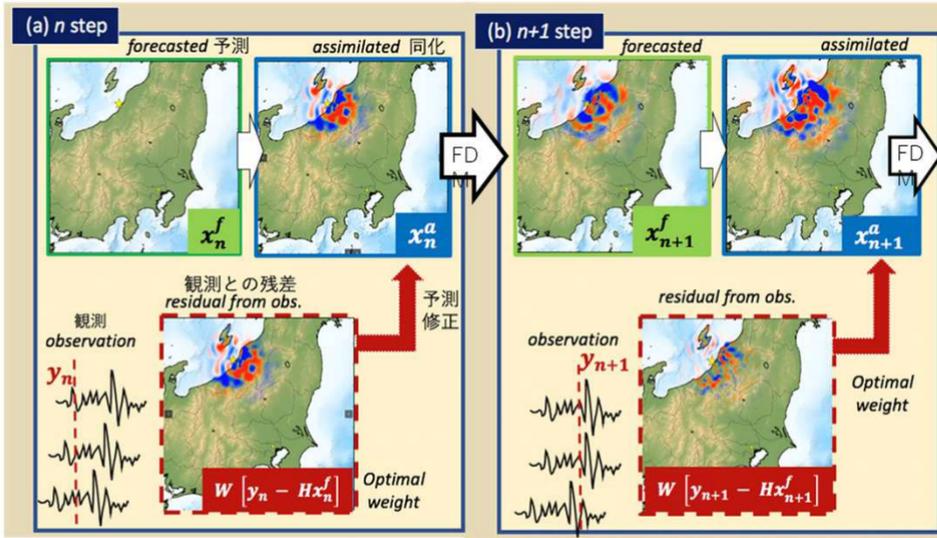
$$\begin{aligned}
 \text{Assim. Comp.} \quad & x_n^a = x_n^f + W(y_n - Hx_n^f) \\
 \text{Comp.} \quad & x_{n+1}^f = Fx_n^a
 \end{aligned}$$

n : Time Step
 W : Weighting Matrix
 F : Wave Propagation simulation

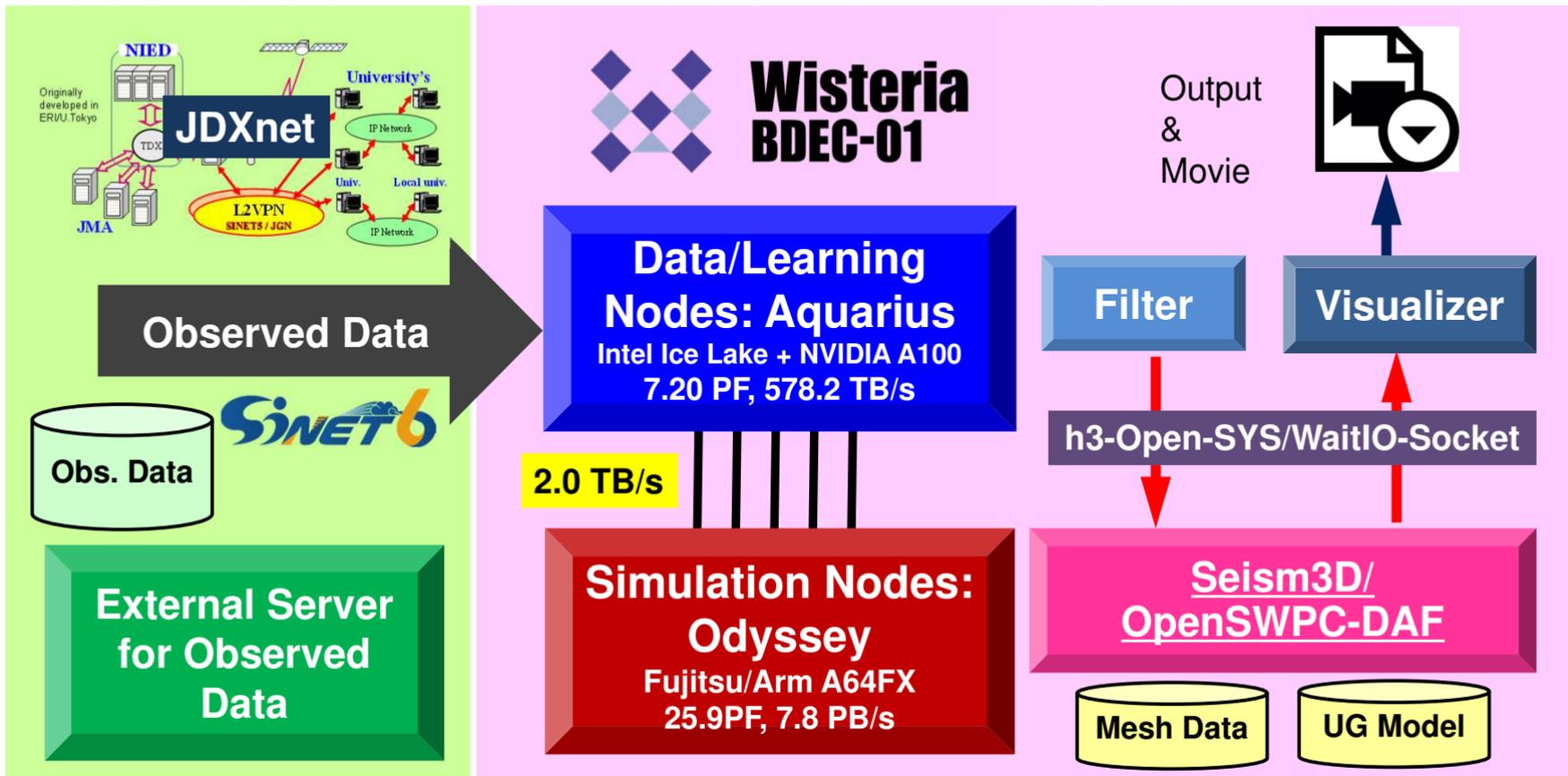
(A+S) Assimilation+Simulation



(Pure S) Pure Simulation/Forecast



3D Earthquake Simulation with Real-Time Data Observation/Assimilation on Wisteria/BDEC-01



Communications by WaitIO-Socket

[Kasai et al. 2021]

Aquarius: SEND

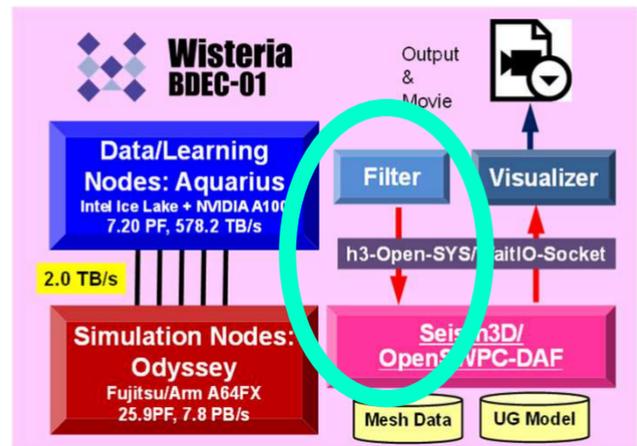
```
program dmy_filter
<省略: 型宣言等>
call mpi_init (ierr)
call mpi_comm_size (MPI_COMM_WORLD, nprocs, ierr)
call mpi_comm_rank (MPI_COMM_WORLD, myrank, ierr)
call WAITIO_CREATE_UNIVERSE (WAITIO_COMM_UNIVERSE, ierr)

if (myrank==0) then
open(100,file='./obsfile_list.txt', form='formatted', status='old', iostat=ierr)
do i=1,300
<省略: obsデータ読み込み処理>
print *, "Send obs data ....."
call WAITIO_MPI_ISEND (NTMAX1_o, 1, WAITIO_MPI_INTEGER, 2,1, WAITIO_COMM_UNIVERSE,req(1,1), ierr)
call WAITIO_MPI_ISEND (DT_o, 1, WAITIO_MPI_FLOAT, 2,2, WAITIO_COMM_UNIVERSE,req(1,2), ierr)
call WAITIO_MPI_ISEND (NST_o, 1, WAITIO_MPI_INTEGER, 2,3, WAITIO_COMM_UNIVERSE,req(1,3), ierr)
call WAITIO_MPI_ISEND (AT_o, 1, WAITIO_MPI_FLOAT, 2,4, WAITIO_COMM_UNIVERSE,req(1,4), ierr)
call WAITIO_MPI_ISEND (T0_o, 1, WAITIO_MPI_FLOAT, 2,5, WAITIO_COMM_UNIVERSE,req(1,5), ierr)
call WAITIO_MPI_ISEND (ISO_X_o, NSMAX, WAITIO_MPI_INTEGER, 2,6, WAITIO_COMM_UNIVERSE,req(1,6), ierr)
call WAITIO_MPI_ISEND (ISO_Y_o, NSMAX, WAITIO_MPI_INTEGER, 2,7, WAITIO_COMM_UNIVERSE,req(1,7), ierr)
call WAITIO_MPI_ISEND (ISO_Z_o, NSMAX, WAITIO_MPI_INTEGER, 2,8, WAITIO_COMM_UNIVERSE,req(1,8), ierr)
call WAITIO_MPI_ISEND (ISTX_o, NST, WAITIO_MPI_INTEGER, 2,9, WAITIO_COMM_UNIVERSE,req(1,9), ierr)
call WAITIO_MPI_ISEND (ISTY_o, NST, WAITIO_MPI_INTEGER, 2,10, WAITIO_COMM_UNIVERSE,req(1,10), ierr)
call WAITIO_MPI_ISEND (ISTZ_o, NST, WAITIO_MPI_INTEGER, 2,11, WAITIO_COMM_UNIVERSE,req(1,11), ierr)
call WAITIO_MPI_ISEND (STC_o, 6*NST, WAITIO_MPI_INTEGER, 2,12, WAITIO_COMM_UNIVERSE,req(1,12), ierr)
call WAITIO_MPI_ISEND (VxAll_obs, NST*NOBS_LEN, WAITIO_MPI_FLOAT, 2,13, WAITIO_COMM_UNIVERSE,req(1,13), ierr)
call WAITIO_MPI_ISEND (VyAll_obs, NST*NOBS_LEN, WAITIO_MPI_FLOAT, 2,14, WAITIO_COMM_UNIVERSE,req(1,14), ierr)
call WAITIO_MPI_ISEND (VzAll_obs, NST*NOBS_LEN, WAITIO_MPI_FLOAT, 2,15, WAITIO_COMM_UNIVERSE,req(1,15), ierr)
call WAITIO_MPI_WAITALL (15,req, status, ierr)
call sleep(1)
enddo
close (100)
endif
call WAITIO_FINALIZE (ierr)
call mpi_finalize (ierr)
end
```

Odyssey: RECV

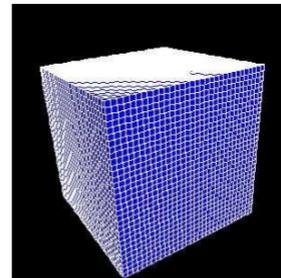
```
call WAITIO_MPI_RECV (NTMAX1_o, 1, WAITIO_MPI_INTEGER, 0,1, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (DT_o, 1, WAITIO_MPI_FLOAT, 0,2, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (NST_o, 1, WAITIO_MPI_INTEGER, 0,3, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (AT_o, 1, WAITIO_MPI_FLOAT, 0,4, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (T0_o, 1, WAITIO_MPI_FLOAT, 0,5, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (ISO_X_o, NSMAX, WAITIO_MPI_INTEGER, 0,6, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (ISO_Y_o, NSMAX, WAITIO_MPI_INTEGER, 0,7, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (ISO_Z_o, NSMAX, WAITIO_MPI_INTEGER, 0,8, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (ISTX_o, NST, WAITIO_MPI_INTEGER, 0,9, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (ISTY_o, NST, WAITIO_MPI_INTEGER, 0,10, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (ISTZ_o, NST, WAITIO_MPI_INTEGER, 0,11, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (STC_o, 6*NST, WAITIO_MPI_INTEGER, 0,12, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (VxAll_obs, NST*NOBS_LEN, WAITIO_MPI_FLOAT, 0,13, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (VyAll_obs, NST*NOBS_LEN, WAITIO_MPI_FLOAT, 0,14, WAITIO_COMM_UNIVERSE,...)
call WAITIO_MPI_RECV (VzAll_obs, NST*NOBS_LEN, WAITIO_MPI_FLOAT, 0,15, WAITIO_COMM_UNIVERSE,...)
```

16:20-16:35 Shinji Sumimoto (U.Tokyo)



Example: Off Niigata 2007 Mw6.6 Earthquake

- Observed Data: Stored in External Server
- Aquarius receives observed data, and apply filtering
- “Data Assimilation + Simulation (A+S)”, and “Forecast by Simulation (Pure S)” are separated codes, while same number of computing nodes were used on Odyssey
- Movies were created after simulations (O(10) sec.)



Seism3D/OpenSWPC-DAF

– 3D FDM + Optimal Interpolation Technique for Data Assimilation

– Each Mesh: 240m × 240m × 240m

– 1,920 × 1,920 × 240 meshes (8.85 × 10⁸)

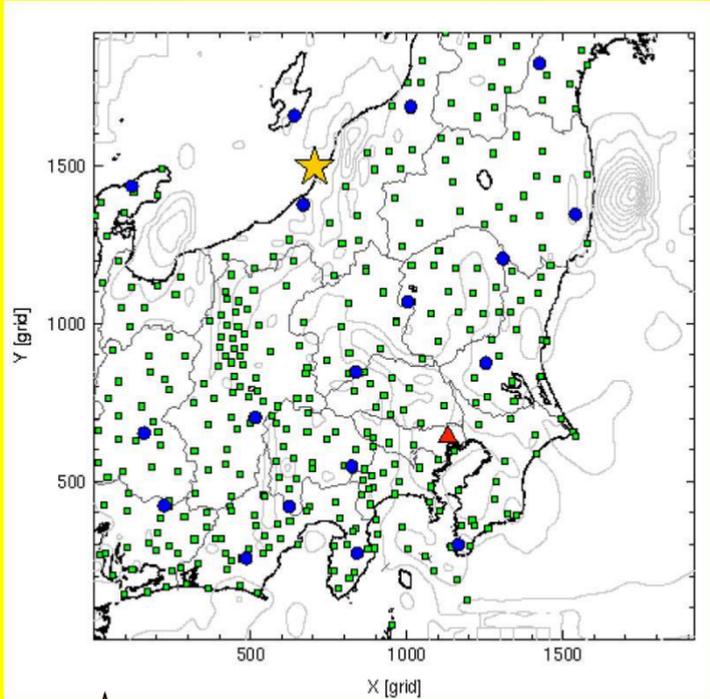
– 460.8 km × 460.8 km × 57.6 km

$$v_p^n = v_p^{n-1} + \frac{1}{\rho} \left(\frac{\partial \sigma_{xp}^{n-1/2}}{\partial x} + \frac{\partial \sigma_{yp}^{n-1/2}}{\partial y} + \frac{\partial \sigma_{zp}^{n-1/2}}{\partial z} \right) \Delta t \quad (p = x, y, z)$$

$$\begin{array}{l} \text{Assim. Comp.} \quad \text{Residual} \quad \text{Obs.} \quad \text{Comp.} \quad n: \text{Time Step} \\ \mathbf{x}_n^a = \mathbf{x}_n^f + \mathbf{W}(\mathbf{y}_n - \mathbf{H}\mathbf{x}_n^f) \quad \mathbf{W}: \text{Weighting Matrix} \\ \text{Comp.} \quad \text{Assim.} \\ \mathbf{x}_{n+1}^f = \mathbf{F}\mathbf{x}_n^a \quad \mathbf{F}: \text{Wave Propagation simulation} \end{array}$$

Off Niigata 2007 Mw6.6 Earthquake

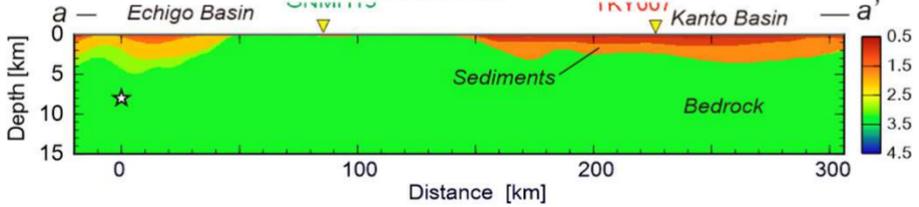
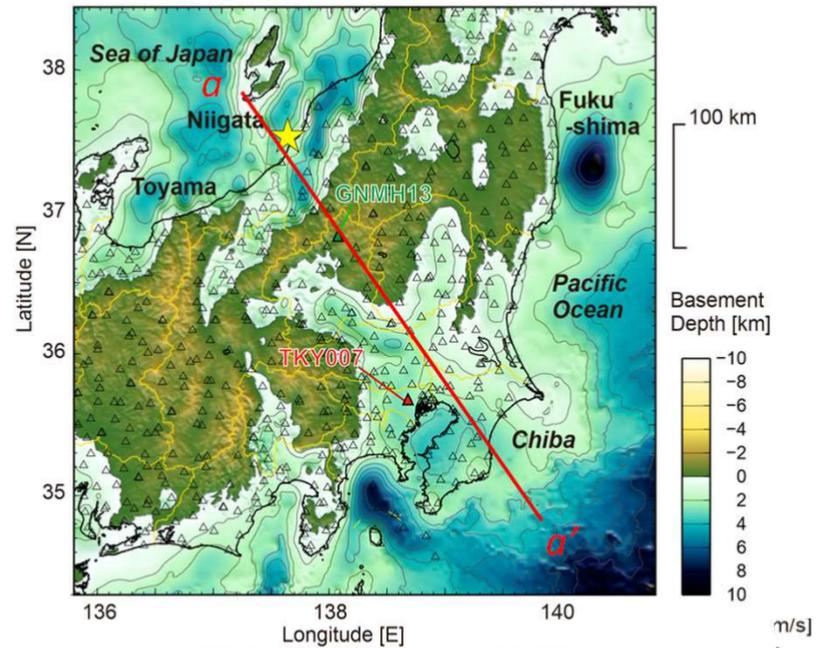
[c/o Prof. T. Furumura, ERI/U.Tokyo]



★ Epicenter

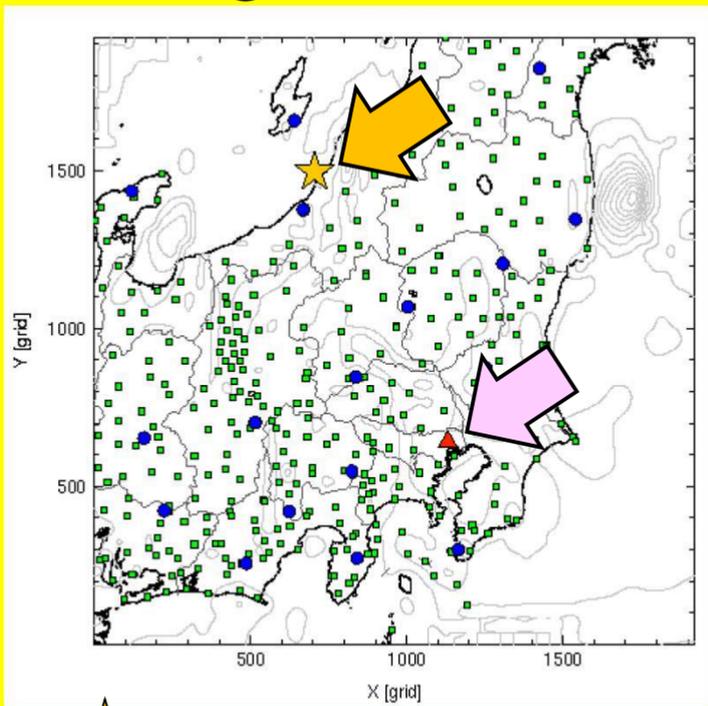
■ Hi-net (Short Period) 349 pts

● F-net (Broadband) 18 pts



Off Niigata 2007 Mw6.6 Earthquake

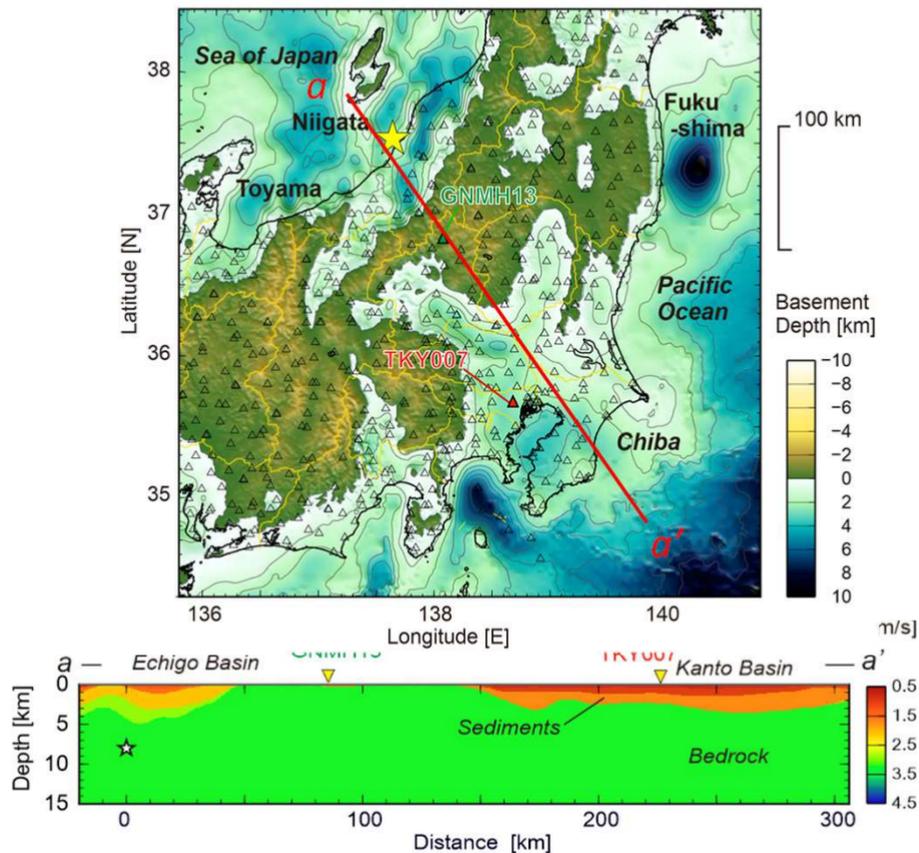
[c/o Prof. T. Furumura,
ERI/U.Tokyo]



★ Epicenter

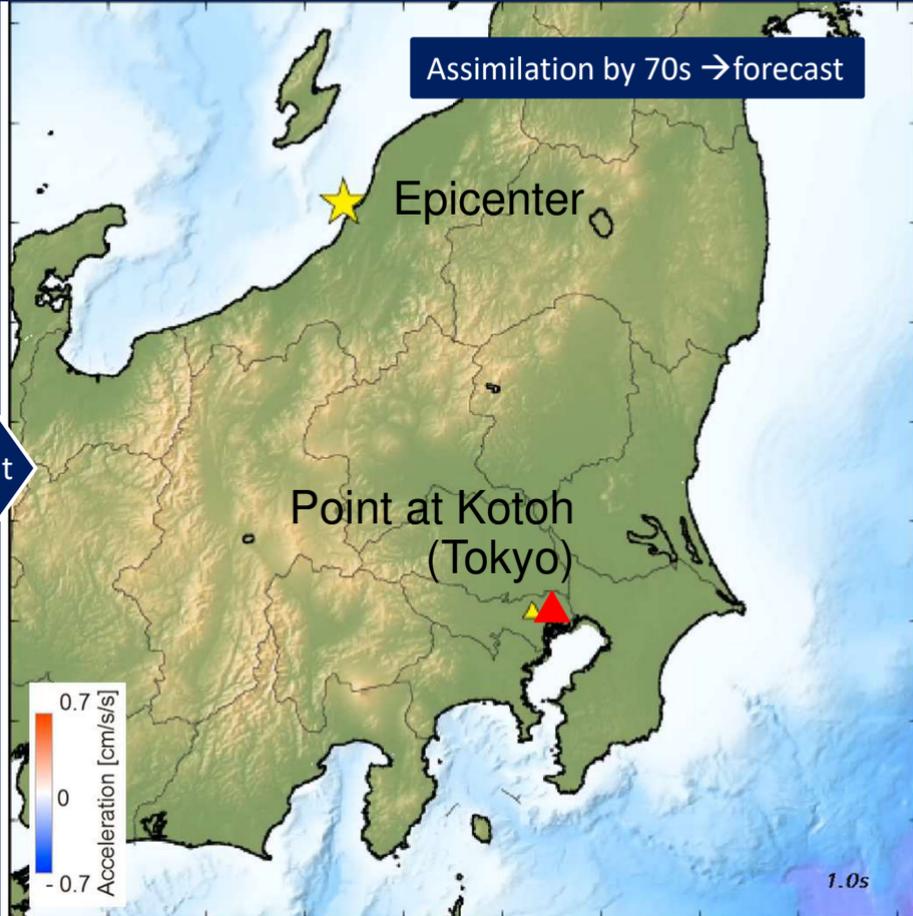
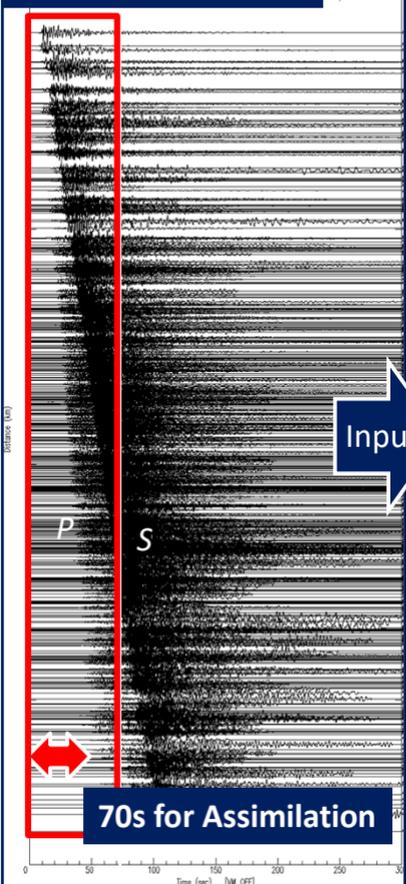
■ Hi-net (Short Period) 349 pts

● F-net (Broadband) 18 pts

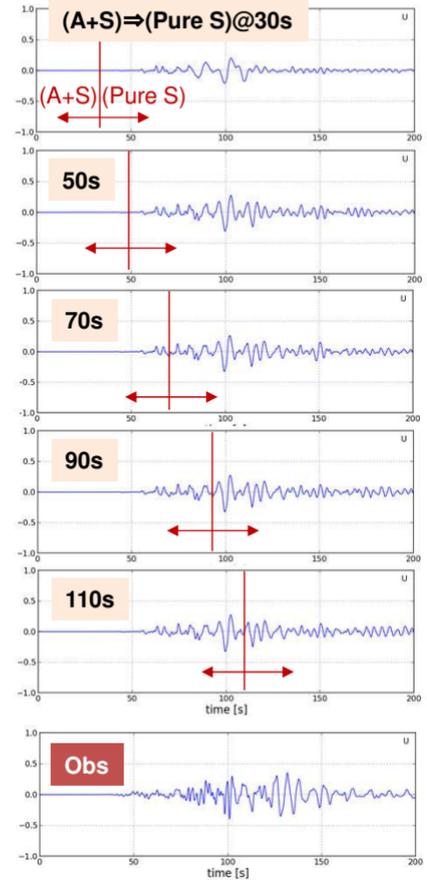


Data Assimilation + Pure Simulation/Forecast

482 K-NET, KiK-net Observation

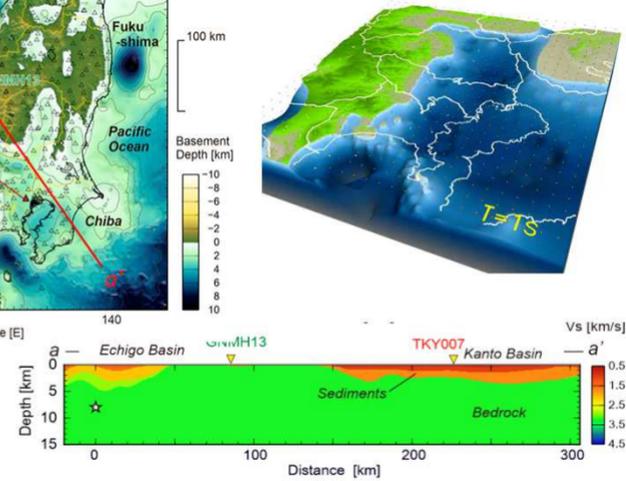
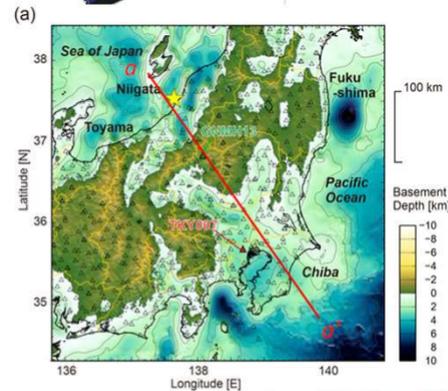
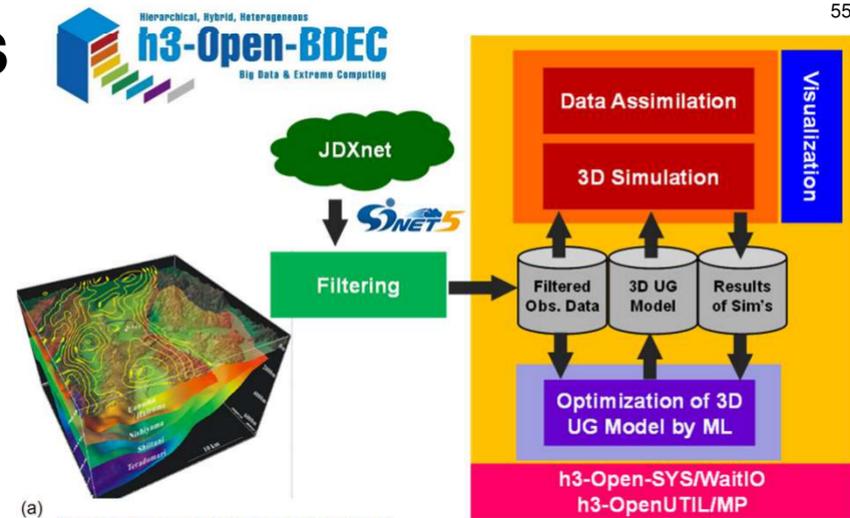


Results at Kotoh ▲ (N.KOTH)
N 35° 37.0'
E 139° 46.9'



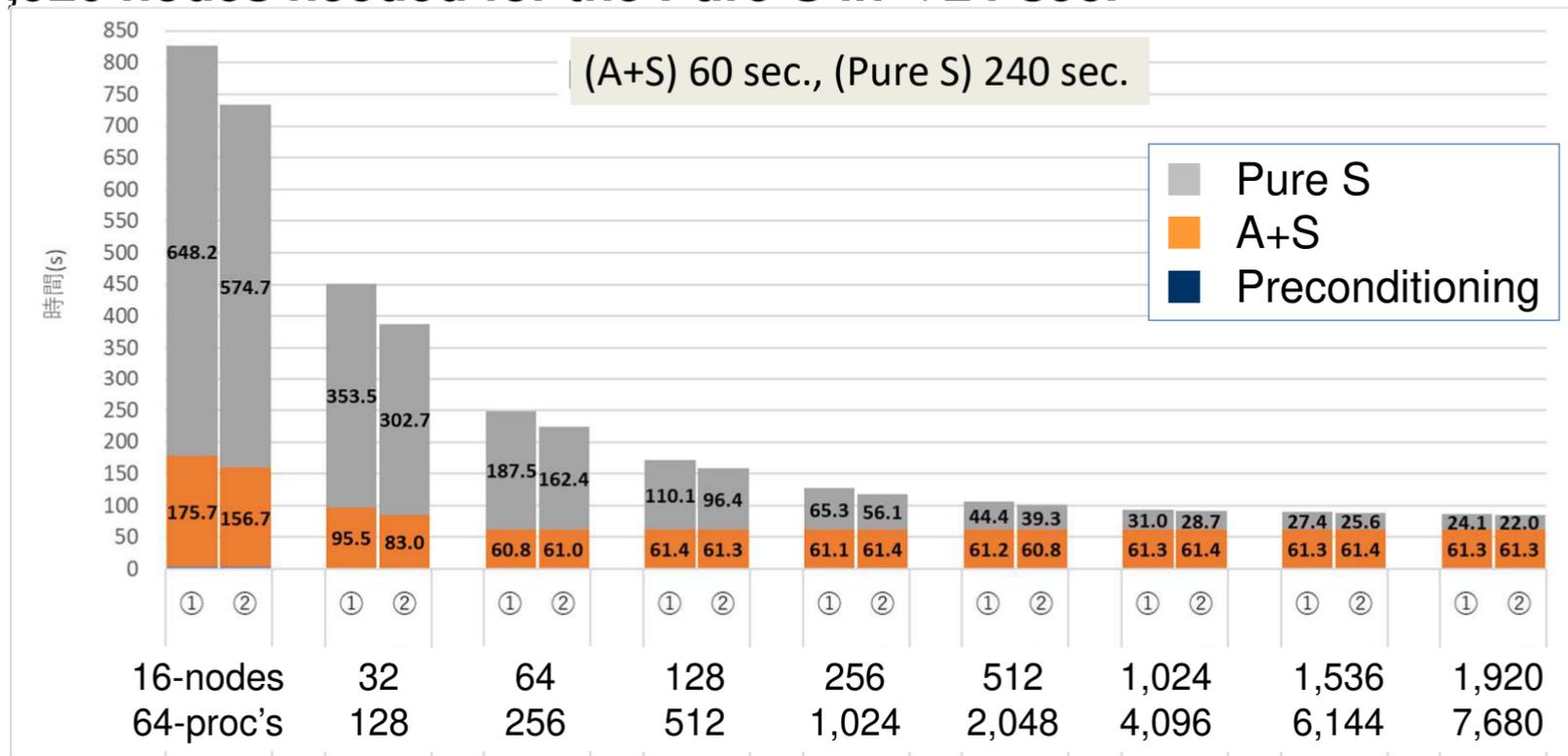
Future Directions towards Integration of (S+D+L)

- Accurate Prediction of Seismic Wave Propagation with Real-Time Data Observation/Assimilation
 - Emergency Info. for Safer Evacuation
 - 10x faster than real phenomena with $O(10^3)$ nodes of supercomputers



(A+S) for 60-sec and (Pure S) for 240-sec on Odyssey, ①②: without/with scalar tuning

1,920 nodes needed for the Pure-S in < 24-sec.

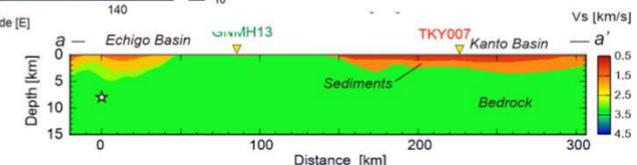
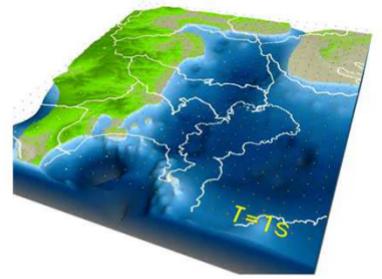
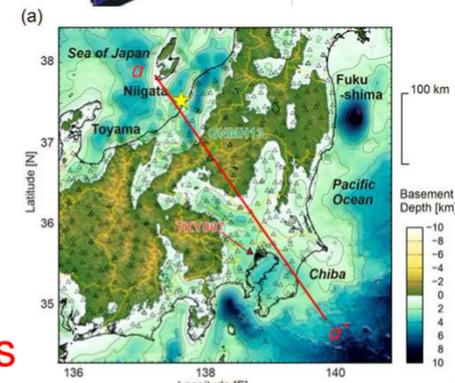
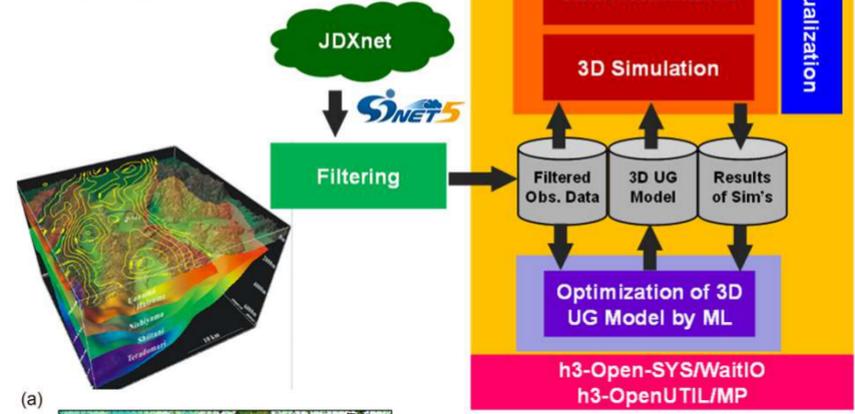


Future Directions towards Integration of (S+D+L)

- Accurate Prediction of Seismic Wave Propagation with Real-Time Data Observation/Assimilation
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• 3D Underground Model

- Heterogeneous, Observation is difficult
- Inversion analyses of seismic waves are important for prediction of structure of underground model
- ML may be utilized for acceleration of this prediction based on analyses of small earthquakes in normal time (e.g. $M_w < 3.0$)
- More sophisticated DA method (e.g. 4DVar)



Construction of 3D Underground Model by Data Assimilation/Machine Learning

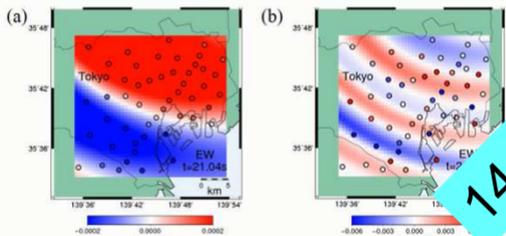
- Local models with smaller meshes should be used

Replica Exchange
Monte Carlo
Nagao et al.

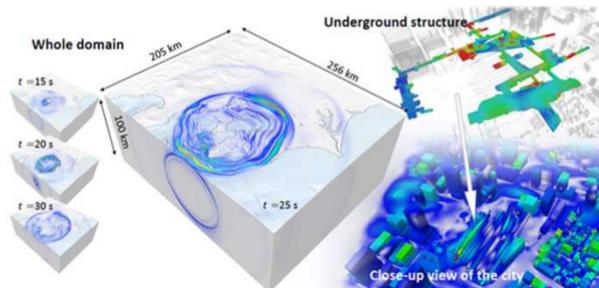
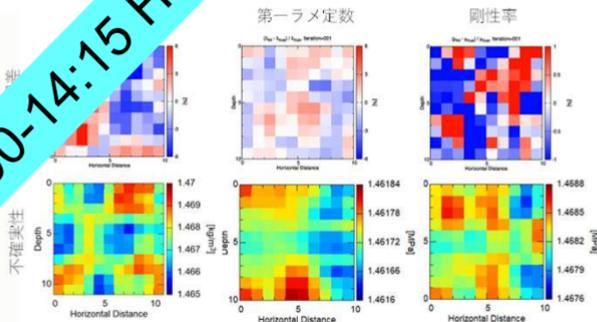
2nd Order Adjoint
Nagao et al.

Large-Scale ML
Ichimura, Fujita
SC22 GB Finalists

14:00-14:15 Hiromichi Nagao (U.Tokyo)



Movie S2. Seismic wavefield in the Tokyo area for the Mw 5.5 earthquake of 16 September 2014 in the northern Kanto area, in the frequency band (a) 0.10–0.20 Hz and (b) 0.10–1.0 Hz, computed with the optimum model parameters, compared to the observations (circles).



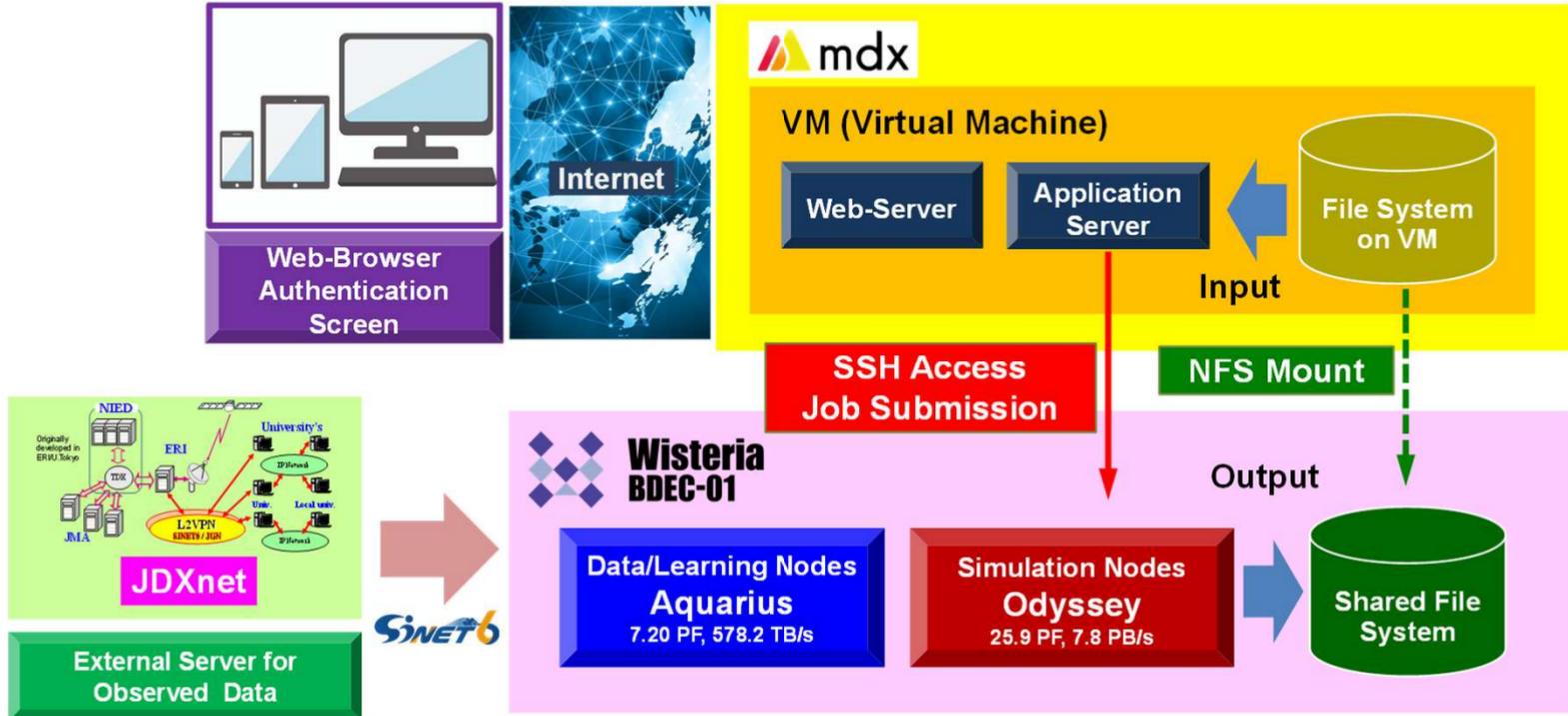
現実的な計算時間・計算機資源で不確実性評価まで可能な新しい4次元変分法の実問題への応用が可能となった

Web-based Simulation System for Outreach Activities



- Web-based simulation system for enlightenment of disaster prevention/mitigation awareness using “3D Earthquake Simulation with Real-Time Data Observation/Assimilation”
- Users including general citizens and high-school/junior-high-school students, access the web-server on the mdx system, and manipulate simulations on the Wisteria/BDEC-01.
- The framework can be utilized in various types of applications.

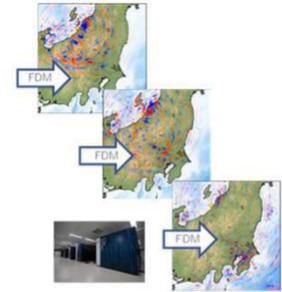
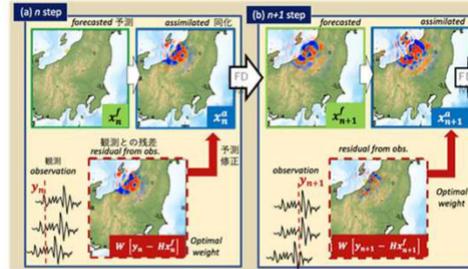
Web-based Simulation System for Outreach Activities



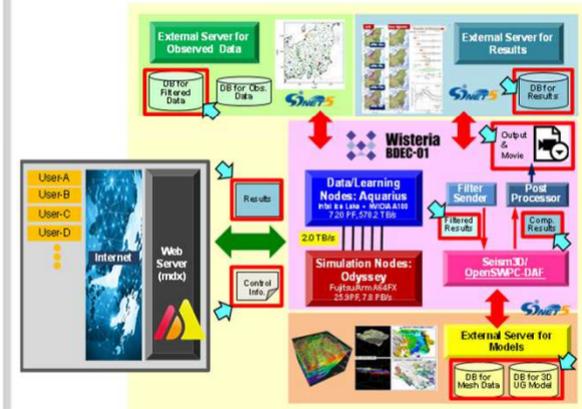
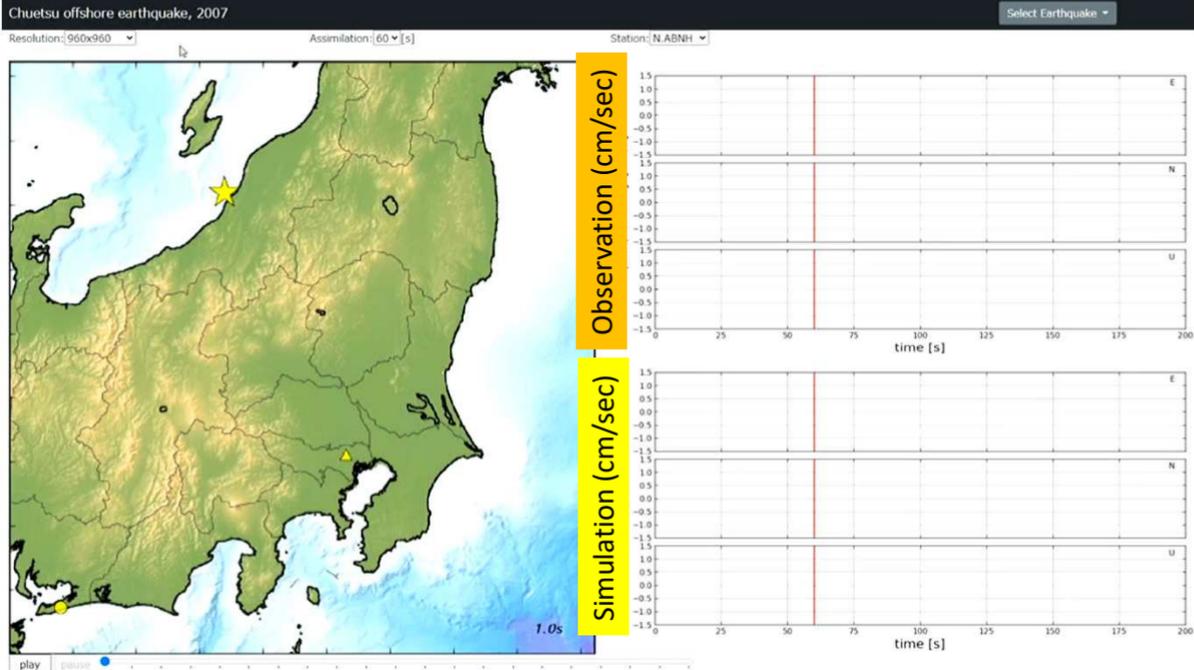
Web-based Simulation System for Outreach Activities (Prototype)

(A+S) Assimilation+Simulation

(Pure S) Pure Simulation/Forecast



01

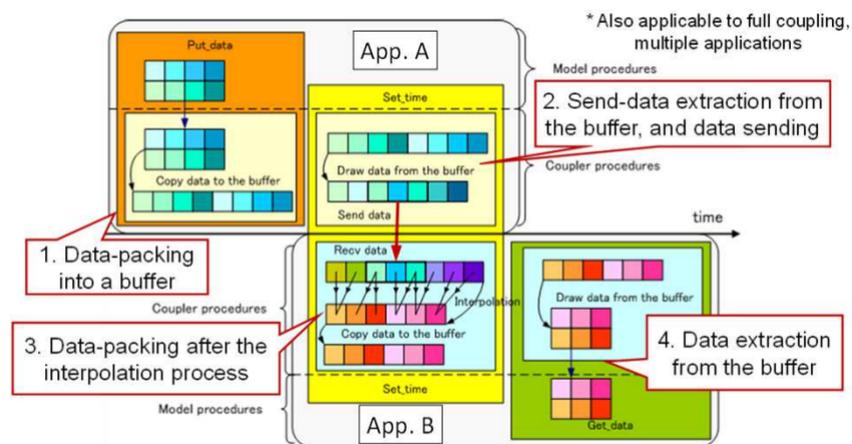


- Integration of (Simulation/Data/Learning)
 - Wisteria/BDEC-01
 - h3-Open-BDEC
- **Applications on Wisteria/BDEC-01 with h3-Open-BDEC**
 - Seismic Wave Propagation
 - **Global Atmosphere**
 - International/Domestic Collaborations
- Integration of (Simulation/Data/Learning) and Beyond
- Summary

Multiphysics Coupler



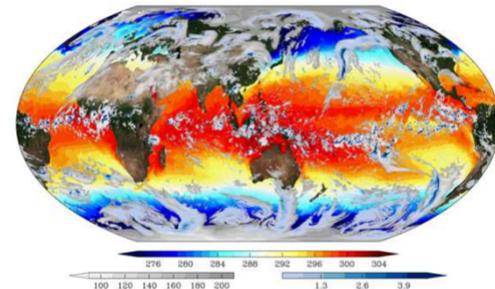
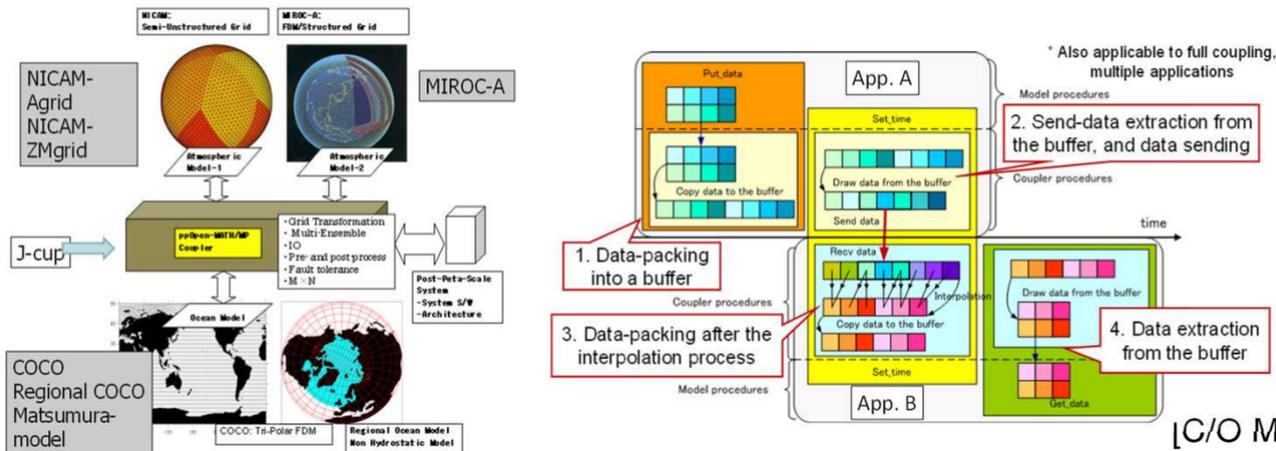
- Traditional Coupler: ppOpen-MATH/MP
 - Weak-Coupling of Multiple (usually two) Applications
 - Each application does a single computation
 - Ocean-Atmosphere
 - Fluid-Structure



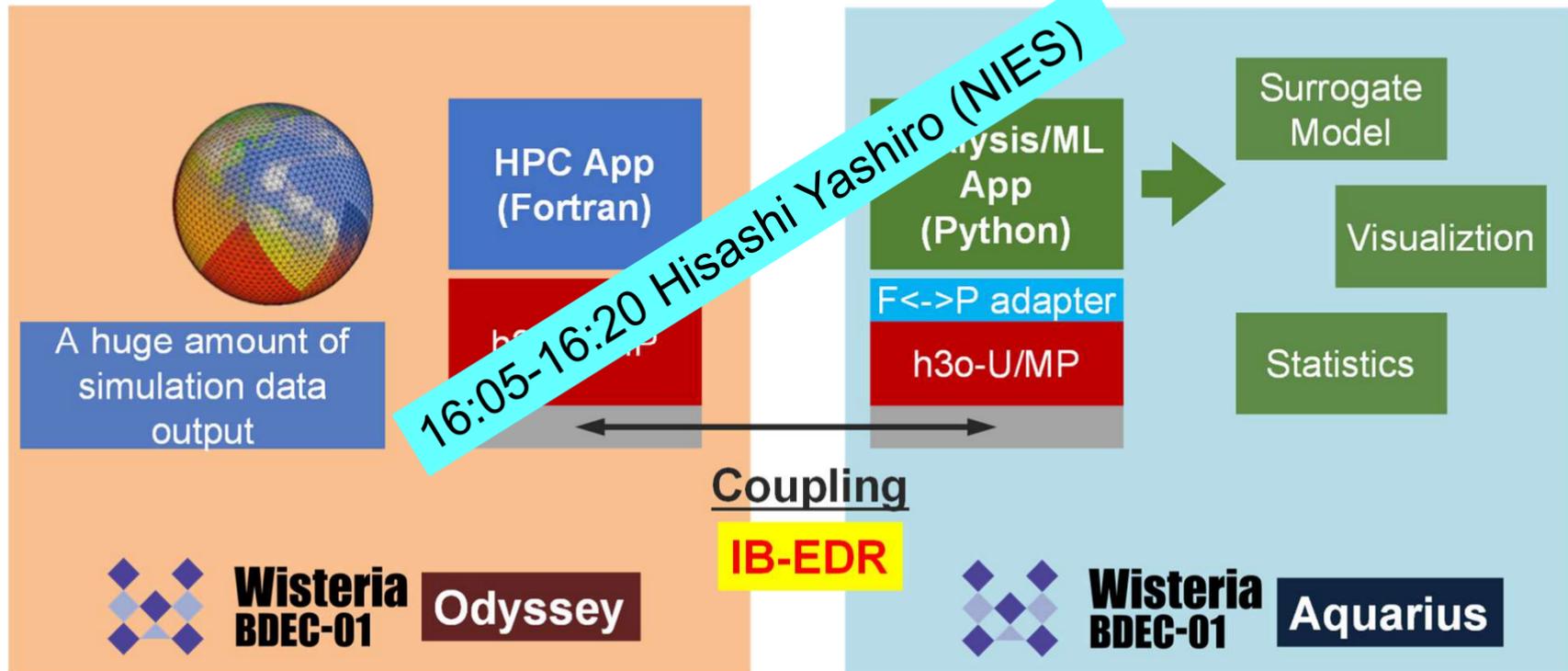
Atmosphere-Ocean Coupling by ppOpen-MATH/MP (Previous Project)



- High-resolution global atmosphere-ocean coupled simulation by NICAM (Atmosphere) and COCO (Ocean) through ppOpen-MATH/MP on the K computer is achieved.
 - ppOpen-MATH/MP is a coupling software for the models employing various discretization method.

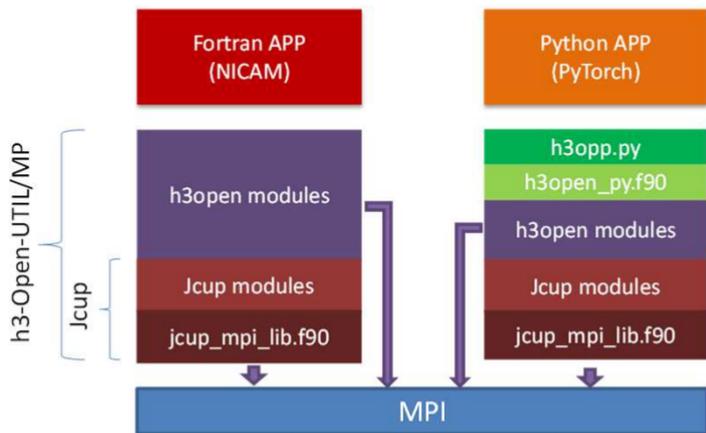


h3-Open-UTIL/MP (h3o-U/MP) Extended Multiphysics Coupler

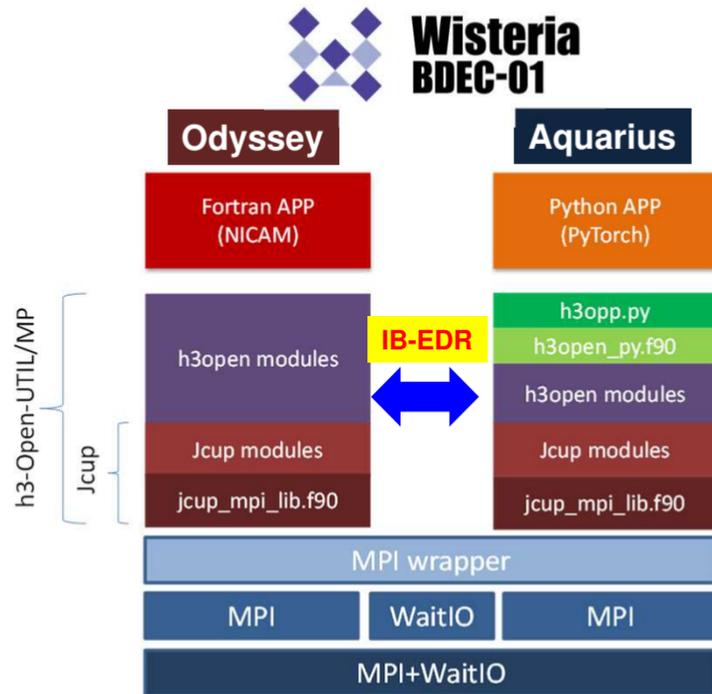
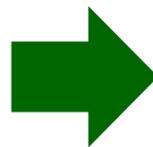


h3-Open-UTIL/MP + h3-Open-SYS/WaitIO-Socket

Available in June 2022



May 2021: MPI Only

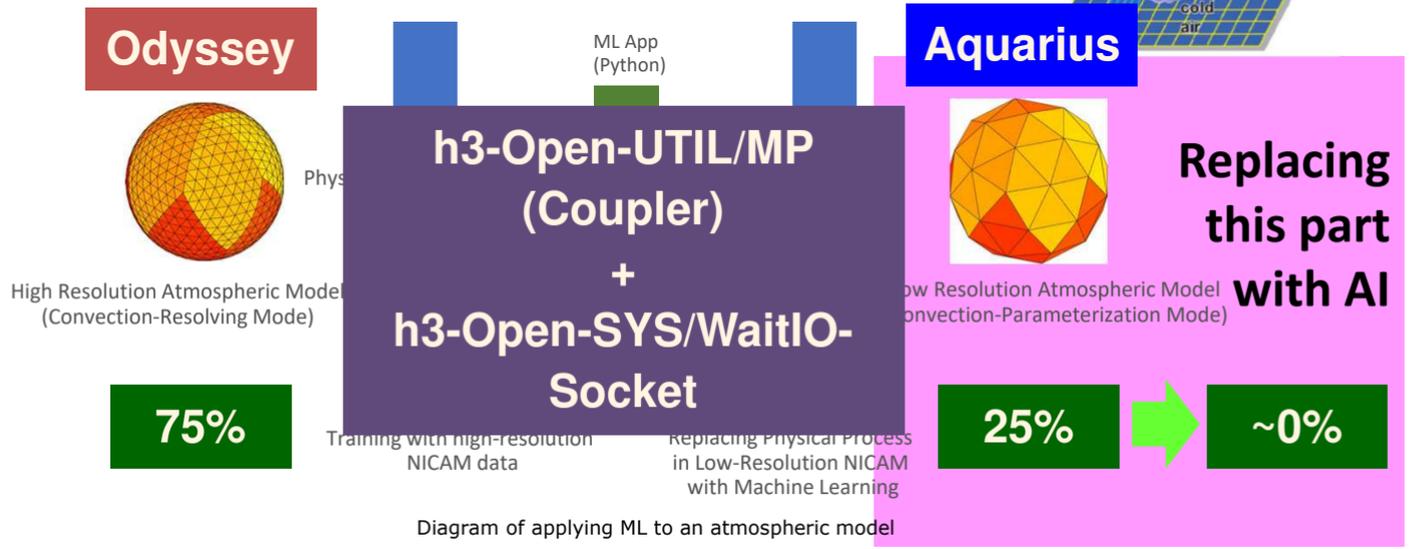
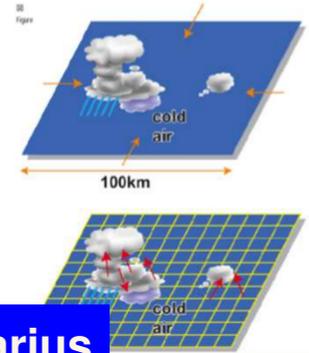


June 2022: Coupler + WaitIO

Atmosphere-ML Coupling

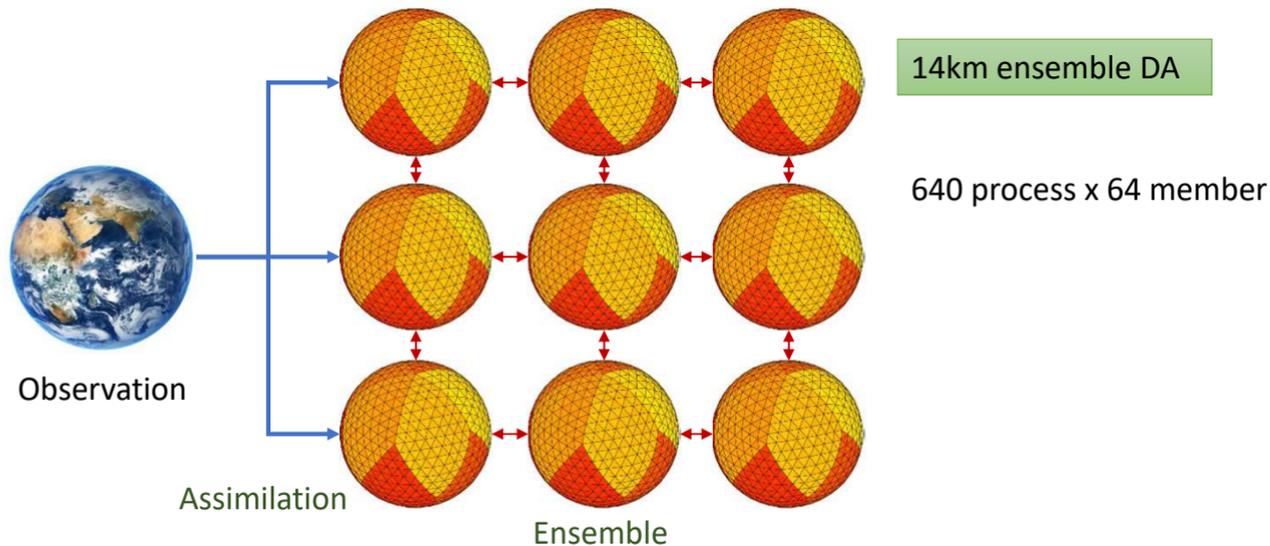
[Yashiro (NIES), Arakawa (ClimTech/U.Tokyo)]

- Motivation of this experiment
 - Two types of Atmospheric models: Cloud resolving VS Cloud parameterizing
 - Cloud resolving model is difficult to use for climate simulation
 - Parameterized model has many assumptions
 - Replacing low-resolution cloud processes calculation with ML!



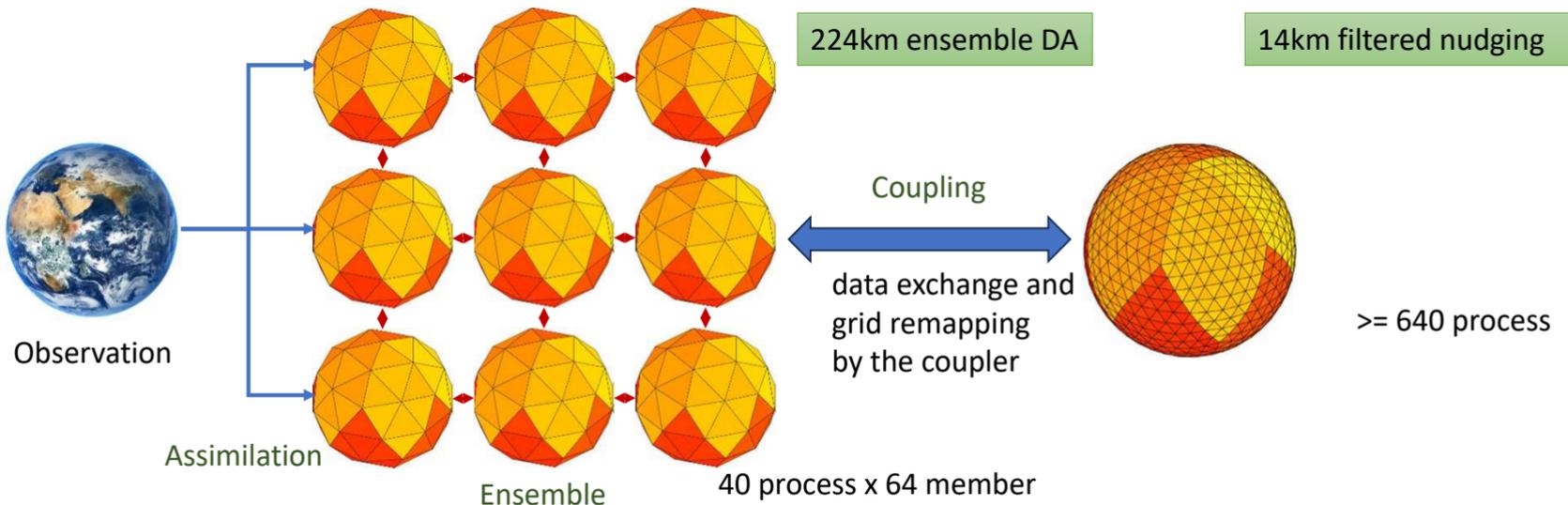
Ensemble-Based Data Assimilation

- Ensemble Data Assimilation of Atmospheric model
 - Data Assimilation + Ensemble Calculation
 - Effective technique to enhance forecast accuracy
- Problems with high-resolution ensemble
 - High-resolution ensemble requires significant resources (time and/or CPU)
 - Potential for poor reproducibility of large-scale fields



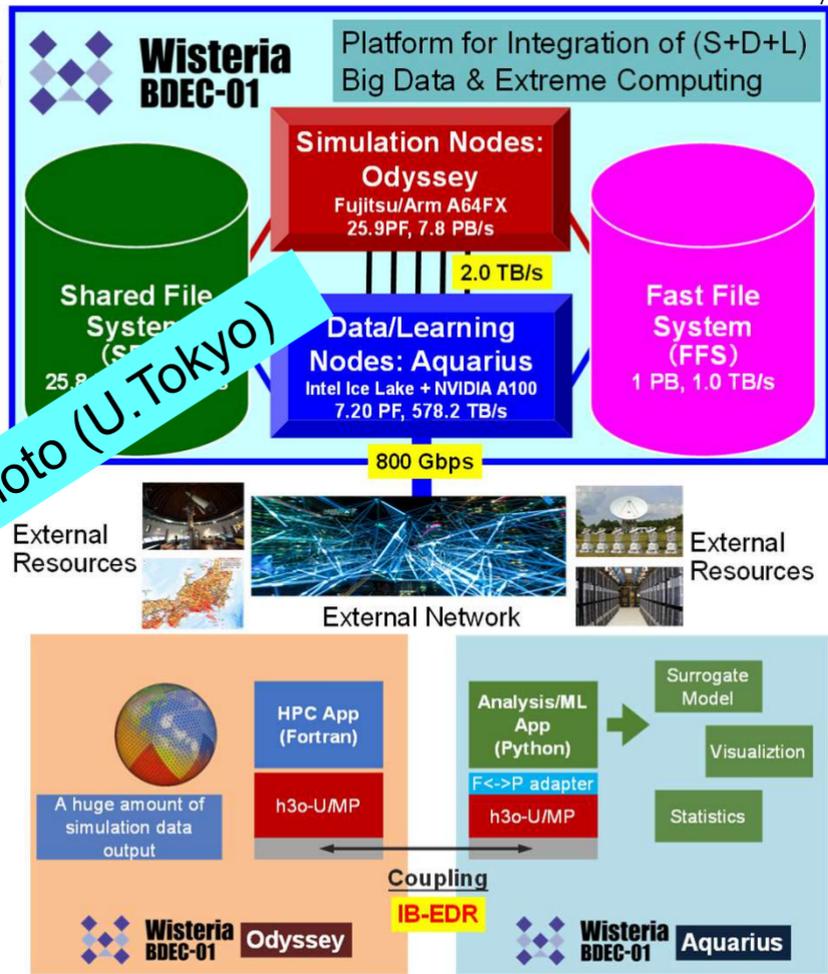
Ensemble Coupling

- Low-resolution ensemble + high-resolution calculation
 - 224km ensemble (40 process x 64 ensemble) + 14km simulation (≥ 640 process)
 - Fewer computational resources
 - More accurate reproduction of large-scale fields



How to run the workloads

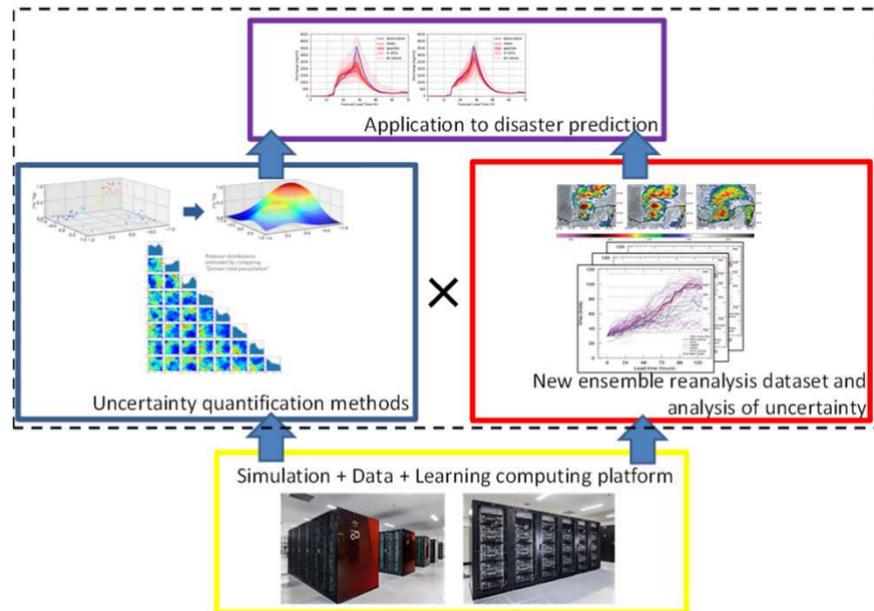
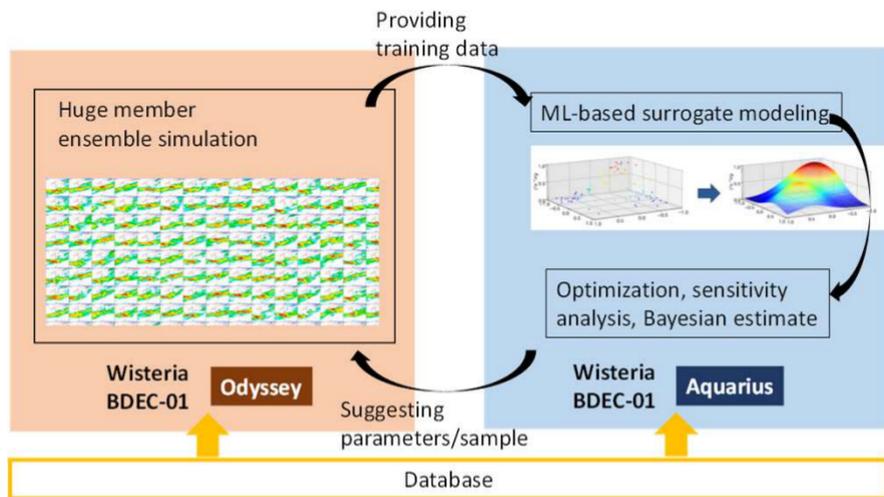
- Total Number of Nodes
 - Odyssey: 7,680 nodes: not so crowded
 - Aquarius: 45 nodes, 360 GPUs, very crowded
- One node of Aquarius is reserved for this type of workload on the integration of (S+D+L)
- 2 separate jobs (Odyssey and Aquarius) should be submitted
- If both jobs “grab” resources, execution starts at 16:20-16:35 Shinji Sumimoto (U.Tokyo)
- More flexible (& complicated) policy needed



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Uncertainty Quantification of Extreme Weather Prediction

Y. Sawada (U.Tokyo)



FY.2023-2025, JHPCN Project

Innovative Computational Science by Integration of Simulation/Data/Learning under Heterogeneous Computing Env.



東京大学
THE UNIVERSITY OF TOKYO



東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO



名古屋大学
NAGOYA UNIVERSITY



九州大学
KYUSHU UNIVERSITY



国立研究開発法人
国立環境研究所
National Institute for Environmental Studies



HITACHI
Inspire the Next



FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG



JÜLICH
FORSCHUNGSZENTRUM



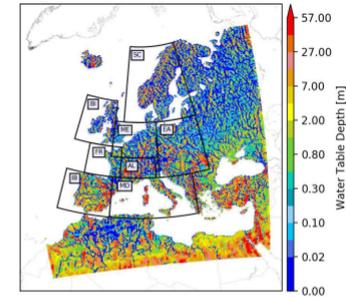
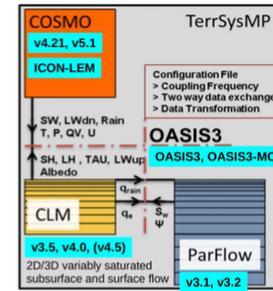
Institut
Ruđer
Bošković



- ✓ Jülich Supercomputing Centre (JSC)
- ✓ Rudjer Boskovic Institute, Centre for Informatics and Computing, Croatia
- ✓ Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
- ✓ French Atomic Energy Commission (CEA)

Target Applications

- JSC 
 - Terrestrial Systems Modeling Platform (TSMMP)
 - Coupling: Groundwater Flow & Atmosphere
 - <https://www.terrsysmp.org/>
 - Chebyshev Accelerated Subspace Eigensolver (ChASE)
 - Quantum Chemistry, Heterogeneous Environment
 - <https://github.com/ChASE-library>
 - Brain Aneurysm Simulations
 - Multiscale, Multiphysics
 - CFD Codes (m-AIA) at JSC
 - <https://www.hpccoe.eu/2021/06/04/m-ai/>
- CEA 
 - Selection of inhibitors of the SARS-CoV-2 Main Protease
 - BigDFT + Polaris/Gromacs



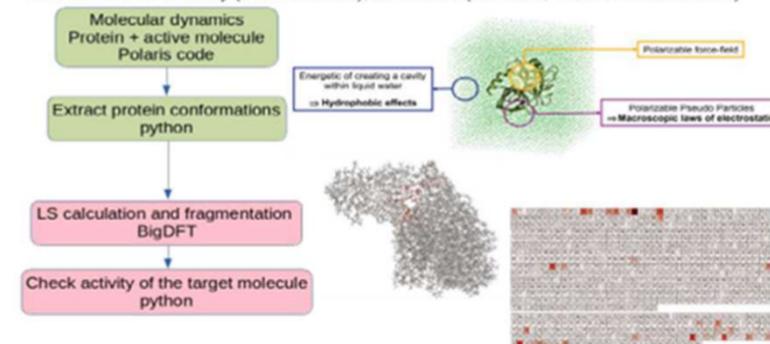
ALGORITHM 1: THE CHASE algorithm: SI plus *our original contributions*

Require: Hermitian matrix A , number of desired eigenpairs nev , threshold tolerance for residuals tol , initial polynomial degree deg , search space increment inc , *optres* and *optm* flags, vector matrix $V = [V_1 \dots V_{nev}]$ and estimates p_1 and p_{max}

Ensure: nev extremal eigenpairs (λ, \tilde{V}) , with $\lambda = [\lambda_1 \dots \lambda_{nev}]$ and $\tilde{V} = [\tilde{V}_1 \dots \tilde{V}_{nev}]$ and their residuals $(Res(\tilde{V}_1, \lambda_1) \dots Res(\tilde{V}_{nev}, \lambda_{nev}))$

- 1: $m_{initial} = deg$ ▷ INITIAL CONSTANT DEGREE
- 2: $(\hat{V}_{opt}, \hat{p}_1, \hat{p}_{max}, \hat{r}_1) \leftarrow \text{LARGEST}(\hat{A}, \text{optres})$ ▷ INITIAL AND OPTIONAL INPUT
- 3: while $size(\hat{r}_1) < nev$ do
- 4: $\hat{V} \leftarrow \text{FILTER}(\hat{A}, \hat{V}_{opt}, \hat{p}_1, \hat{p}_{max}, \hat{V}, m, \text{optm})$ ▷ USE ARRAY OF DEGREES
- 5: $\hat{Q} \leftarrow \text{ORTHONORMALIZE}(\hat{V}, \hat{V})$ ▷ QR FACTORIZATION
- 6: $\hat{Q} = [\hat{Q}_{opt} | \hat{Q}_{rest}]$ ▷ REDUCE TO ACTIVE SUBSPACE
- 7: $(\hat{V}, \hat{\lambda}) \leftarrow \text{ANALYZE}(\hat{A}, \hat{Q})$
- 8: Compute the residuals $Res(\hat{V}, \hat{\lambda})$
- 9: $(\hat{V}, \hat{\lambda}, \hat{r}_1) \leftarrow \text{DEFLATION}(\hat{Q}, \text{LOCKING}(\hat{V}, \hat{\lambda}), Res(\hat{V}, \hat{\lambda}), \hat{V})$
- 10: $p_1 \leftarrow \min(\hat{\lambda}, \lambda)$; $p_{max} \leftarrow \max(\hat{\lambda}, \lambda)$
- 11: $c \leftarrow \frac{deg - p_{max}}{deg - p_1}$; $\ell \leftarrow \frac{deg - p_{max}}{deg - p_1}$
- 12: for $\alpha = 1 \rightarrow size(\hat{r}_1)$ do
- 13: $m_\alpha \leftarrow \text{DEGREE}(\hat{r}_1, \hat{V}, \hat{\lambda}, \hat{\lambda}_\alpha, c, \ell)$ ▷ COMPUTE POLYNOMIAL DEGREE
- 14: end for
- 15: Sort $Res(\hat{V}, \hat{\lambda}), \hat{V}, \hat{\lambda}, m$ according to m
- 16: end while

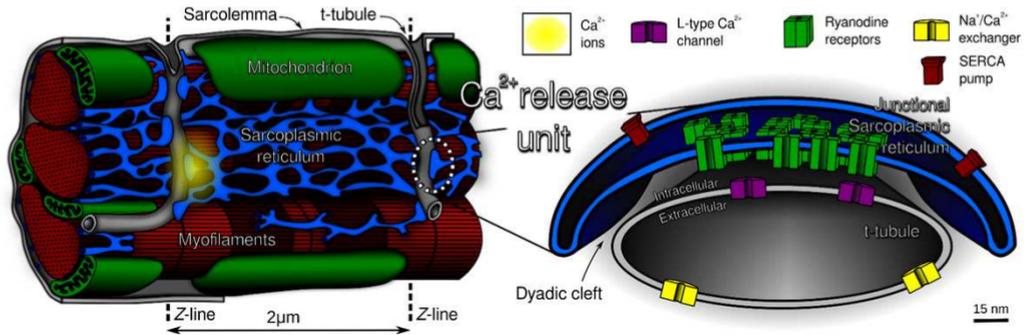
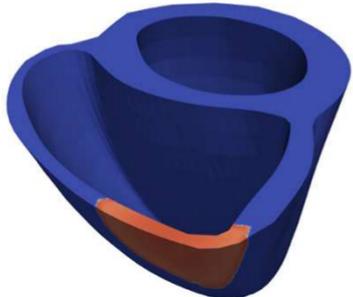
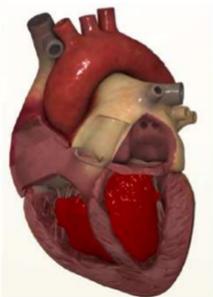
One monoclonal antibody (1400 Residues), 3h walltime (32 nodes, 4096 AMR Rome cores)



Collaboration since FY.2018

High resolution simulation of cardiac electrophysiology on realistic whole-heart geometries

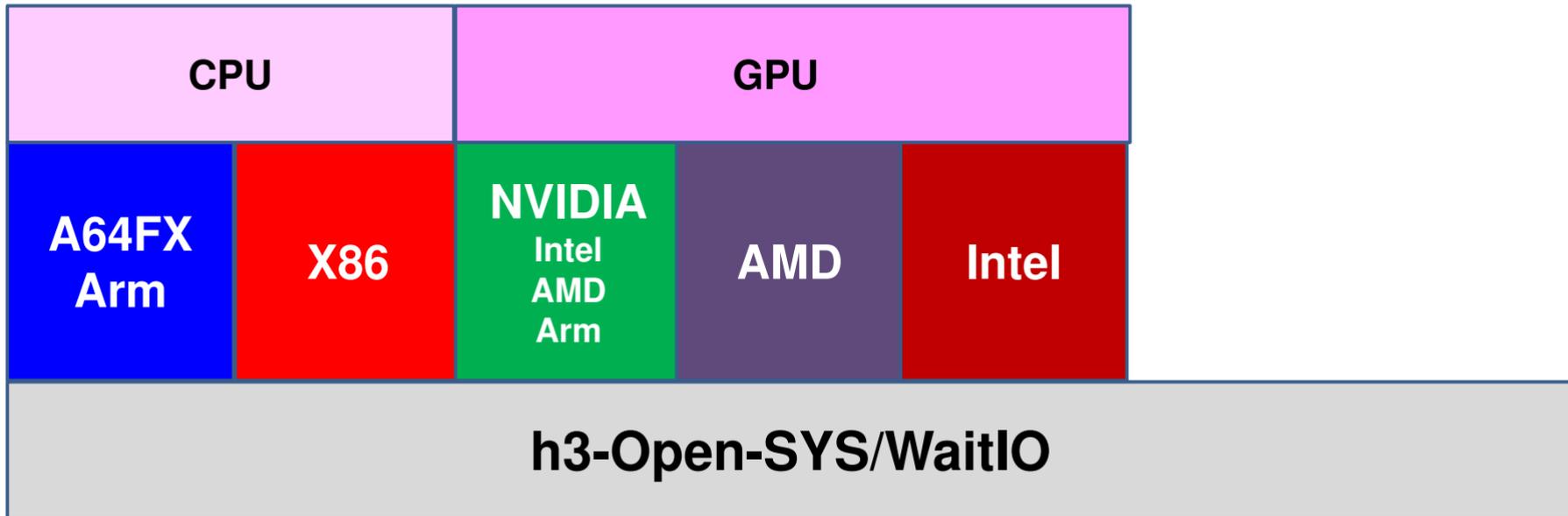
- Coordinated electrical activities are vital for the heart
- Computer-enabled “in-silico” experimentation is important for studying the physiological mechanism and the cause of diseases
- Need biophysically accurate simulations of **cardiac electrophysiology**
 - Extremely fine spatial and temporal resolutions → huge computations
 - Realistic 3D geometry of the heart → unstructured computational mesh



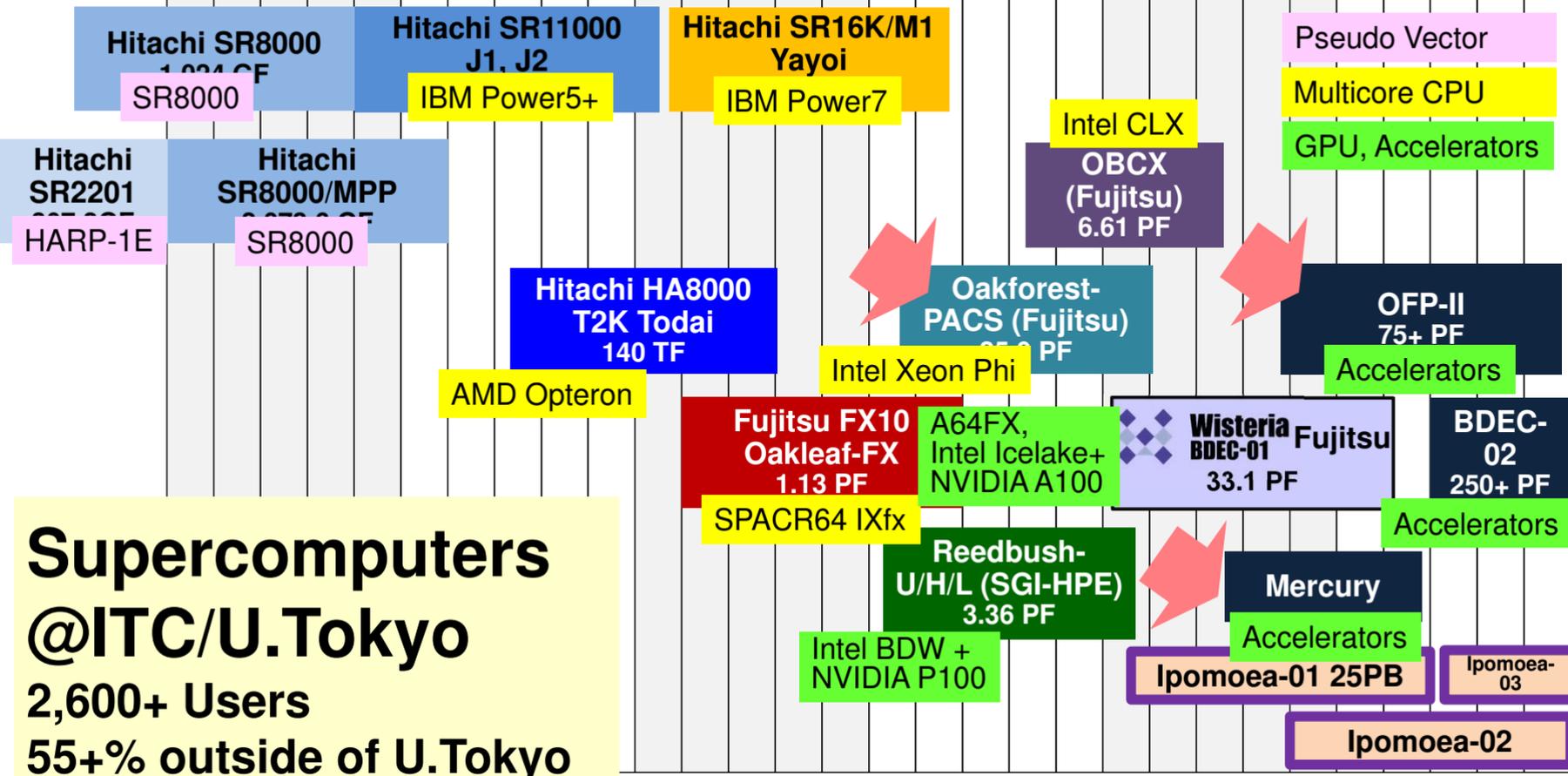
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- Summary

Anything is possible with WaitIO

WaitIO over Internet/cloud is possible



2001-2005	2006-2010	2011-2015	2016-2020	2021-2025	2026-2030
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Supercomputers @ITC/U.Tokyo
 2,600+ Users
 55+% outside of U.Tokyo

OFP-II (1/2)

Bid opened on November 9th, Fujitsu awarded



Group-A: CPU Only: Intel Xeon Max 9480 (SPR)

- Node: Intel Xeon Max 9480 (1.9GHz, 56c) x 2
 - 6.8 TF, 128 GiB, 3,200 GB/sec (HBM2e only)

– Total

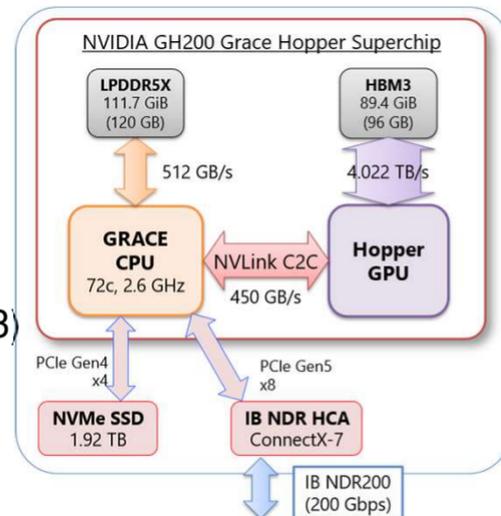
- 190 nodes, 1.3 PF, IB-NDR 200
- 372 TB/sec for STREAM Triad (Peak: 608 TB/sec)

Group-B: CPU+GPU: NVIDIA GH200

- Node: NVIDIA GH200 Grace-Hopper Superchip
 - Grace: 72c, 2.9 TF, 111.7 GiB, 512 GB/sec (LPDDR5X)
 - H100: 66.9 TF DP-Tensor Core, 89.4 GiB, 4,022 GB/sec (HBM3)
 - NVMe SSD for each GPU: 1.9TB, 8.0GB/sec

– Total (Aggregated Performance: CPU+GPU)

- 1,120 nodes, 78.2 PF, 5.07 PB/sec, IB-NDR 200



OFP-II (2/2)

Bid opened on November 9th, Fujitsu awarded



筑波大学
University of Tsukuba



東京大学
THE UNIVERSITY OF TOKYO

- **File System: DDN EXA Scaler, Lustre FS**
 - 10.3 PB (NVMe SSD) 1.0TB/sec, “Ipomoea-01” with 26 PB is also available
- **All nodes in Group-A/B are connected with Full Bisection Bandwidth**
 - $(400\text{Gbps}/8) \times (32 \times 20 + 16 \times 1) = 32.8 \text{ TB/sec}$
- **Operation starts in January 2025, h3-Open-SYS/WaitIO will be adopted for communication between Group-A and Group-B**

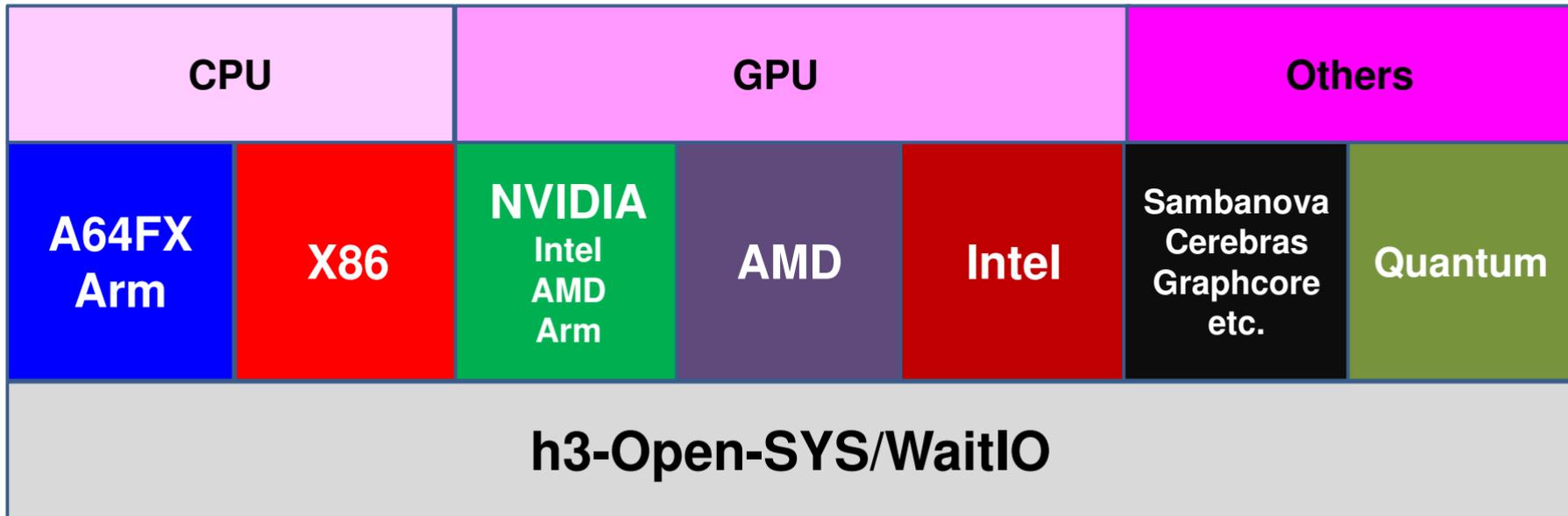
IB-NDR (400Gbps)		
IB-NDR200 (200)		IB-HDR (200)
Group-A Intel Xeon Max (HBM2e) 2 x 190 1.3 PF, 608 TB/sec	Group-B NVIDIA GH200 1,120 78.2 PF, 5.07 PB/sec	File System DDN EXA Scaler 10.3 PB, 1.0TB/sec

Ipomoea-01
Common Shared Storage
26 PB



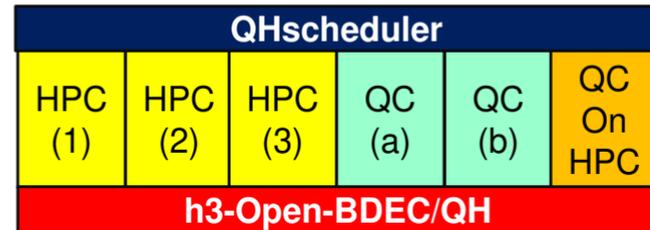
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WaitIO over Internet/cloud is possible



System SW for QC-HPC Hybrid Environment (1/2)

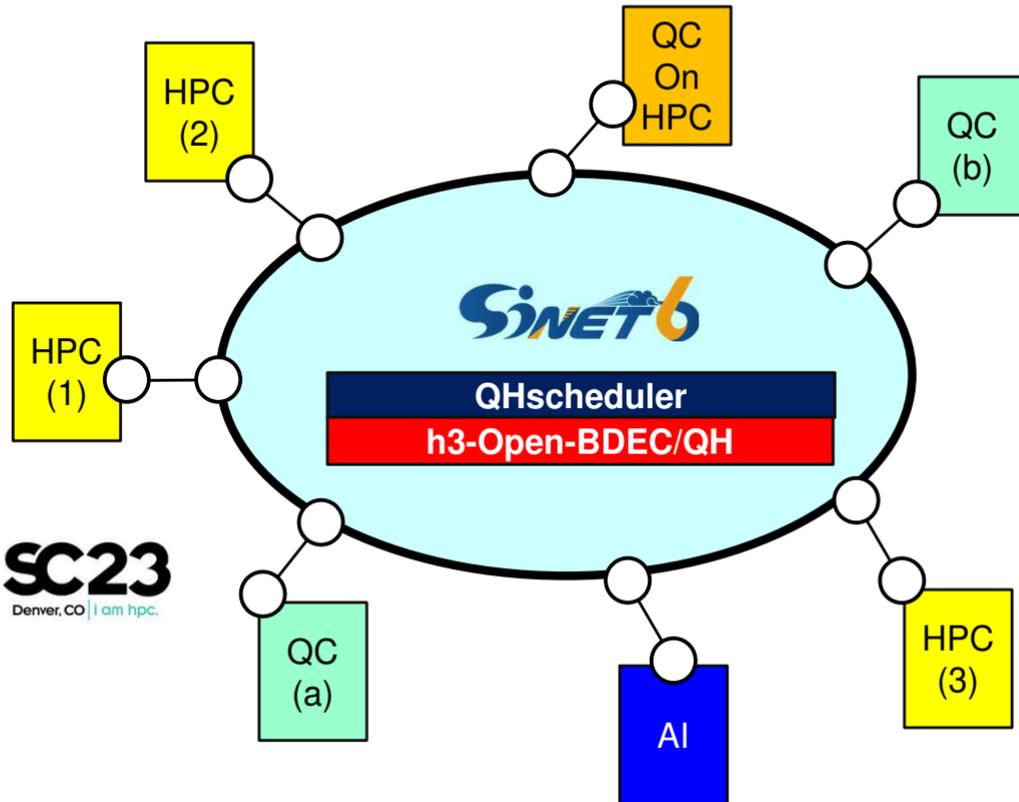
- **Quantum Computer = Accelerator of Supercomputers: QC-HPC Hybrid**
- System SW for Efficient & Smooth Operation of QC (Quantum Computer, including simulators on supercomputers)-HPC Hybrid Environment
 - QHscheduler: A job scheduler that can simultaneously use multiple computer resources distributed in remote locations
 - h3-Open-BDEC/QH: Coupling to efficiently implement and integrate communication and data transfer between QC-HPC on-line and in real time
 - Collaboration with RIKEN R-CCS, funded by Japanese Government
- Target Application
 - AI for HPC, combined workload
 - Simulations in Computational Science
 - Quantum Machine Learning
 - Quantum Simulations, Error Correction



System SW for QC-HPC Hybrid Environment (2/2)

• Innovations

- This is the world's first attempt to link multiple supercomputers and quantum computers installed at different sites in real time.
- In particular, by using multiple QCs simultaneously, it is possible to form a virtual QC with higher processing capacity.
 - Many people are thinking about same thing all over the world
- This idea can be extended to any types of systems



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Summary

- Integration of (Simulation/Data/Learning) at ITC/U.Tokyo
- Wisteria/BDEC-01
- h3-Open-BDEC
- Domestic/International Collaborations

- Challenges towards Quantum Computing

Activities

- Publications

- Peer Reviewed Journal Papers/Proceedings 58
- Presentations (International/Domestic) 89
- Invited Talks (International/Domestic) 33
- Book 1

- Awards

- Shinji Sumimoto, Takashi Arakawa, Yoshio Sakaguchi, Hiroya Matsuba, Hisashi Yashiro, Toshihiro Hanawa, and Kengo Nakajima, A System-Wide Communication to Couple Multiple MPI Programs for Heterogeneous Computing, The 23rd International Conference on Parallel and Distributed Computing, Applications and Technologies(PDCAT' 22), **Best Paper Award**
- Kengo Nakajima, SCA (Supercomputing Asia) HPC Pioneer & Achievement Award (Japan), 2023

Invited/Keynote Talks by KN after April 2023

- HPC Workshop for Nuclear Explosion Monitoring 2023, CTBTO (Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization), Vienna, Austria, May 2023
- 2023 Japan Geoscience Union Meeting, Makuhari, Japan, May 2023
- The 6th International Workshop on Nonhydrostatic Models (NHM-WS 2023), Sapporo, Japan, August 2023
- Accelerated Computing Summit 2023 (OACS), Online, October 2023
- The Initiative for Design Evolution, AIST, Online, October 2023
- 14th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Heterogeneous Systems (ScalAH23) in conjunction with SC23, Denver, CO, USA, November 2023
- 24th Northeast Asia Symposium 2023, Guangzhou, China, November 2023
- WCCM 2024 (16th World Congress on Computational Mechanics)/PANCAM 2024 (4th Pan American Congress on Computational Mechanics), Vancouver, Canada, July 2024 (planned)

Final Goal stated in the Proposal (Nov. 2018)

- We aim to reduce the amount of computations and power consumption **by more than 10 times** while maintaining the same accuracy as conventional methods in multi-level simulations that integrate (S+D+L).
 - Mixed Precision/Adaptive Precision
 - Machine Learning, Hierarchical Data Driven Approach
 - Heterogeneous Computing
- Self evaluation so far ... although we still have 4 months left
 - ○○

13:00 - 13:30	Kengo Nakajima (The University of Tokyo) Integration of Simulation/Data/Learning and Beyond
13:30 - 13:45	Takeshi Iwashita (Online) (Hokkaido University, Kyoto University) Research activities of Hokkaido University group for next-generation linear solvers -mixed precision computing, accelerators, subspace correction techniques-
13:45 - 14:00	Takahiro Katagiri (Nagoya University) Exploring AI for Auto-tuning through Sparse Matrix Image Information
14:00 - 14:15	Hirromichi Nagao (The University of Tokyo) Deep Learning to Extract Earthquakes and Low-Frequency Tremors in Continuous Seismic Waveforms
14:15 - 14:30	Takashi Shimokawabe (The University of Tokyo) Fast Prediction Methods for Fluid Simulation Results Using Deep Neural Networks
14:30 - 15:00	Richard Vuduc (Georgia Institute of Technology, USA) (Keynote Talk) Data-movement accelerators for scientific computing problems
15:00 - 15:20	(Discussion)
15:20 - 15:35	(Break)

15:35 - 15:50	Takeshi Ogita (Online) (Waseda University) Verified Solutions of Large Sparse Linear Systems Arising from 3D Poisson Equation
15:50 - 16:05	Masatoshi Kawai (Online) (Nagoya University) Effectiveness of low/adaptive precision with ICCG method
16:05 - 16:20	Hisashi Yashiro (Online) (National Institute for Environmental Studies) Algorithmic transformation from physical models to data-driven models using the coupling library: a case of a climate model
16:20 - 16:35	Shinji Sumimoto (The University of Tokyo) h3-Open-SYS/WaitIO: A System-wide Heterogeneous Communication Library to Couple Multiple MPI programs
16:35 - 16:50	Hayato Shiba (Online) (University of Hyogo) Deep learning of simulated glassy dynamics
16:50 - 17:20	Xing Cai (Simula Research Laboratory, Norway) (Keynote Talk) Towards high-performance unstructured-mesh computations
17:20 - 17:40	(Discussion)
17:40 - 17:45	(Closing)

Invited Speakers

- Richard Vuduc
 - Professor
 - School of Computational Science and Engineering, Georgia Institute of Technology, USA



- Xing Cai
 - Professor/Chief Research Scientist/Head of Department
 - High Performance Computing Department, Simula Research Laboratory, Norway

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