



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



# Integration of (Simulation + Data + Learning) for Innovative Scientific Computing by h3-Open-BDEC on Wisteria/BDEC-01



**Wisteria**  
**BDEC-01**

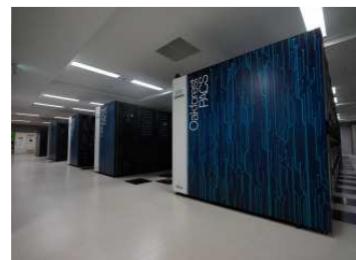


**Kengo Nakajima**  
Information Technology Center  
The University of Tokyo

# 3 Systems at the end of March 2021

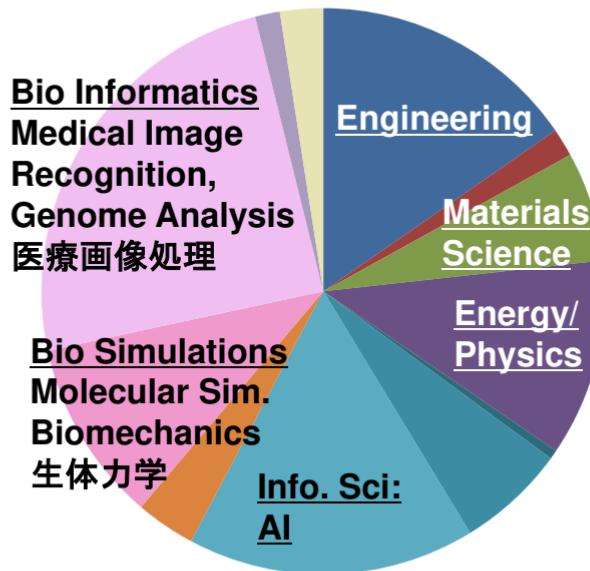
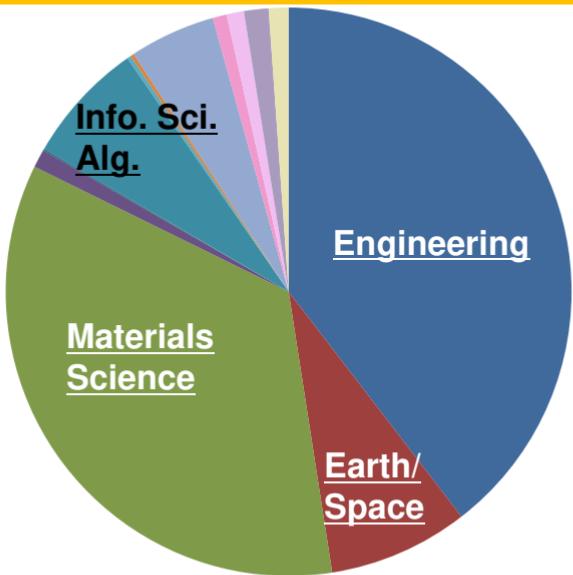
2,600+ users (55+% from outside of U.Tokyo)

- Reedbush (HPE, Intel BDW + NVIDIA P100 (Pascal))
  - Integrated Supercomputer Sys. for Data Analyses & Scientific Simulations
    - Jul.2016-Nov.2021 (Plan)
  - Our first GPU System, DDN IME (Burst Buffer)
  - Reedbush-U: CPU only, 420 nodes, 508 TF (Jul.2016~, retired June 2020)
  - Reedbush-H: 120 nodes, 2 GPUs/node: 1.42 PF (Mar.2017~Nov.2021)
  - Reedbush-L: 64 nodes, 4 GPUs/node: 1.43 PF (Oct.2017~Nov.2021)
- Oakforest-PACS (OFP) (Fujitsu, Intel Xeon Phi (KNL))
  - JCAHPC (U.Tsukuba & U.Tokyo)
  - 25 PF, #22 in 56<sup>th</sup> TOP 500 (November 2020) (#4 in Japan), Omni-Path Architecture, DDN IME (Burst Buffer), Sept.2016~Mar.2022
- Oakbridge-CX (OBCX) (Fujitsu, Intel Xeon Platinum 8280, CLX)
  - Massively Parallel Supercomputer System
  - 6.61 PF, #69 in 56<sup>th</sup> TOP 500, July 2019-June 2023
  - SSD's are installed to 128 nodes (out of 1,368)



# Research Area based on CPU Hours (FY.2019)

## Traditional CSE: Memory Bound Appl's



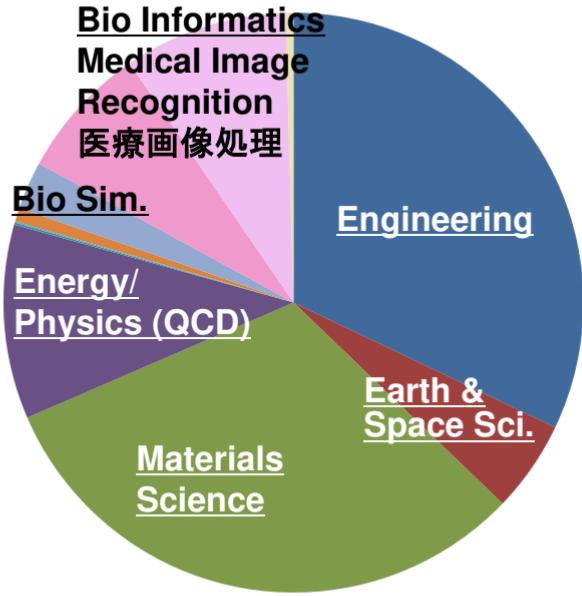
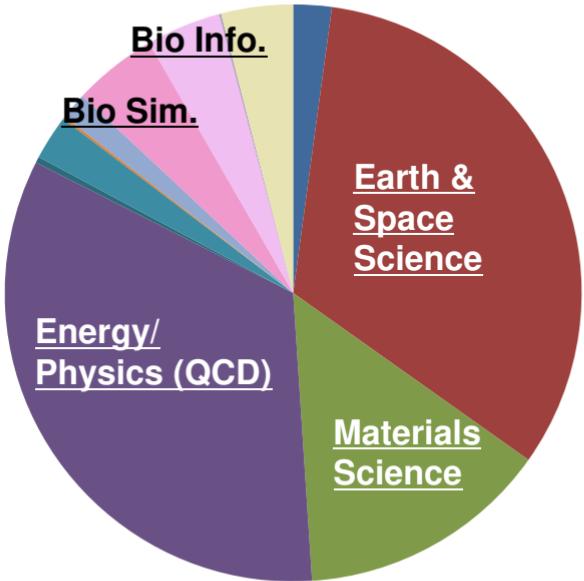
Multicore Cluster  
Intel BDW Only  
(Reedbush-U)

GPU Cluster  
Intel BDW + NVIDIA P100  
(Reedbush-H)



# Research Area based on CPU Hours (FY.2019)

OBCX: October 2019~September 2020



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

**Manycore Cluster**  
Intel Xeon Phi  
(Oakforest-PACS) (OFP)

**Multicore Cluster**  
Intel Xeon CLX  
(Oakbridge-CX) (OBCX)

**Traditional CSE:**  
Memory Bound App's

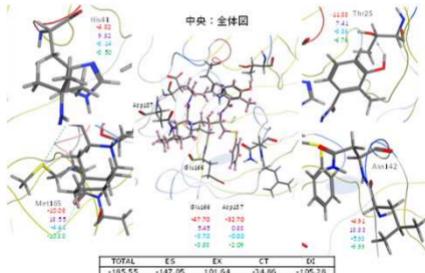
# HPCI Urgent Call for Fighting against COVID-19 in Japan (FY.2020)

by 8 SC Centers of Natl. Univ., AIST etc.

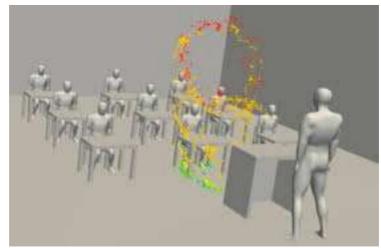
6 of 14 accepted projects use U.Tokyo's Systems



Project Name	PI	System
Fragment molecular orbital calculations on the main protease of COVID-19	Yuji Mochizuki (Rikkyo U.)	OFP
Study on the evaluation of arrhythmogenic risk of COVID-19 candidate drugs	Toshiaki Hisada (UT Heart)	
Prediction of dynamical structure of Spike protein of SARS-COVID19	Yuji Sugita (RIKEN)	
Computer-assisted search for inhibitory agents for SARS-CoV-2	Tyuji Hoshino (Chiba U.)	OBCX
Prediction and Countermeasure for virus droplet Infection under Indoor Environment: Case studies for massively-parallel simulation on Fugaku	Makoto Tsubokura (Kobe U.)	
Spreading of polydisperse droplets in a turbulent puff of saturated exhaled air	Marco Edoardo Rosti (OIST)	

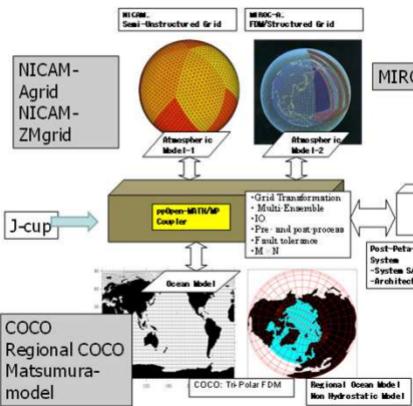
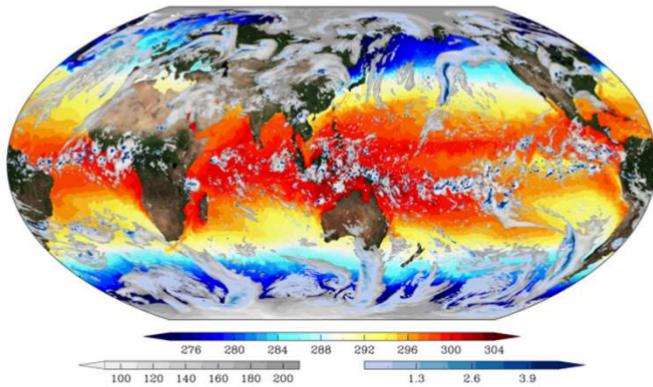


[c/o Prof. Y. Mochizuki (Rikko U.)]

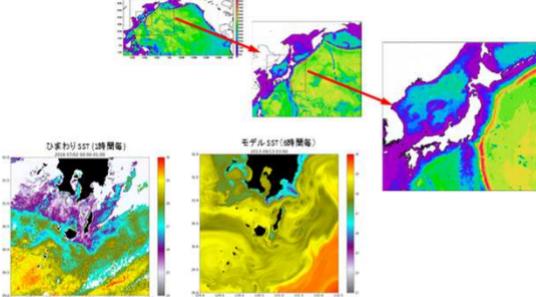
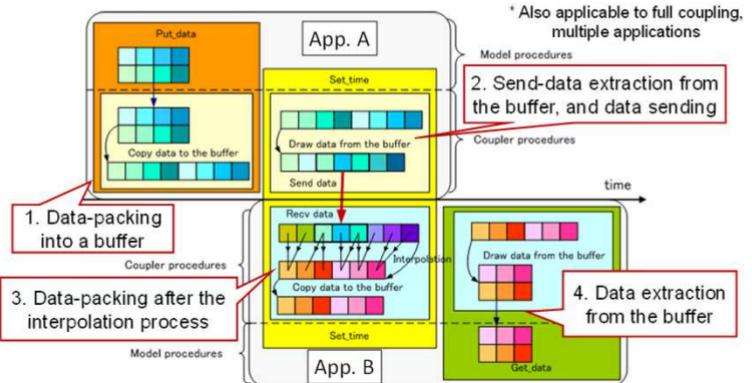
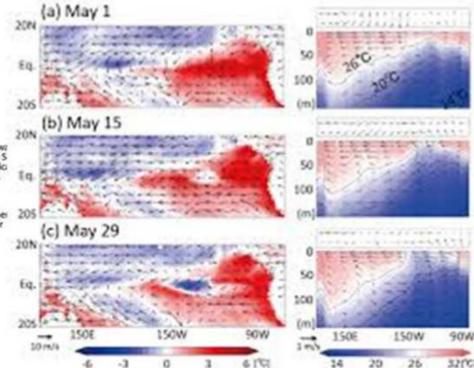
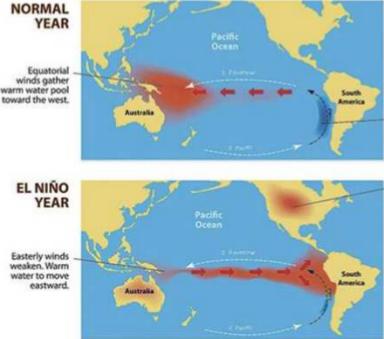


[c/o Prof. M.Tsubokura (Kobe U.)]

# Global Atmosphere-Ocean Coupled Simulations



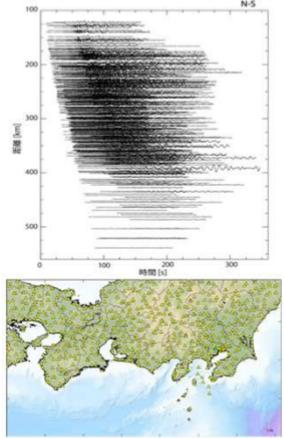
## THE EL NIÑO PHENOMENON



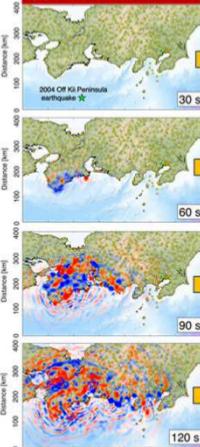
[c/o Prof. M. Sato, Prof. H. Hasumi  
(AORI/U.Tokyo)]

# Solid Earth & Earthquake Simulations

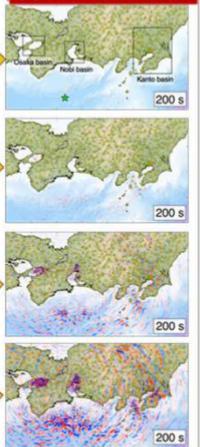
○ Observation (K-NET, KiK-net 446 pts)



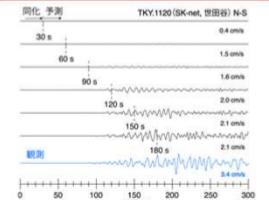
(a) Assimilated



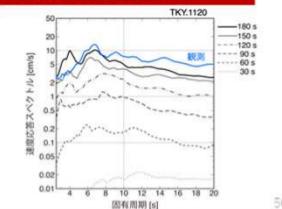
(b) Pure Simulation



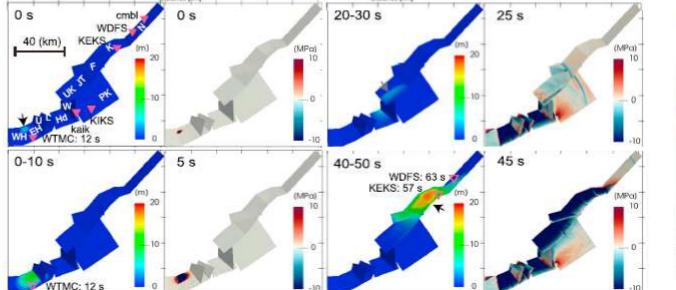
## Long Wave Propagation in Tokyo



## Response Spectrum

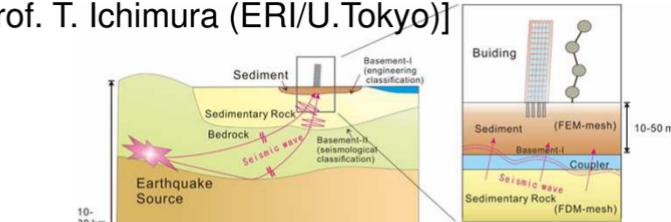


Assimilation at 90 sec. → Pure Simulation

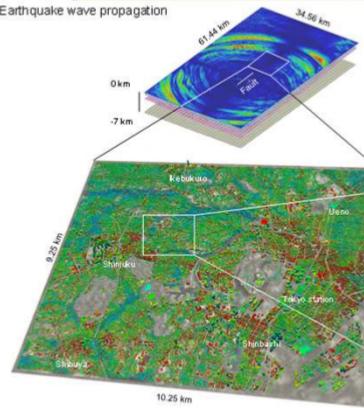


[c/o Prof. R. Ando (U.Tokyo)]

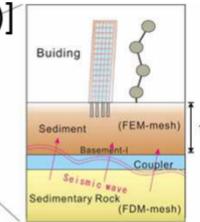
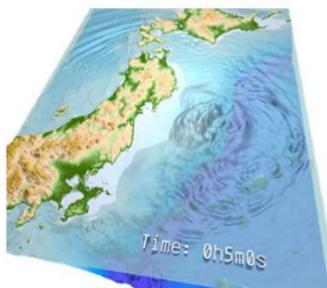
[c/o Prof. T. Furumura,  
Prof. T. Ichimura (ERI/U.Tokyo)]



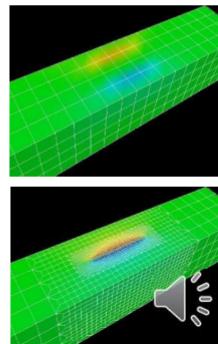
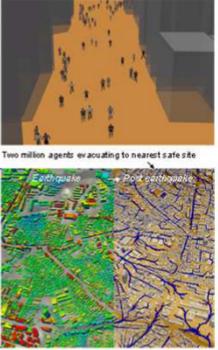
a) Earthquake wave propagation



b) City response simulation



c) Resident evacuation



# Simulation of Geologic CO<sub>2</sub> Storage

[c/o Dr. Hajime Yamamoto  
(Taisei Corporation)]

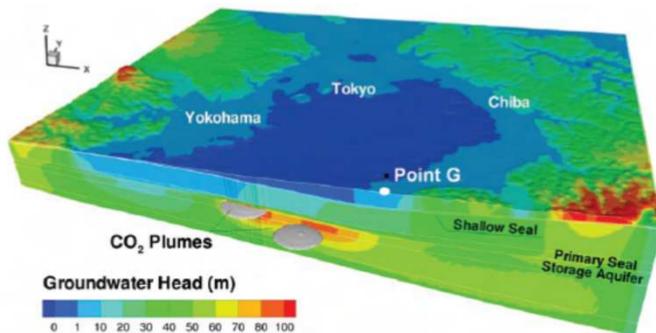
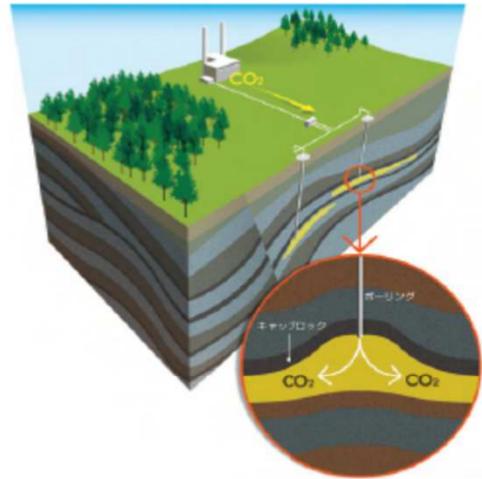


図-4 CO<sub>2</sub>圧入後の地下水圧（全水頭換算）の分布（100 年後）

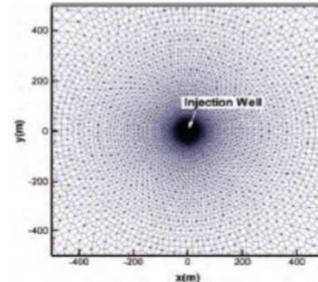
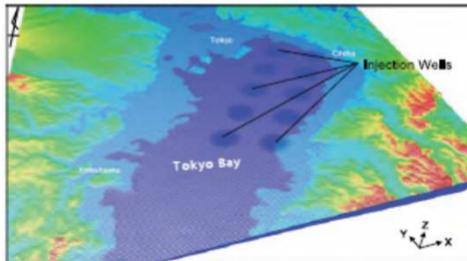
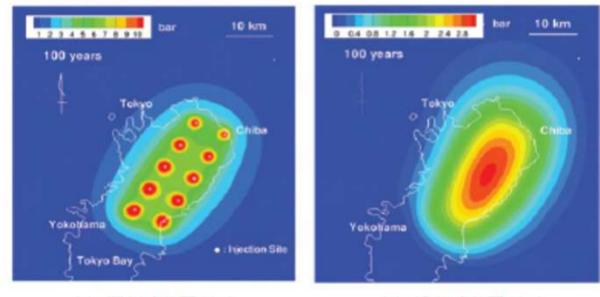
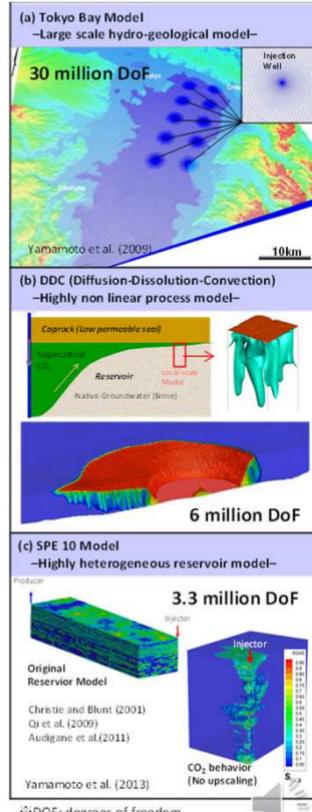


図-5 圧力上昇量の平面分布（初期状態からの増分、圧入開始から 100 年後）

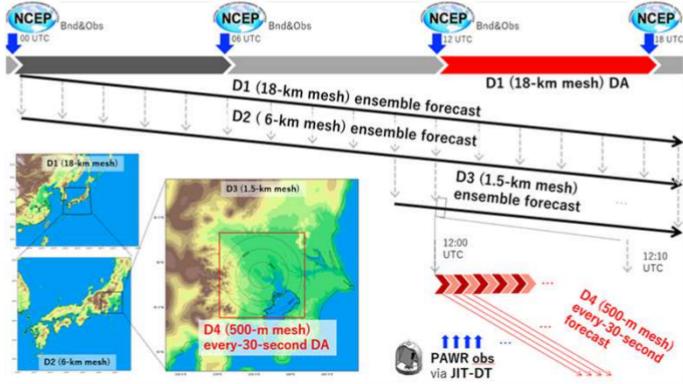


(a) 深部遮蔽層下面

(b) 浅部遮蔽層下面

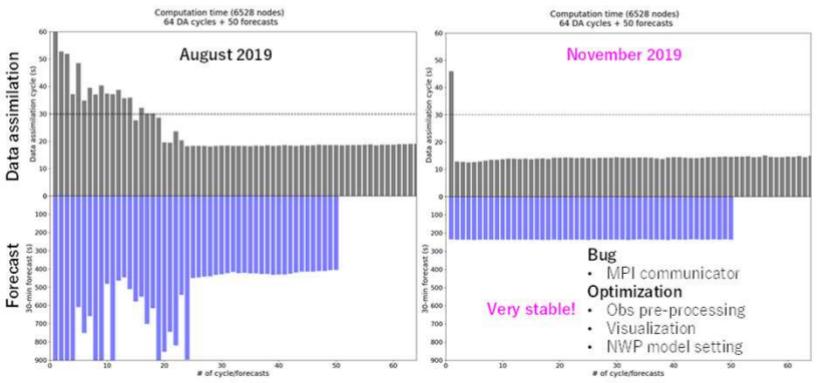


# Real-Time Prediction of Severe Rainstorm by OFP



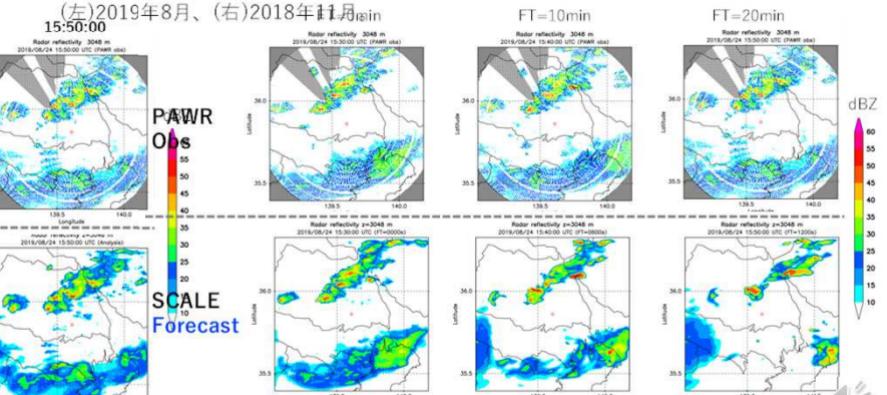
全体のワークフロー

15:30:00      15:40:00



計算性能の向上。上段はデータ同化、下段は30分予報にかかった時間(秒)。

(左)2019年8月、(右)2018年11月



PAWR  
Obs

SCALE-  
LETKF  
Analysis

[c/o Dr. Takemasa Miyoshi  
(RIKEN R-CCS)]

2019年8月24日の事例についてのテスト結果。(上)レーダー観測と(下)SCALE-LETKFによる解析で得られたレーダー反射強度(dBZ)を示す。

# Society 5.0 & BDEC System

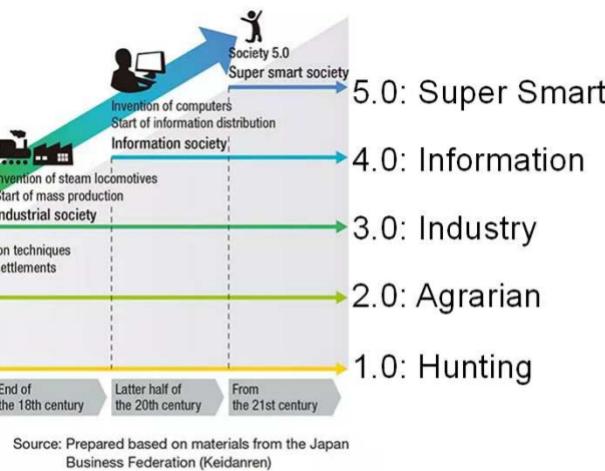
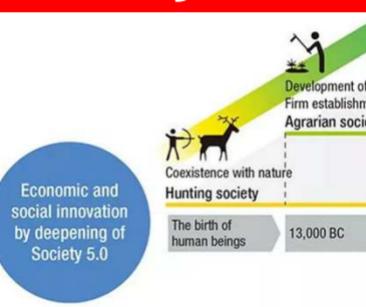
- We are developing an innovative method of computational science towards the Exascale Era/Society 5.0 by integration of (Simulation + Data + Learning (S+D+L)), where ideas of data science and machine learning are introduced to computational science



# Society 5.0: the Cabinet Office of Japan

- Super Smart & Human-centered Society by Digital Innovation (IoT, Big Data, AI etc.) and by Integration of Cyber Space & Physical Space

**HPC is very important for Society 5.0**



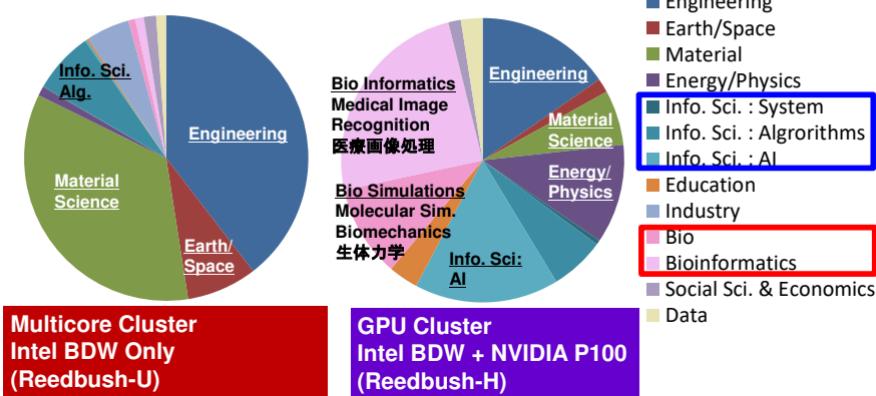
## Society 5.0 for SDGs

Society 5.0 offers a new growth model with a view of “solving social issues” as well as “creating a better future”, which **contributes to the achievement of SDGs**



# Future of Supercomputing

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



- **Integration/Convergence of (Simulation + Data + Learning) (S+D+L) is important towards Society 5.0**

- **BDEC (Big Data & Extreme Computing)**
  - Platform for Integration of (S+D+L)
  - Focusing on S (Simulation)
    - AI for HPC, Sophiscated Simulation
  - Planning started in 2015

**BDEC (Big Data & Extreme Computing)**

**S + D + L**



# Society 5.0 & BDEC System

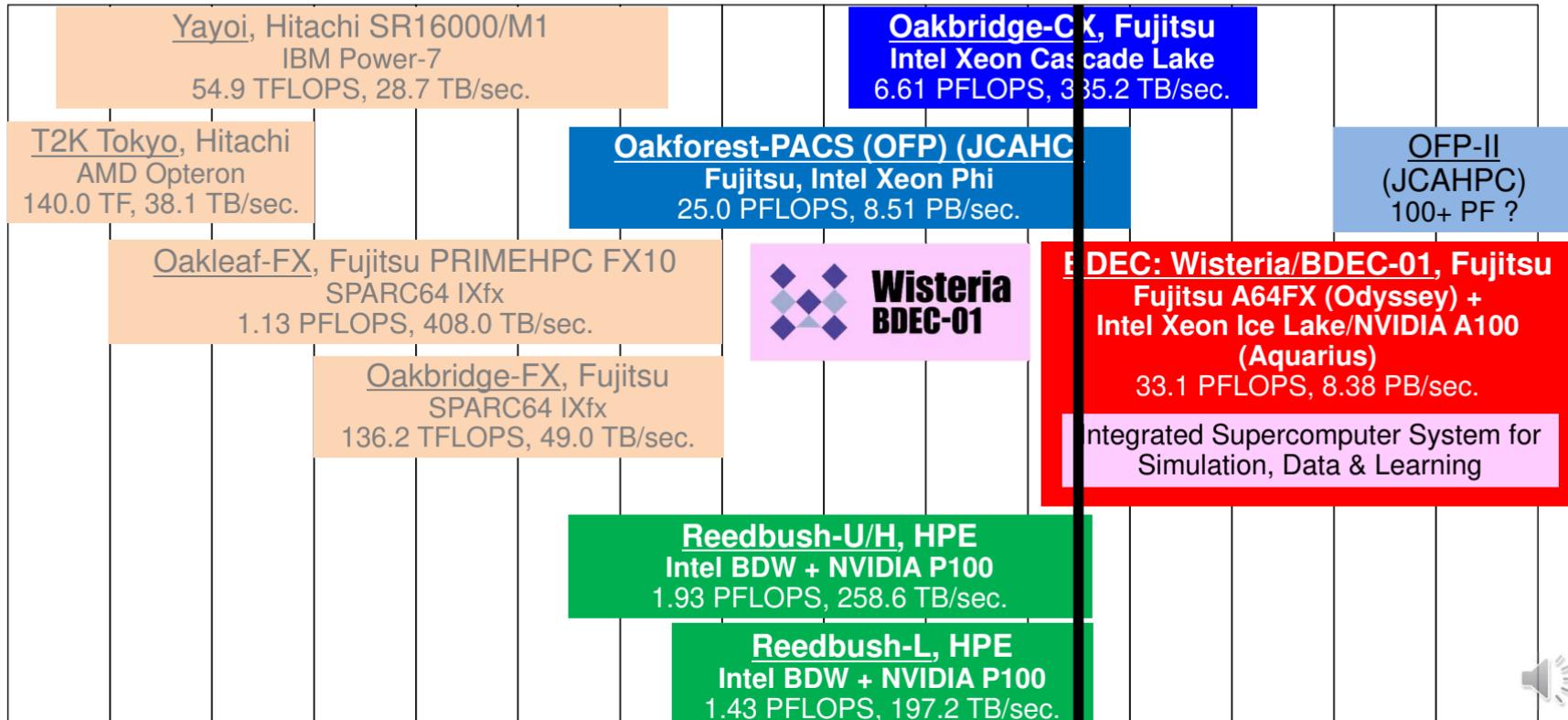
- We are developing an innovative method of computational science towards the Exascale Era/Society 5.0 by integration of (Simulation + Data + Learning (S+D+L)), where ideas of data science and machine learning are introduced to computational science
- **We have been operating 3 systems, and are now introducing the BDEC (Big Data & Extreme Computing) System as the Platform for Integration of (S+D+L)**
  - Wisteria/BDEC-01 with 33.1 PF



# Supercomputers in ITC/U.Tokyo

Information Technology Center, The University of Tokyo

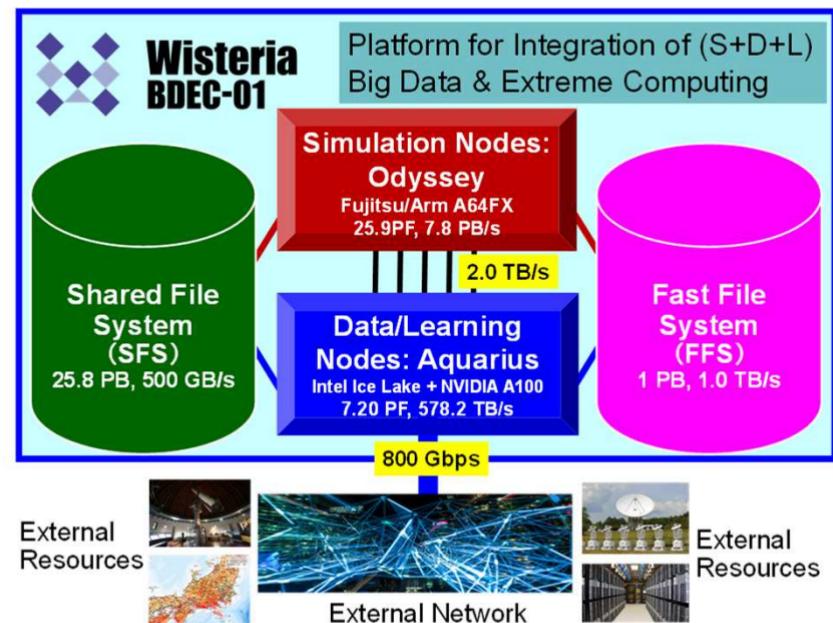
FY11 12 13 14 15 16 17 18 19 20 21 22 23 24 25



# Wisteria/BDEC-01

- Operation starts on May 14, 2021
- 33.1 PF, 8.38 PB/sec by Fujitsu
  - ~4.5 MVA with Cooling, ~360m<sup>2</sup>
- **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 1<sup>st</sup> BDEC System (Big Data & Extreme Computing) Platform for Integration of (S+D+L)



# Rankings@ISC 2021

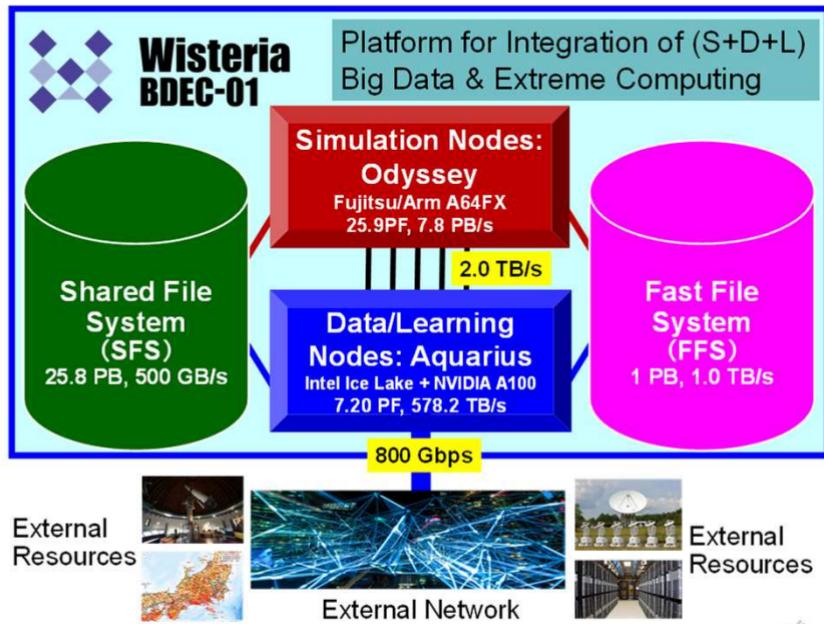
## June 2021



ISC HIGH  
PERFORMANCE  
2021 DIGITAL

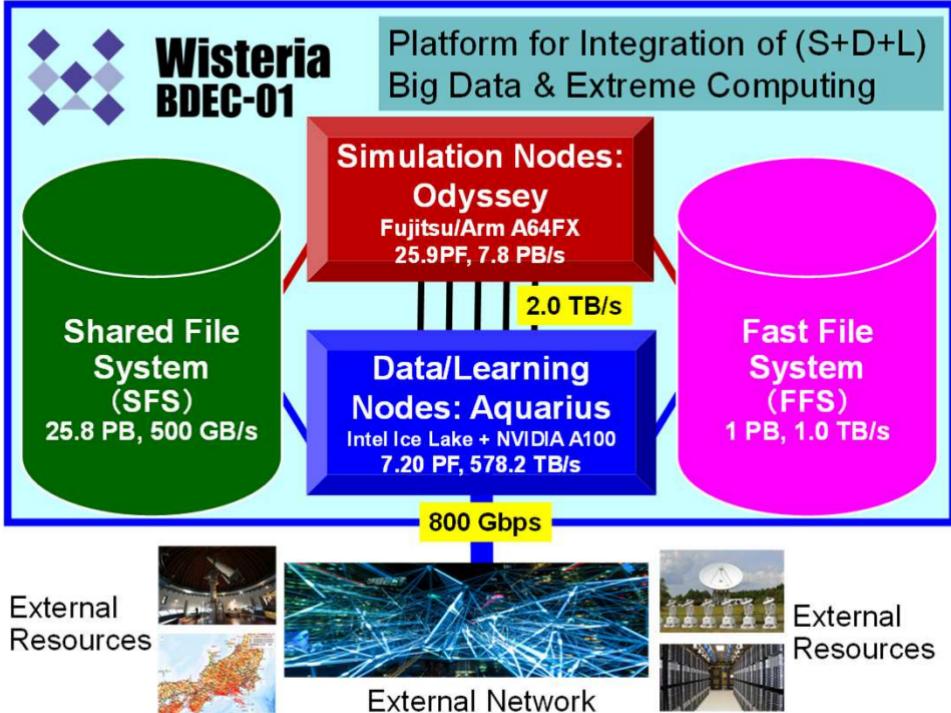
JUNE 24 - JULY 2, 2021  
ISC-HPC.COM

	Odyssey	Aquarius
TOP 500	13	94
Green 500	21	10
HPCG	9	53
Graph 500 BFS	3	-
HPL-AI	7	-

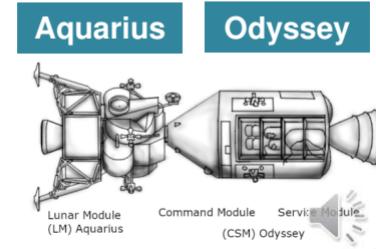


# Wisteria/BDEC-01

## Platform for Integration of (S+D+L)



- Wisteria (紫藤)
  - “Legend of Princess Wisteria” at Lake Teganuma in Kashiwa
- Odyssey
  - Callsign of Apollo 13’s Command Module (CM)
- Aquarius
  - Callsign of Apollo 13’s Luna Module (LM)



**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



**Simulation Codes**

**Simulation Nodes**  
**Odyssey**

Optimized Models & Parameters

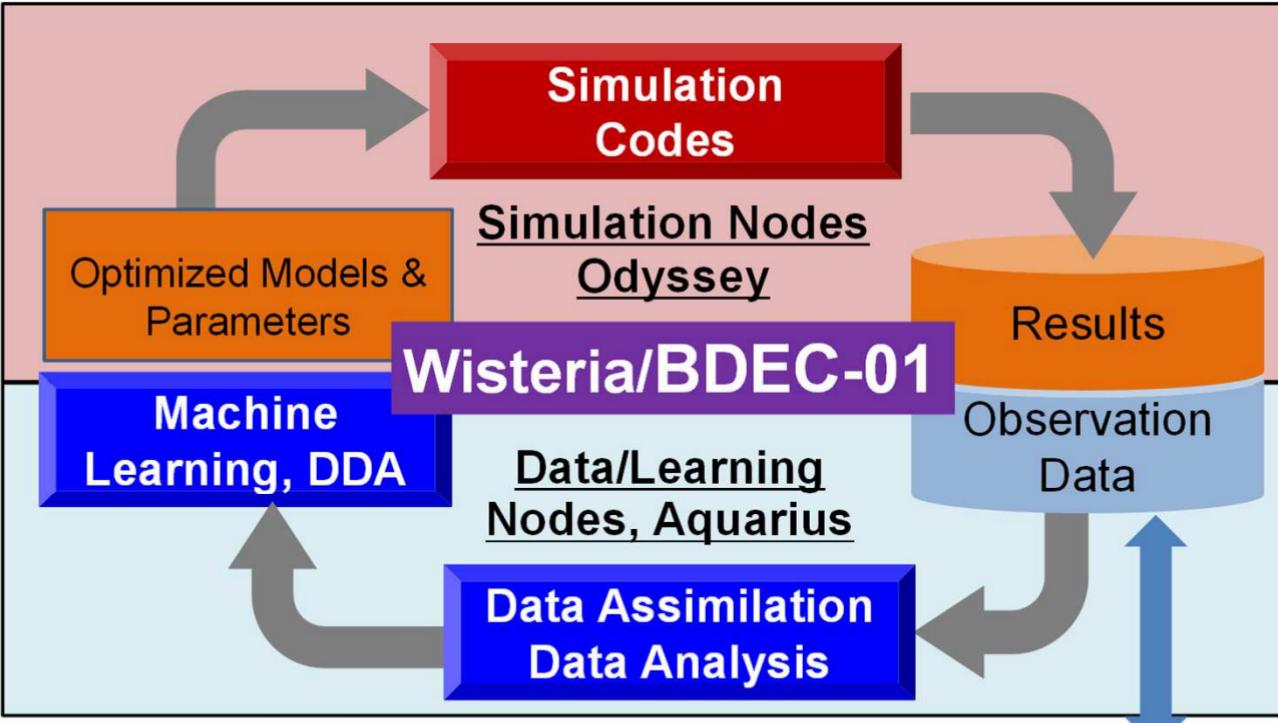
**Machine Learning, DDA**

**Wisteria/BDEC-01**

**Data/Learning Nodes, Aquarius**

**Data Assimilation Data Analysis**

Results  
Observation Data

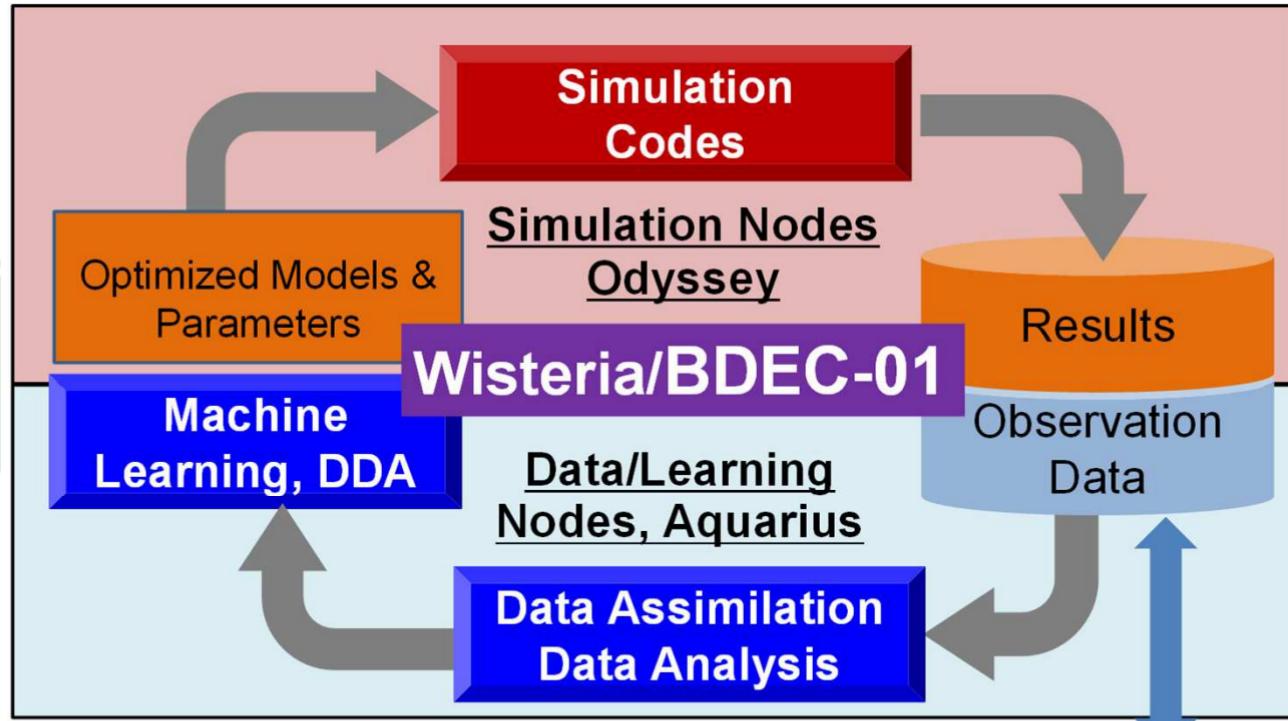


**Simulation Nodes**  
**Odyssey**  
25.9 PF, 7.8 PB/s

**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



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



# h3-Open-BDEC on BDEC System



- We are developing an innovative method of computational science towards the Exascale Era/Society 5.0 by integration of (Simulation + Data + Learning (S+D+L)), where ideas of data science and machine learning are introduced to computational science
- We have been operating 3 systems, and are now introducing the BDEC (Big Data & Extreme Computing) System, Wisteria/BDEC-01, with 33.1 PF as the Platform for Integration of (S+D+L)
- **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 through JSPS Grant-in-Aid for Scientific Research (S) since 2019
  - Leading-PI: Kengo Nakajima (The University of Tokyo)
  - Total Budget: 152.7M JPY= 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 Assimilati...
- Takashi Shimokawabe (ITC/U.Tokyo), Co-PI, ML/hDDA
- Takeshi Ogita (TWCU), Co-PI, Accuracy Verification
- Takahiro Katagiri (Nagoya U), Co-PI, Appropriate Computing
- Hiroya Matsuba (ITC/U.Tokyo), Co-PI, Container



# h3-Open-BDEC

## Innovative Software Platform for Integration of (S+D+L) on BDEC

### h3-Open-BDEC

New Principle for Computations  
Numerical Alg./Library

Simulation + Data + Learning  
App. Dev. Framework

Integration + Communications+ Utilities  
Control & Utility

**h3-Open-MATH**  
Algorithms with High-Performance, High Reliability & Mixed/Adaptive Precision

**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

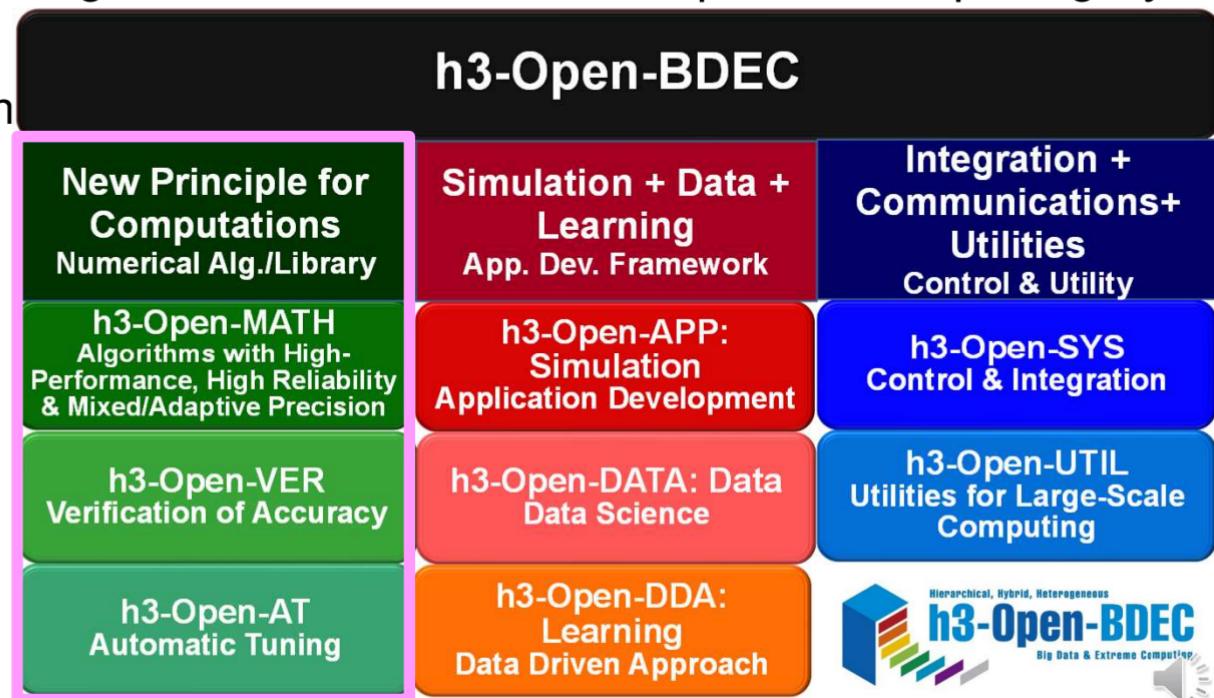
**h3-Open-DDA:**  
Learning  
Data Driven Approach



# h3-Open-BDEC: Two Significant Innovations

① Methods for Numerical Analysis with High-Performance/High-Reliability/Power-Saving based on the New Principle of Computing by

- ✓ Adaptive Precision
- ✓ Accuracy Verification
- ✓ Automatic Tuning



# Approximate Computing with Low/Adaptive/Trans Precision

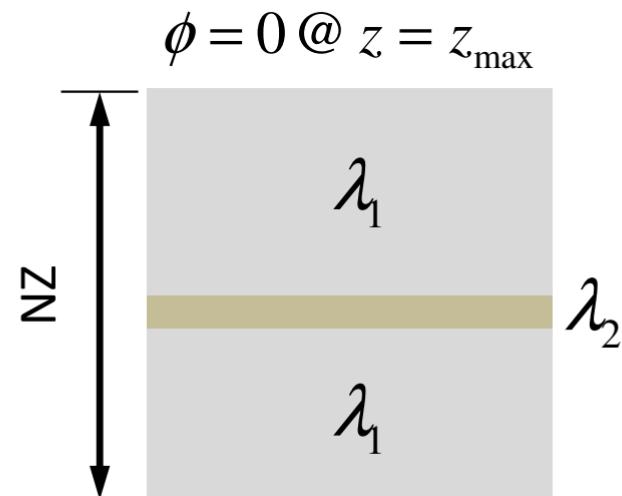
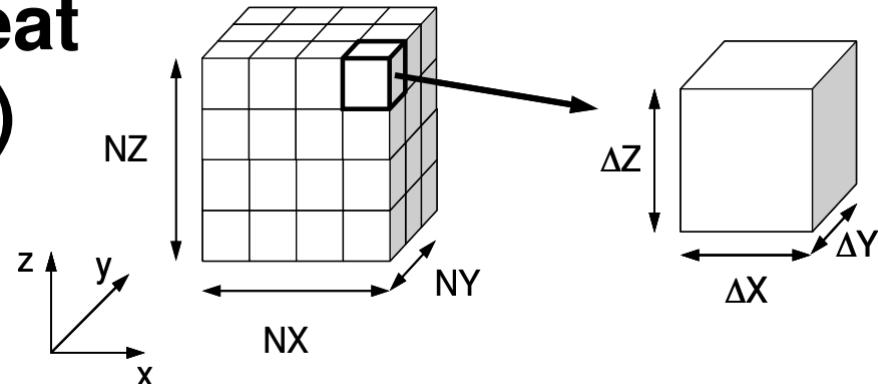
- Mostly, scientific computing has been conducted using FP64 (double precision, DP)
  - Sometimes, problems can be solved by FP32 (single precision, SP) or lower precision
- **Lower precision may save time, energy and memory**
- Approximate Computing
  - Originally for image recognition etc. where accuracy 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)

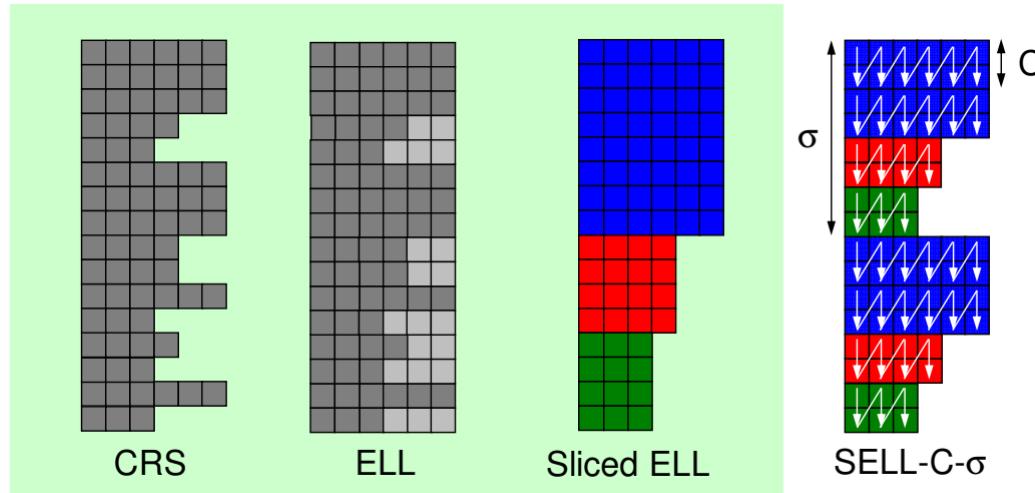
$$\nabla \cdot (\lambda \nabla \phi) + f = 0$$

- 7-point Stencil
- Heterogenous Material Property
  - $\lambda_1/\lambda_2$  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- $\sigma$  etc.)



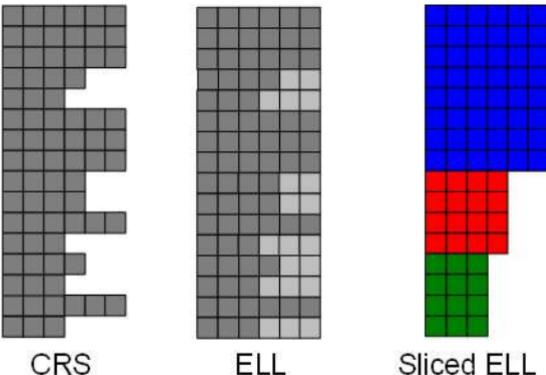
System	Oakforest-PACS	Oakbridge-CX	Oakleaf-7 (FX700)
Abbreviation	OFP	OBCX	OL7
Architecture of CPU	Intel Xeon Phi 7250 (Knights Landing, KNL)	Intel Xeon Platinum 8280 (Cascade Lake, CLX)	Fujitsu A64FX(1.8GHz)
Core#/Socket	68	28	48
Socket#/Node	1	2	1
Peak Performance (DP) (GFLOPS)/Node	3,046	4,838	2,765
Memory Capacity (GB)/Node	MCDRAM: 16 DDR4: 96	192	32
Memory Bandwidth (GB/sec), Stream Triad	MCDRAM: 490 DDR4: 84.5	202	809
Compiler	Intel Parallel Studio 2019		Fujitsu FCC 4.0.0



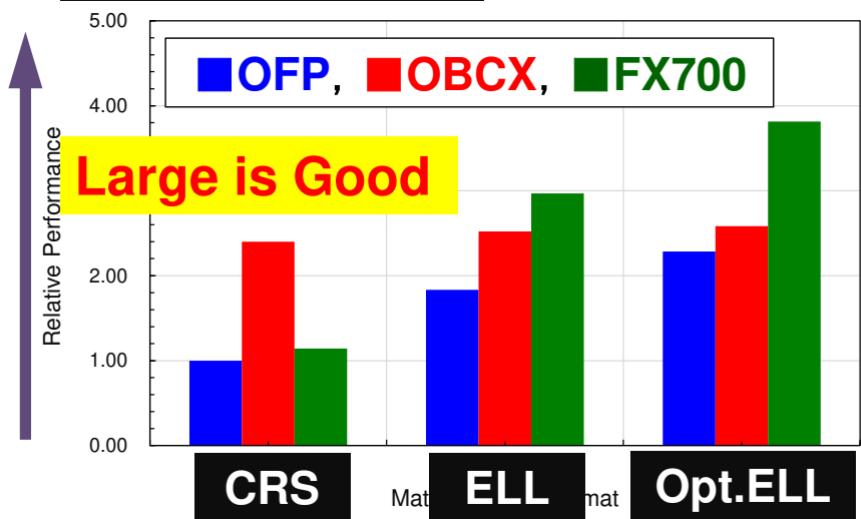
# Ratio of Performance

Elapsed Computation Time for ICCG (DP),  
Normalized by OFP with CRS,  $\lambda_1 / \lambda_2 = 1$

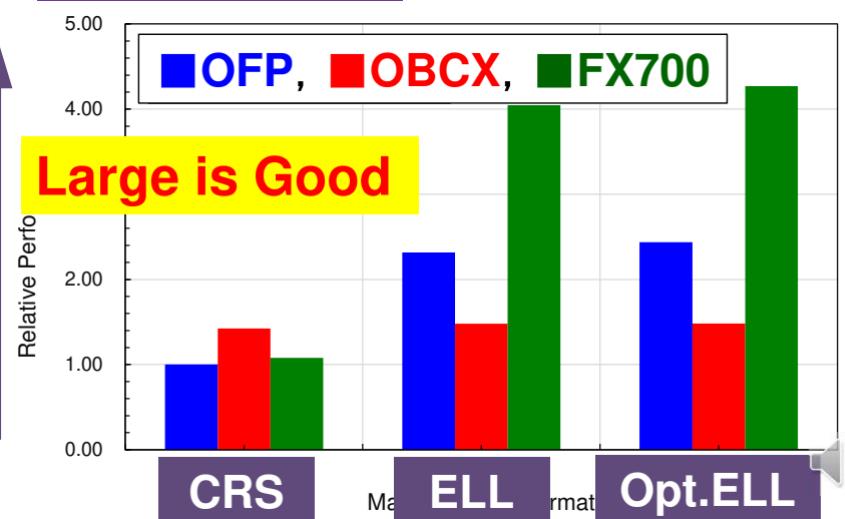
[KN et al. SWoPP 2020]



Medium :  $128^3$



Large :  $256^3$



# Mixed Precision Computing of ICCG Solver for P3D on FX700

	SpMV, DAXPY, Dot Products	Preconditioning	Vectors for Preconditioning
D-D	FP64	FP64	FP64
D-S	FP64	FP32	FP32
D-H	FP64	FP16	FP32
S-S	FP32	FP32	FP32
S-H	FP32	FP16	FP32



# Mixed Precision Computing for P3D on FX700

## Implementation of Forward Substitution (CRS) in ICCG

[KN et al. SWoPP 2020]

**FP64**  
**FP32**  
**FP16**

```

!$omp parallel do private(ip, i)
do ip= 1, PEsmptOT
do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
    Ws(I, Z)= W(i, R)
  enddo
enddo

!$omp parallel private(ic, ip, ip1, I, WVALs, k)
do ic= 1, NCOLORtot
!$omp do
  do ip= 1, PEsmptOT
    ip1= (ip-1)*NCOLORtot + ic
    do i= SMPindex(ip1-1)+1, SMPindex(ip1)
      WVALs= Ws(i, Z)
      do k= indexL(i-1)+1, indexL(i)
        WVALs= WVALs - ALs(k) * Ws(itemL(k), Z)
      enddo
      Ws(I, Z)= WVALs * Ws(i, DD)
    enddo
  enddo
enddo

!$omp end parallel

(Backward Substitution)

!$omp parallel do private(ip, i)
do ip= 1, PEsmptOT
do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
    W(I, Z)= Ws(I, Z)
  enddo
enddo

```

**D-S**

```

!$omp parallel do private(ip, i)
do ip= 1, PEsmptOT
do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
    Ws(I, Z)= W(i, R)
  enddo
enddo

!$omp parallel private(ic, ip, ip1, i, WVALs, k)
do ic= 1, NCOLORtot
!$omp do
  do ip= 1, PEsmptOT
    ip1= (ip-1)*NCOLORtot + ic
    do i= SMPindex(ip1-1)+1, SMPindex(ip1)
      WVALs= Ws(i, Z)
      do k= indexL(i-1)+1, indexL(i)
        WVALs= WVALs - ALh(k) * Ws(itemL(k), Z)
      enddo
      Ws(i, Z)= WVALs * Wh(i, DD)
    enddo
  enddo
enddo

!$omp end parallel

```

**S-H**

```

!$omp parallel do private(ip, i)
do ip= 1, PEsmptOT
do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
    Ws(I, Z)= W(i, R)
  enddo
enddo

!$omp parallel private(ic, ip, ip1, i, WVALs, k)
do ic= 1, NCOLORtot
!$omp do
  do ip= 1, PEsmptOT
    ip1= (ip-1)*NCOLORtot + ic
    do i= SMPindex(ip1-1)+1, SMPindex(ip1)
      WVALs= Ws(i, Z)
      do k= indexL(i-1)+1, indexL(i)
        WVALs= WVALs - ALh(k) * Ws(itemL(k), Z)
      enddo
      Ws(i, Z)= WVALs * Wh(i, DD)
    enddo
  enddo
enddo

!$omp end parallel

```

**D-H**

```

!$omp parallel do private(ip, i)
do ip= 1, PEsmptOT
do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
    W(I, Z)= Ws(I, Z)
  enddo
enddo

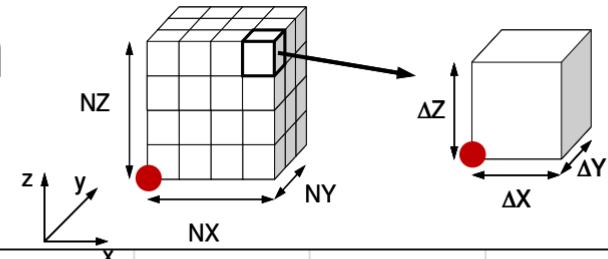
!$omp parallel do private(ip, i)
do ip= 1, PEsmptOT
do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
    W(I, Z)= Ws(I, Z)
  enddo
enddo

```

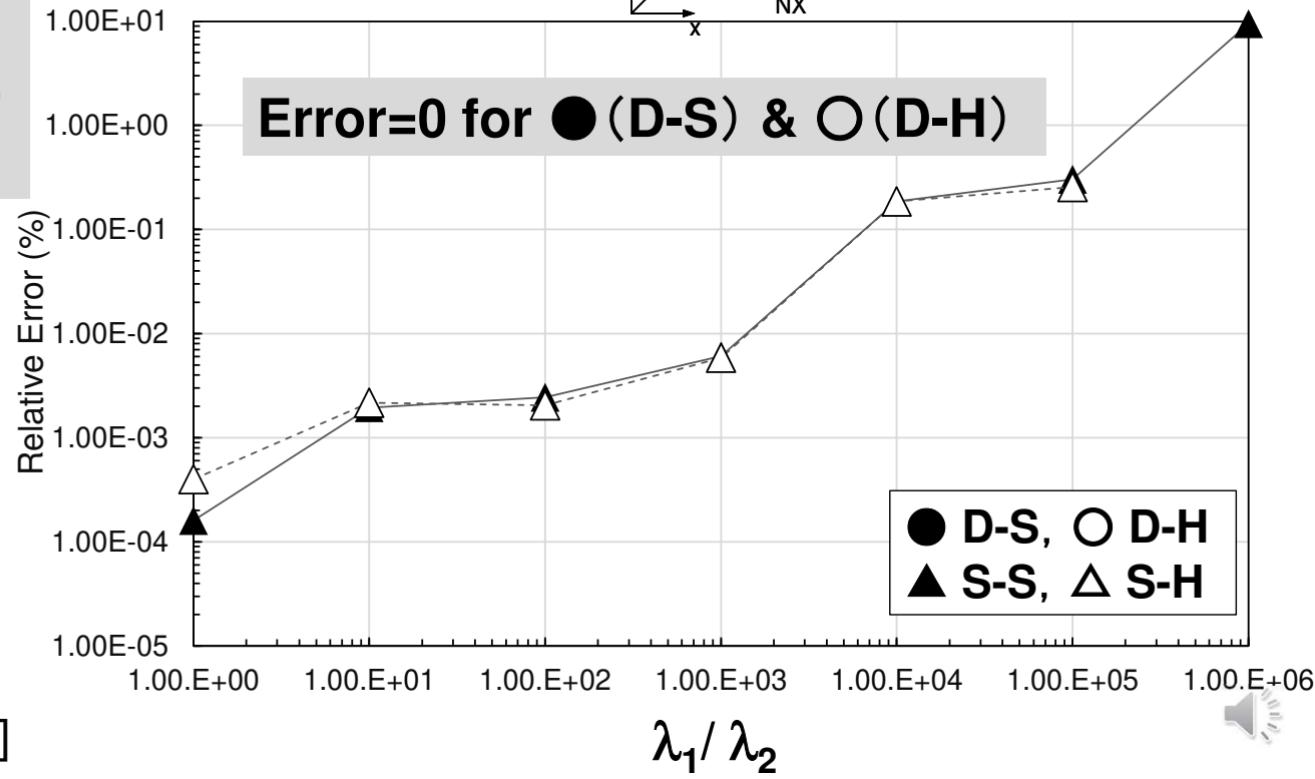


# Mixed Precision Computation

D-H/S-H do not converge at  $\lambda_1 / \lambda_2 = 10^6$



**Relative Error (%) compared to D-D @ ●**



# Mixed Precision Computation

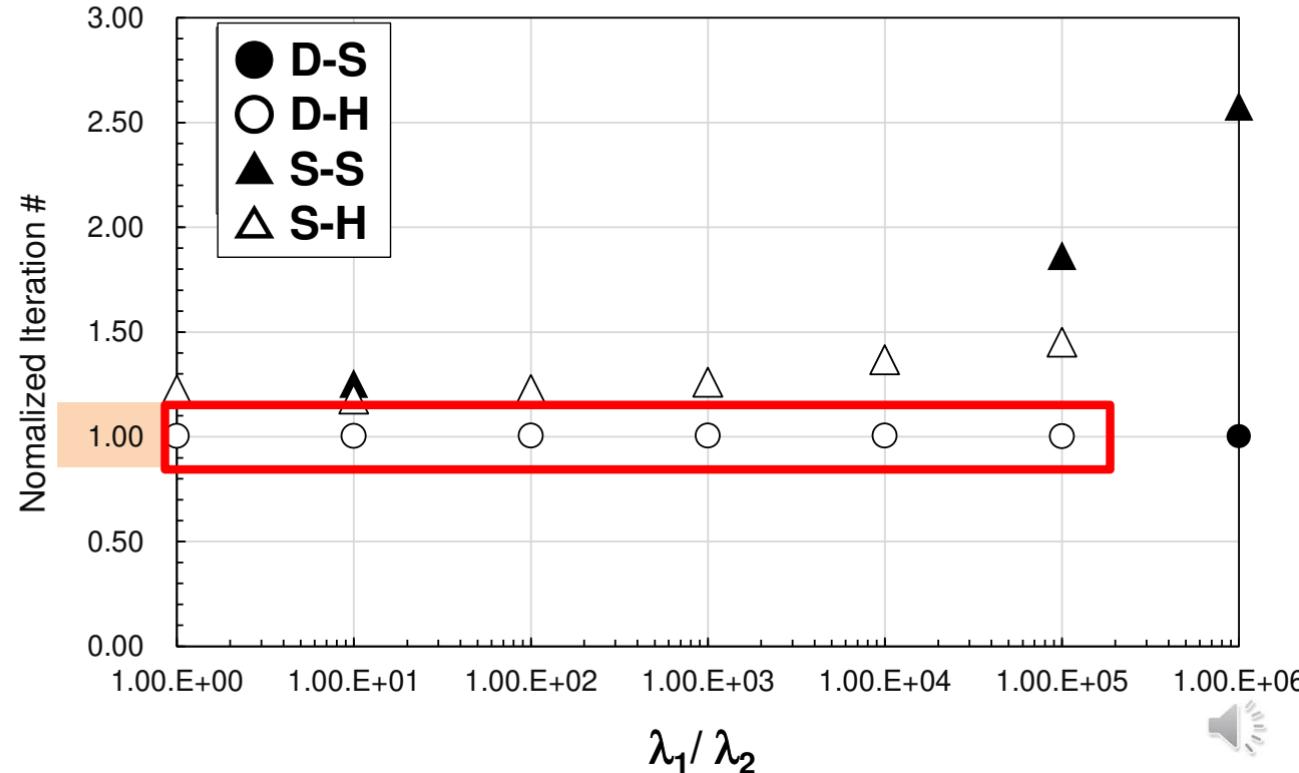
[KN et al. SWoPP 2020]

D-H/S-H do not converge at  $\lambda_1 / \lambda_2 = 10^6$

**Number of Iterations (Normalized by that of D-D)**

● ~ ○ ~ D-D, ▲ ~ △

**Results of (D-S, D-H) agree with those of D-D (if  $\lambda_1 / \lambda_2 \leq 10^5$ )**



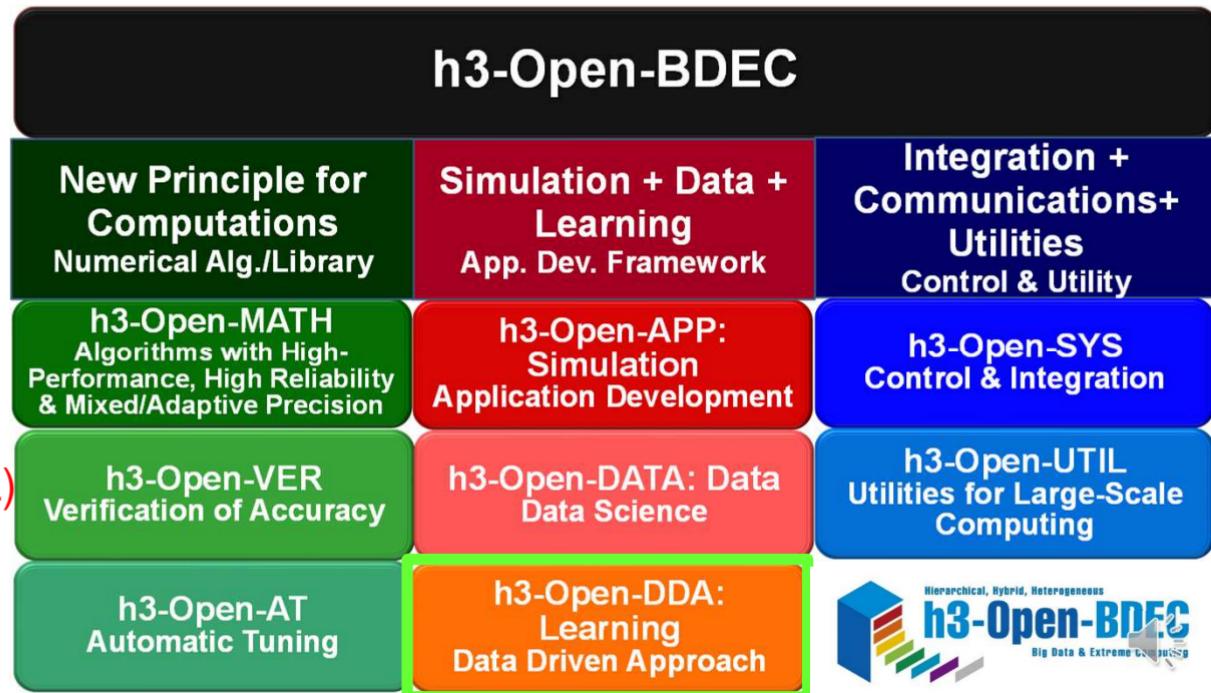
# h3-Open-BDEC: Two Significant Innovations

① Methods for Numerical Analysis with High-Performance/High-Reliability/Power-Saving based on the New Principle of Computing by

- ✓ Adaptive Precision
- ✓ Accuracy Verification
- ✓ Automatic Tuning

② Hierarchical Data Driven Approach (*hDDA*) based on machine learning

- ✓ Integration of (S+D+L)  
AI for HPC



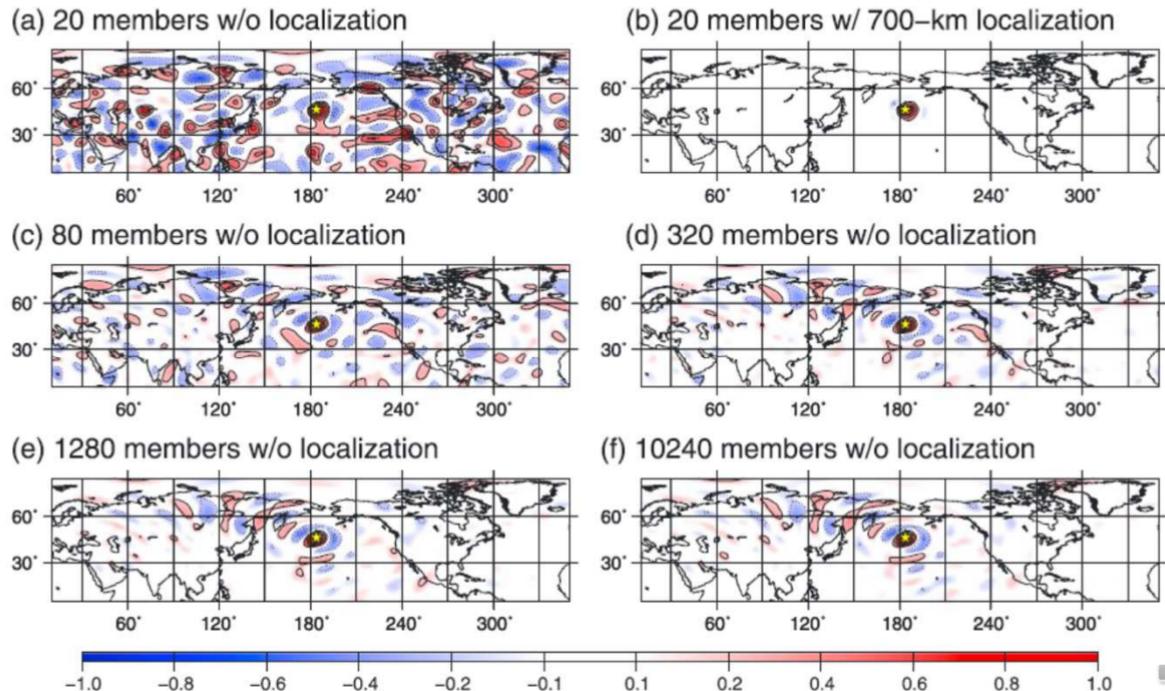
# Real-World Scientific Simulations

- Non-Linear: Huge Number of Parameter Studies needed
  - ✓ Reduction of cases is very crucial

## • Data Assimilation

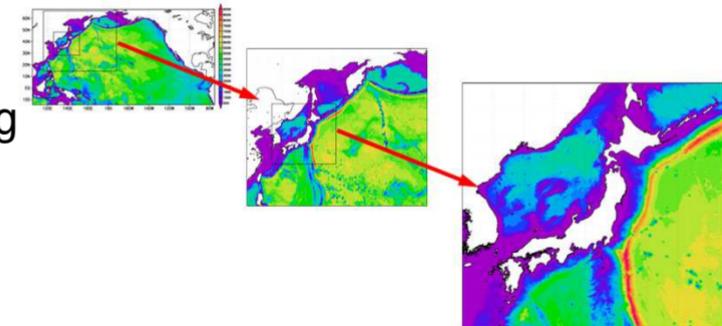
- ✓ Mid-Range Weather Prediction: 50-100 Ensemble Cases, 1,000 needed for accurate solution.
- ✓ 50-100 (or fewer) may be enough for accurate solution, if opt. parameters are selected (e.g. by ML),

[Miyoshi et al. 2014]

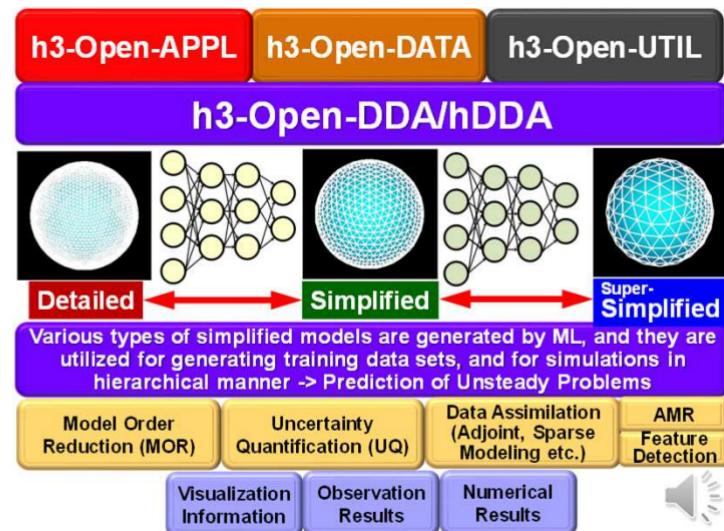


# Hierarchical Data Driven Approach: *hDDA*

- Data Driven Approach (DDA)
  - Technique of AI/ML is introduced for predicting the results of simulations with different parameters.
  - DDA generally requires  $O(10^3\text{-}10^4)$  runs for generation of training data.



- **hDDA (Hierarchical DDA)**
  - Simplified models with coarser meshes (but preserving original features of physics) for efficient training are constructed automatically by Machine Learning using:
    - Feature Detection, AMR
    - MOR (Model Order Reduction)
    - UQ (Uncertainty Quantification)
    - Sparse Modeling



# Acceleration of Transient CFD Simulations using ML/CNN Integration of (S+D+L), AI for HPC

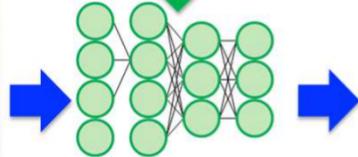
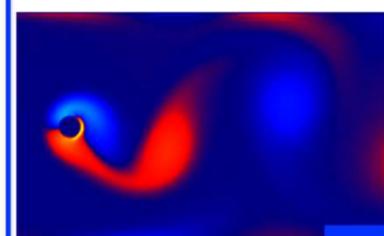


## Datasets

$$f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) + \Omega_i(x, t)$$

$$\Omega_i(x, t) = -\frac{1}{\tau} (f_i(x, t) - f_i^{eq}(x, t))$$

## Training



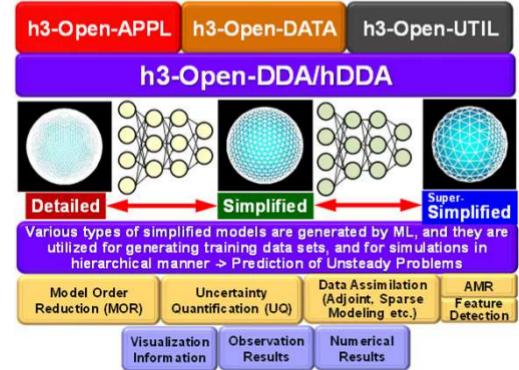
CNN to predict simulation results

## Prediction

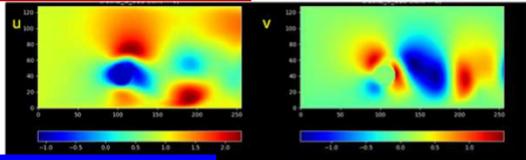
Prediction of the Results  
after 10+ Time Steps ...

Prediction of Time  
Evolution

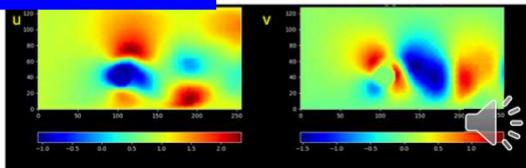
NN may become “faster simulator”



## Simulations: LBM



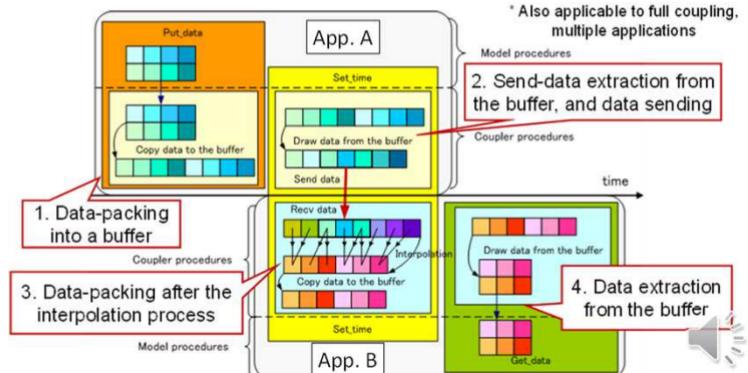
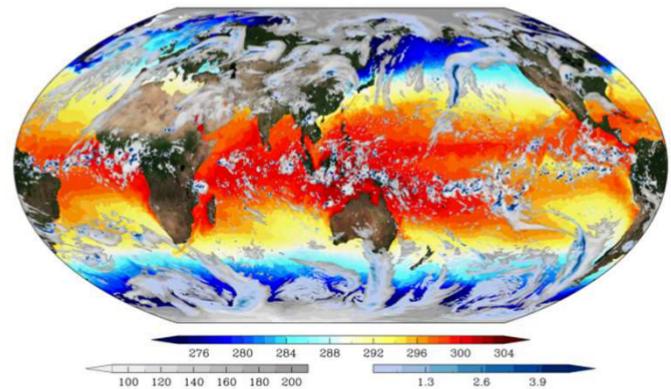
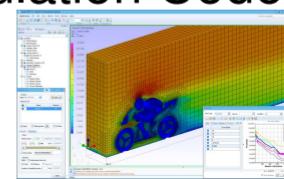
## CNN Predictions



# Possible Applications (S+D+L) on Wisteria/BDEC-01 with h3-Open-BDEC

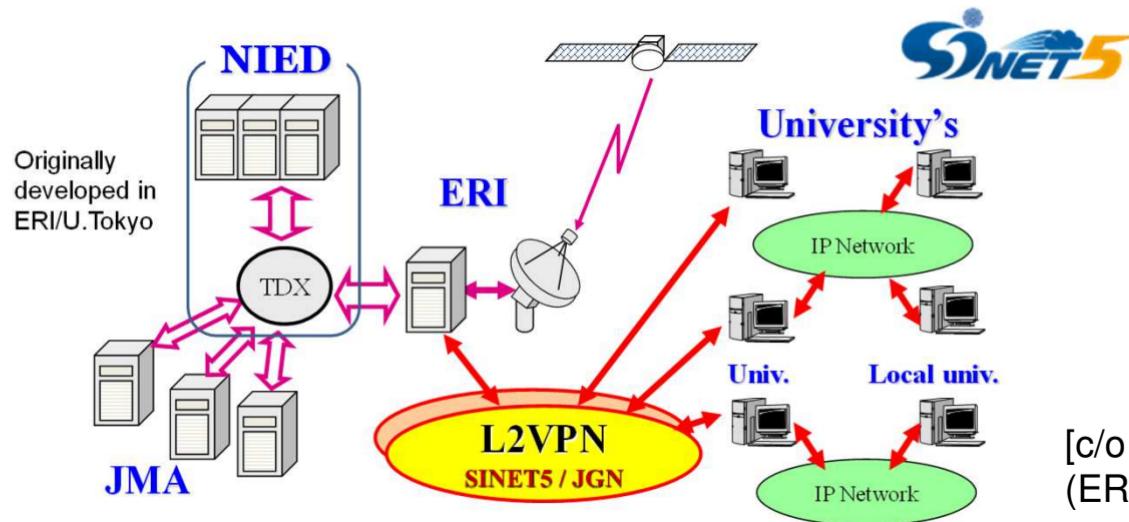


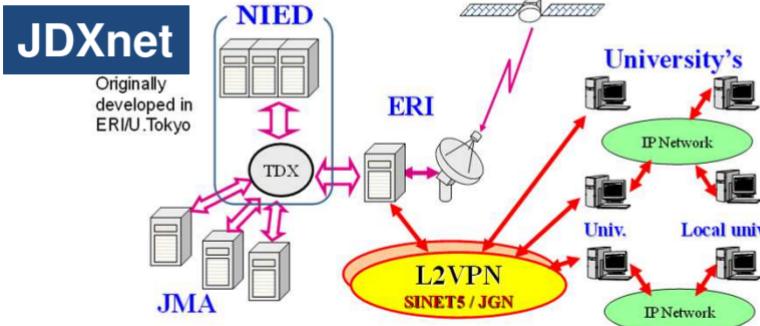
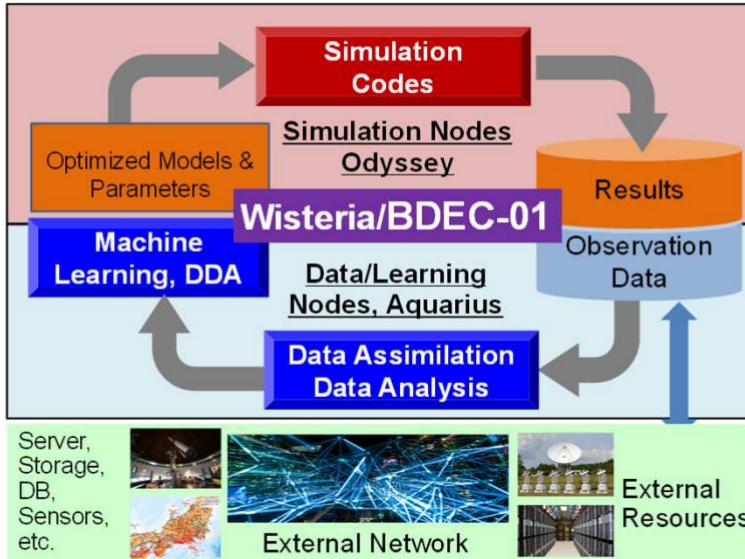
- Simulations with Data Assimilation
  - Very Typical Example of (S+D+L)
- Atmosphere-Ocean Coupling for Weather and Climate Simulations
  - AORI/U.Tokyo, RIKEN R-CCS, NIES
- **Earthquake Simulations with Real-Time Data Assimilation**
  - ERI/U. Tokyo
- Real-Time Disaster Simulations
  - Flood, Tsunami
- (S+D+L) for Existing Simulation Codes (Open Source Software)
  - OpenFOAM



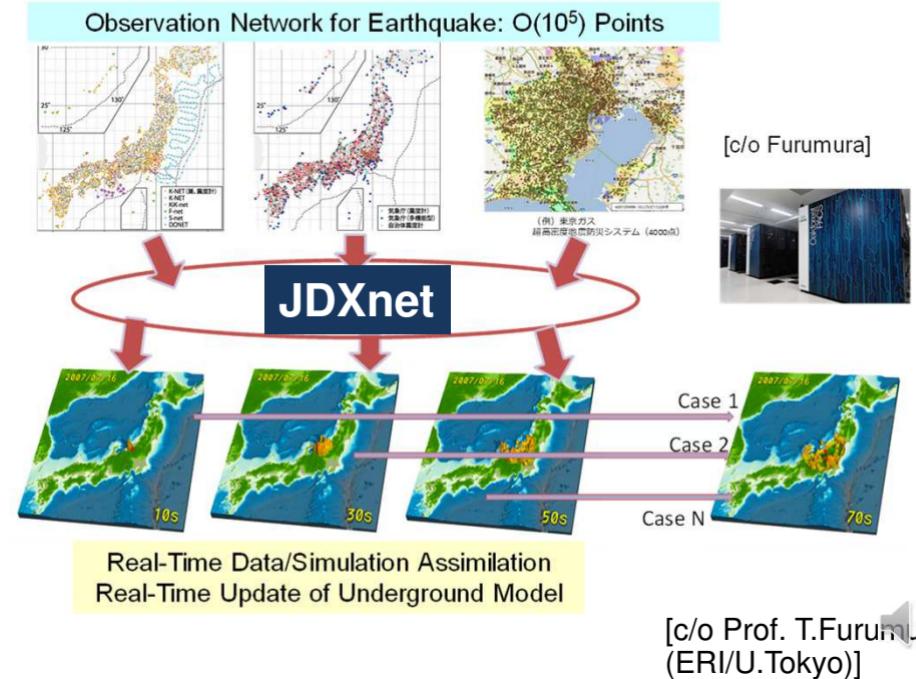
# Real-Time Sharing of Seismic Observation is possible in Japan by JDXnet with SINET

- Seismic Observation Data (100Hz/3-dir's/ $O(10^3)$  observation points) by JDXnet is available through SINET in Real Time
  - $O(10^2)$  GB/day
  - $O(10^5)$  pts in future including stations operated by industry





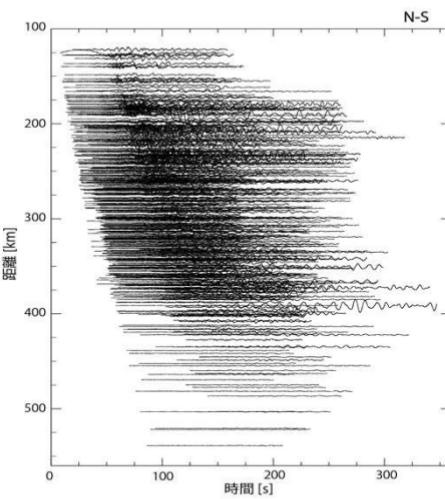
# 3D Earthquake Simulation with Real-Time Data Observation/Assimilation



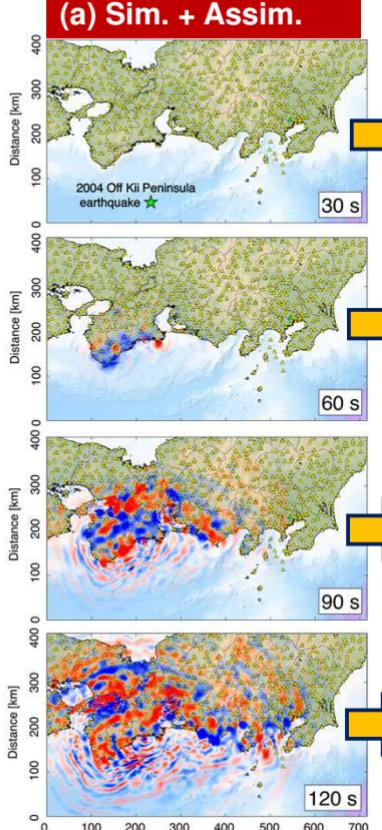
[c/o Prof. T.Furumura  
(ERI/U.Tokyo)]

# Example of Real-Time Assimilation of (Obs.+Comp.): 2004 Kii Peninsula Earthquake (Mw 7.4) [c/o Oba & Furumura]

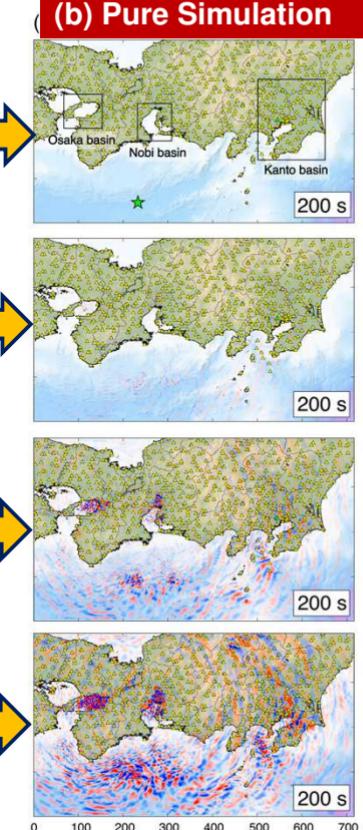
○ Observation (K-NET, KiK-net 446 pts)



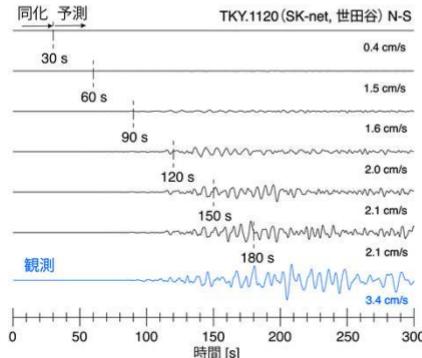
(a) Sim. + Assim.



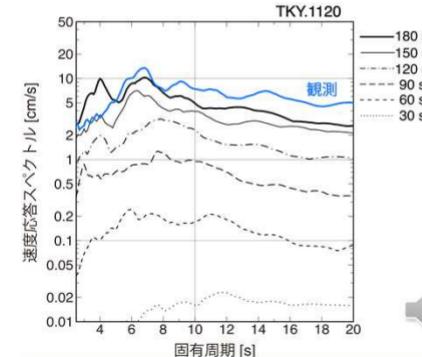
(b) Pure Simulation



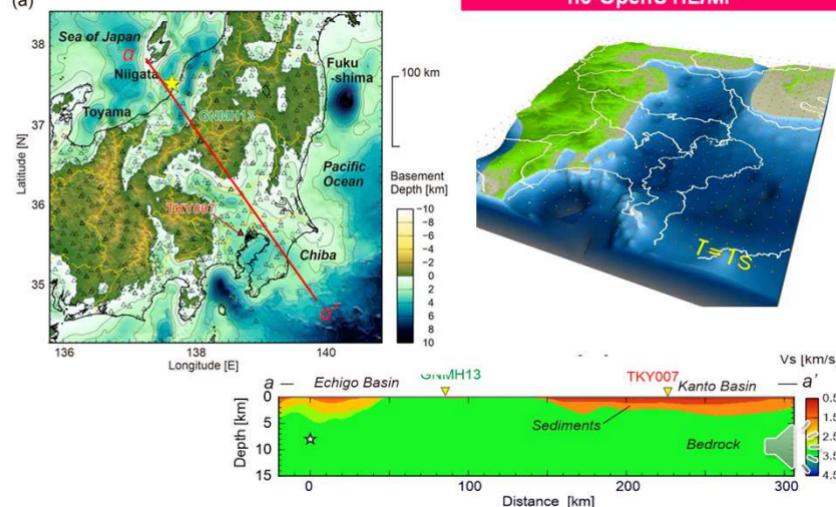
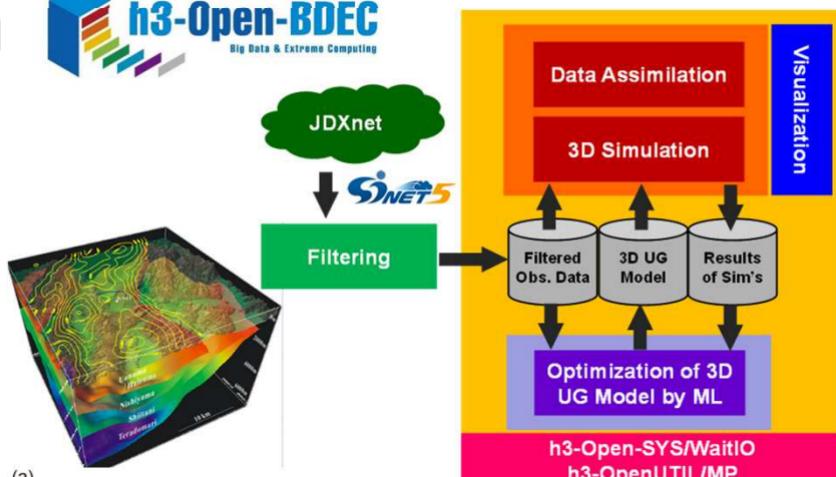
Long Wave Propagation in Tokyo



Response Spectrum

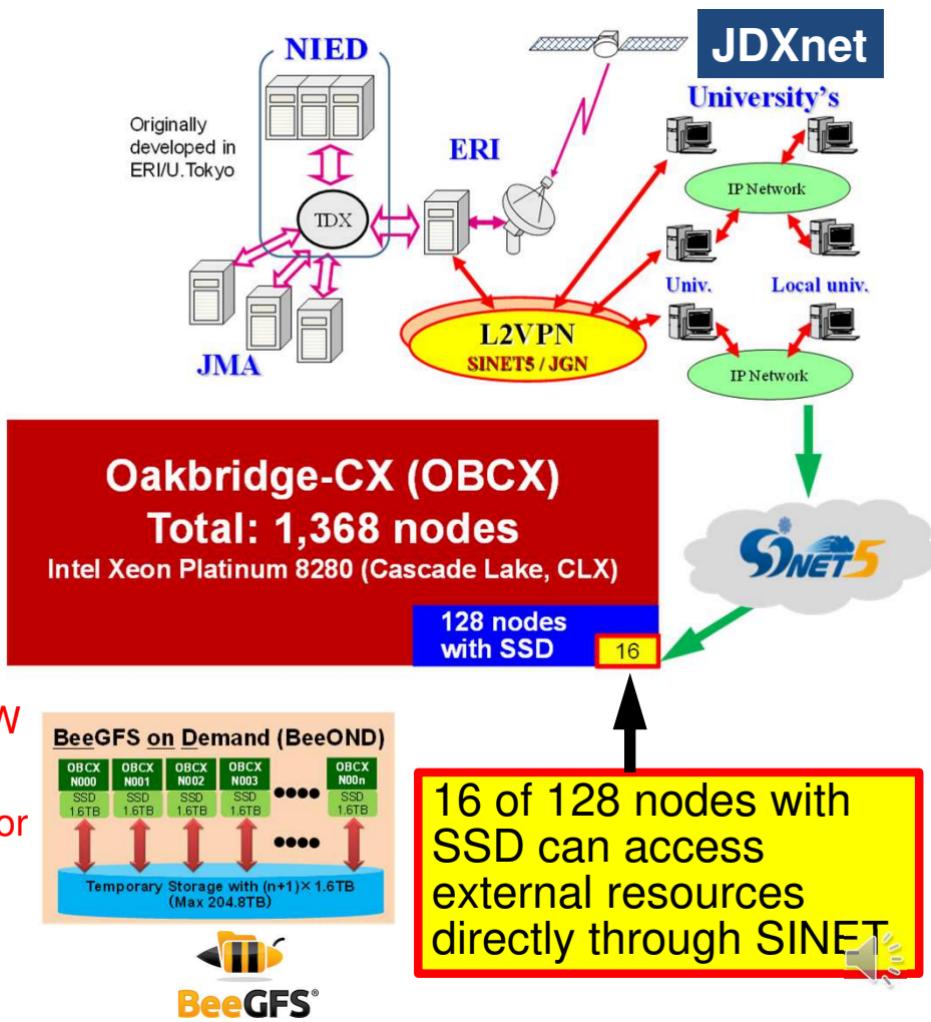


# 3D Earthquake Simulation with Real-Time Data Observation/Assimilation



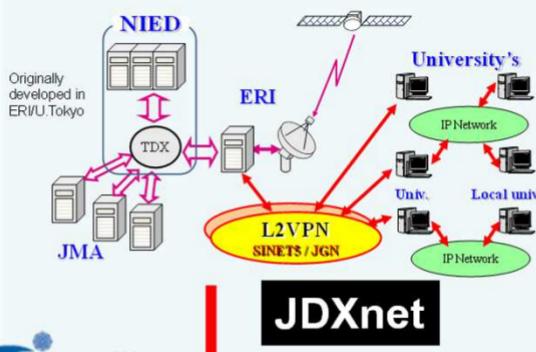
# Preliminary Works on Oakbridge-CX (OBCX)

- Intel Xeon Platinum 8280 (Cascade Lake, CLX), Fujitsu
  - 1,368 nodes, 6.61 PF peak, 385.1 TB/sec, 4.2+ PF for HPL
  - #69 in 56<sup>th</sup> Top500 (Nov.2020)**
  - Fast Cache: SSD's for 128 nodes: Intel SSD, BeeGFS: 200+TB Fast FS
    - 1.6 TB/node, 3.20/1.32 GB/s/node for R/W
    - 16 of these nodes can directly access external resources (server, storage, sensor network etc.) through SINET
- Switching to Wisteria/BDEC-01 after May 2021

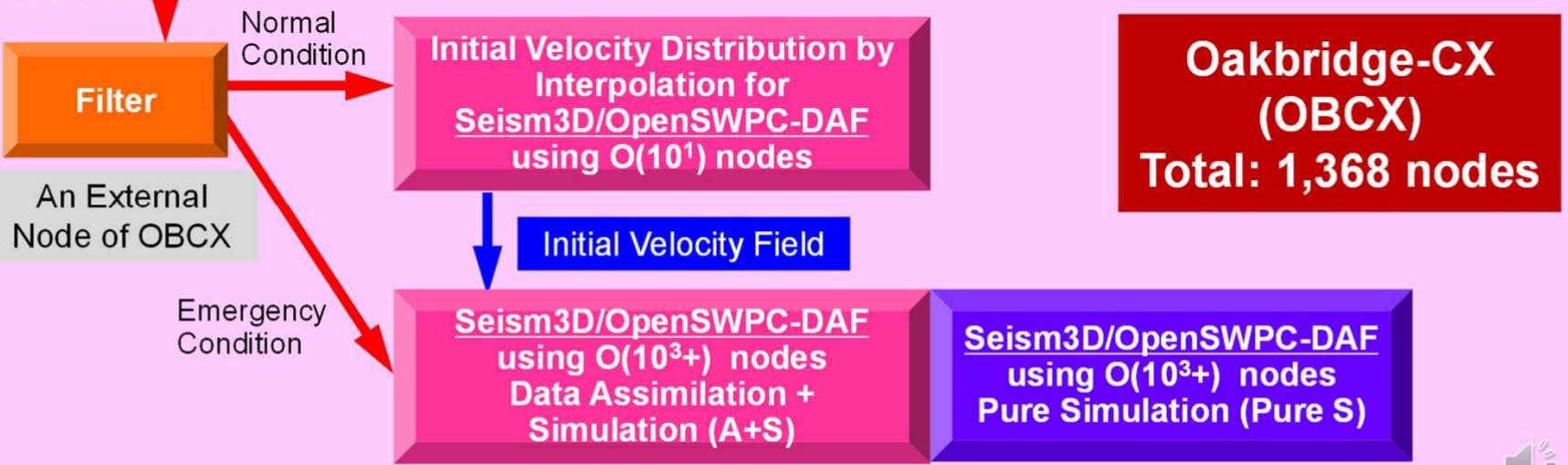


# 3D Simulation + Real-Time Data Assimilation on OBCX

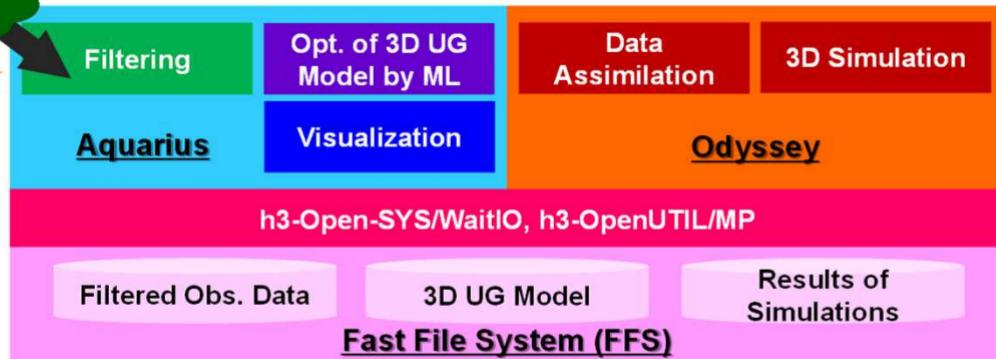
## Seism3D/OpenSWPC-DAF: 3D FDM (Finite-Difference Method)



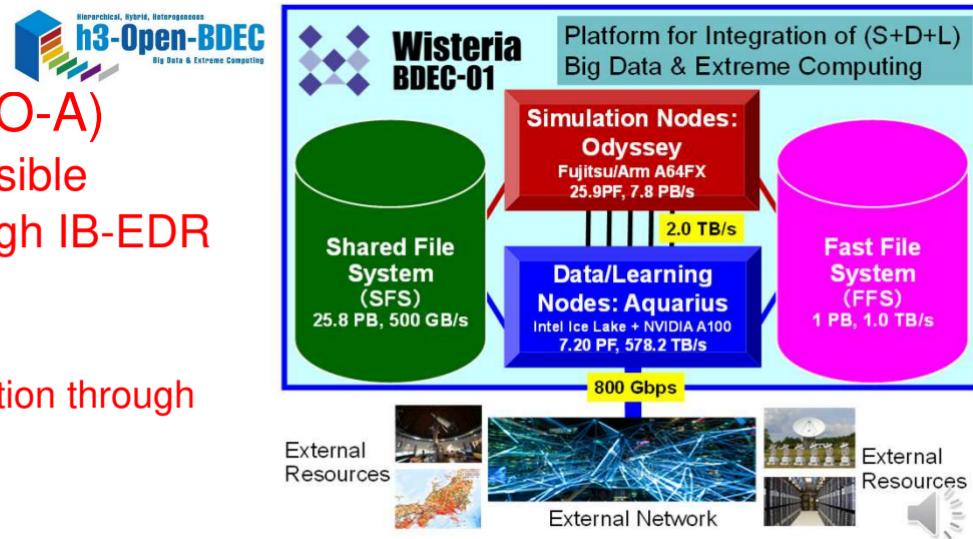
**JDxnet**



# Computing on Wisteria/BDEC-01



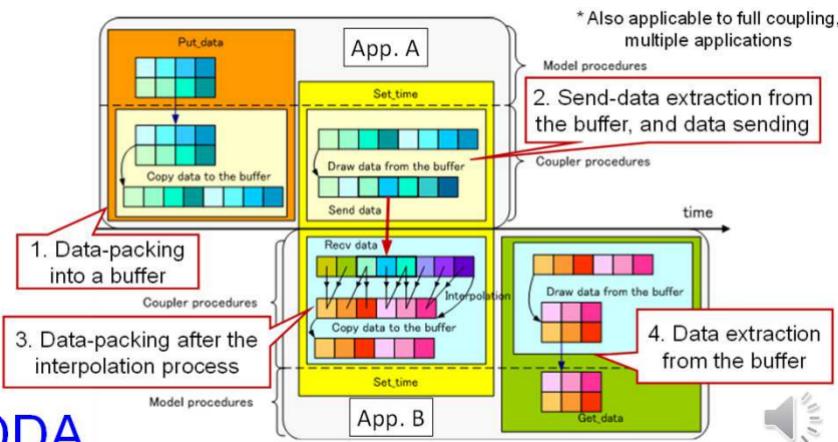
- Wisteria/BDEC-01
  - Aquarius (GPU: NVIDIA A100)
    - Filtering, ML, Visualization
  - Odyssey (CPU: A64FX)
    - Data Assimilation, Simulation
- Combining Odyssey-Aquarius (O-A)
  - Single MPI Job over O-A is impossible
  - Actually, O-A are connected through IB-EDR with 2TB/sec.
  - h3-Open-SYS/WaitIO
    - Library for Inter-Process Communication through IB-EDR with MPI-like interface
  - h3-Open-UTIL/MP
    - Multiphysics Coupler



# h3-Open-UTIL/MP

## Multilevel Coupler/Data Assimilation

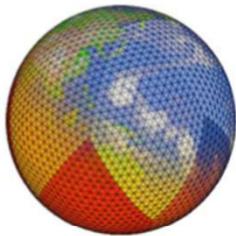
- Current Coupler: ppOpen-MATH/MP
  - Weak-Coupling of Multiple (usually two) Applications
    - Each application does a single computation
- h3-Open-UTIL/MP
  - Data Assimilation (Multiple Computations: Ensemble)
  - Assimilation of Computations with Different Resolutions
    - h3-Open-DATA, h3-Open-APP
  - Data Assimilation by Coupled Codes
    - e.g. Atmosphere-Ocean
- Data Assimilation: h3-Open-DATA
  - Karman Filter, Particle Karman Filter
  - LETKF
  - Adjoint Method
- Generation of Simplified Models in hDDA



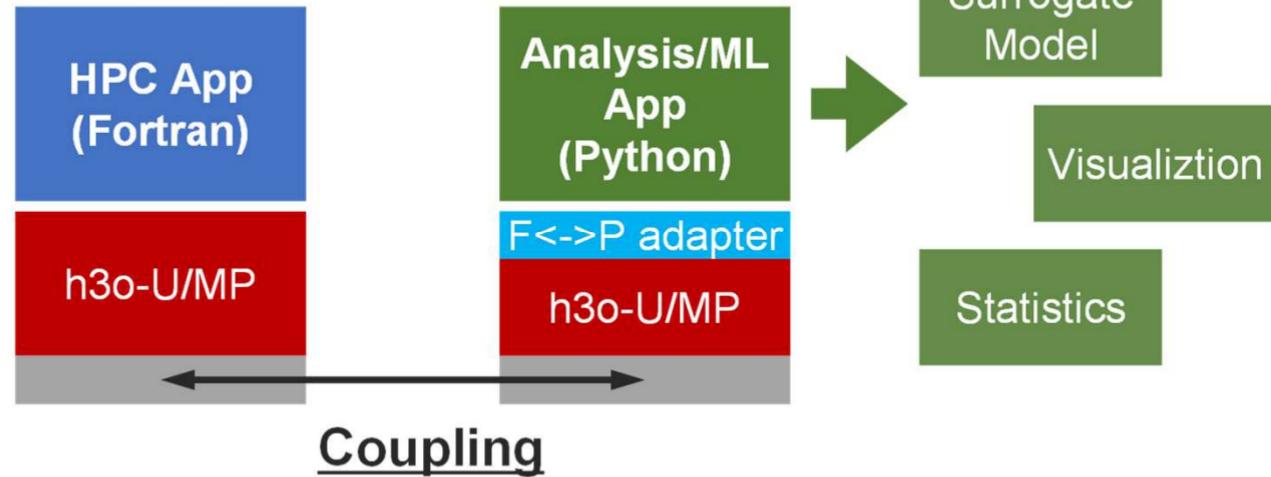
# **h3-Open-UTIL/MP (h3o-U/MP)**

**(HPC+AI) Coupling**

**[Dr. H. Yashiro, NIES]**



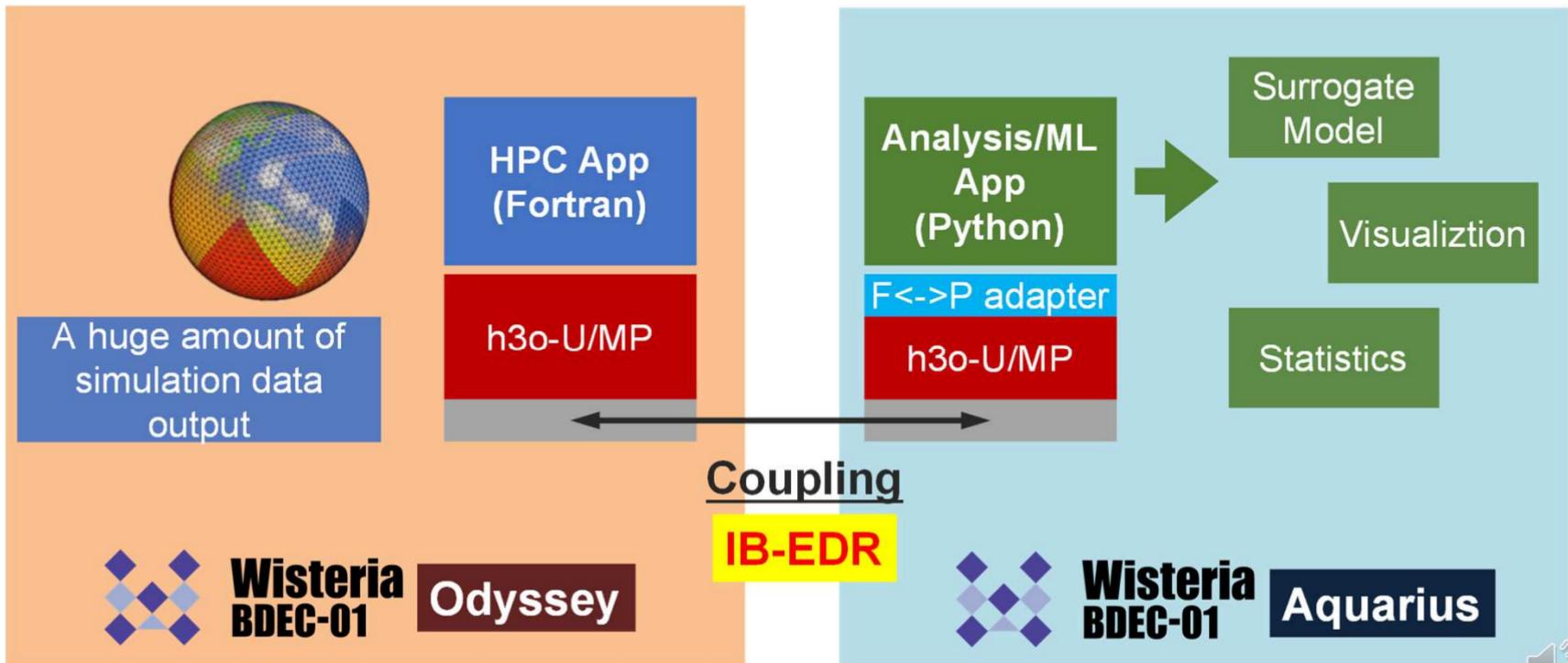
A huge amount of  
simulation data  
output



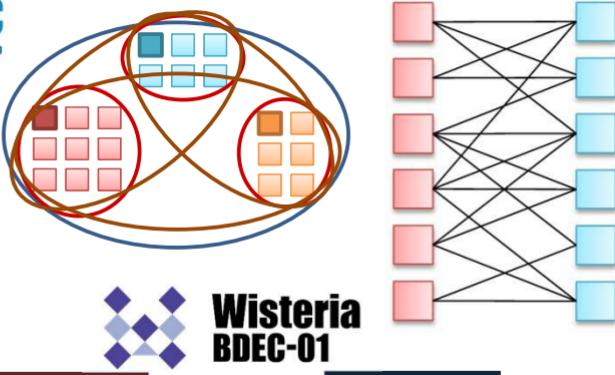
- Providing on-the-fly input/output/training data to the Analysis/ML tools
  - Easy to apply to existing HPC applications
  - Easy access to existing Python-based tools for AI/ML



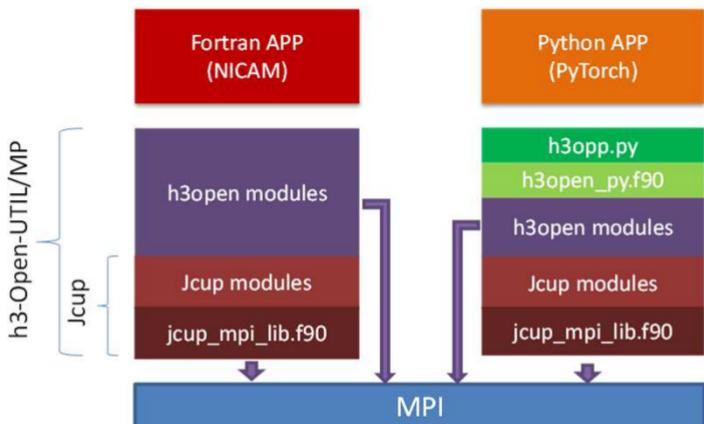
# **h3-Open-UTIL/MP (h3o-U/MP) + h3-Open-SYS/WaitIO**



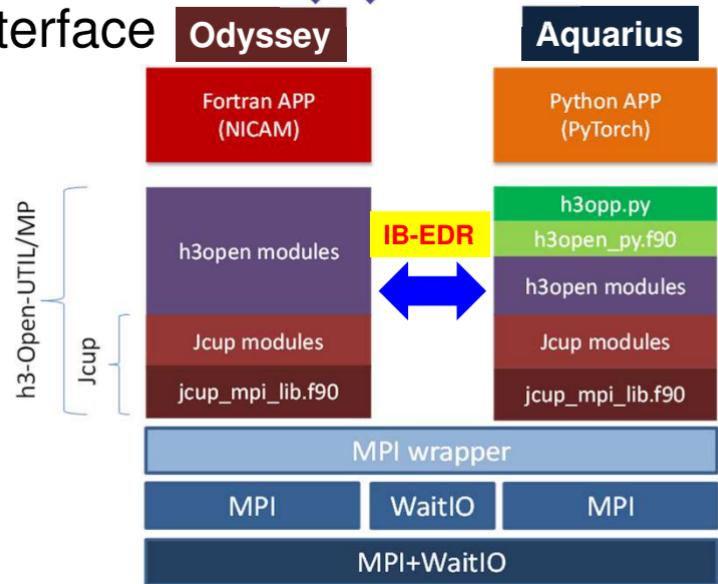
# h3-Open-UTIL/MP + h3-Open-SYS/WaitIO



- Current Status: Single MPI Job
- Direct Communication between Odyssey-Aquarius through IB-EDR by h3-Open-SYS/WaitIO, which provides MPI-like Interface



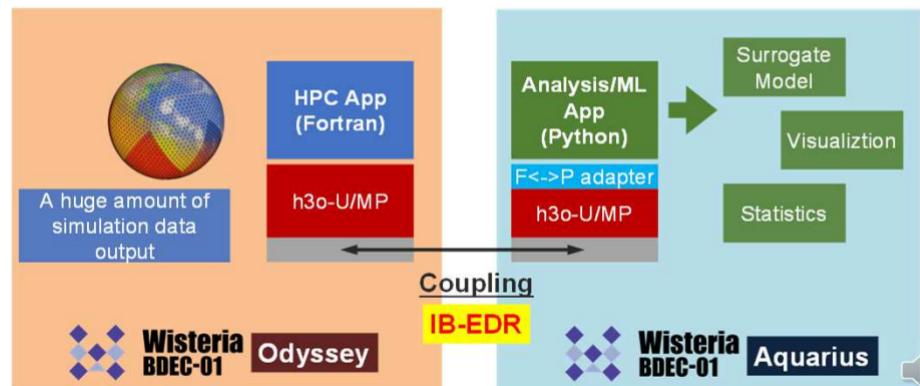
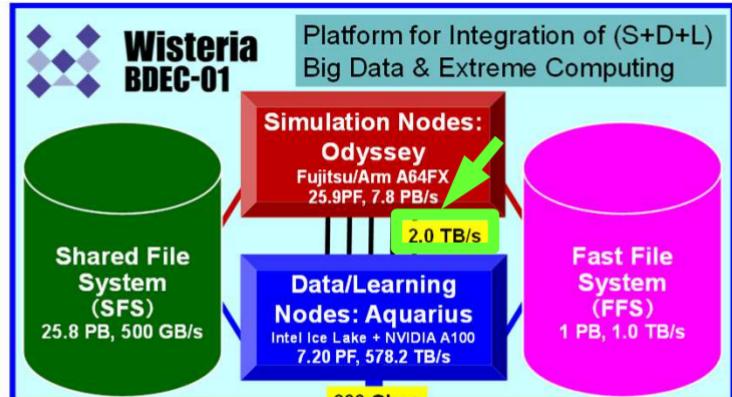
Current Status: Single MPI Job



# Schedule for Public Use

## Collaborations are Welcome !!

- h3-Open-SYS/WaitIO
  - October 2021, O-A Direct Communication by MPI-like Interface
- h3-Open-UTIL/MP (HPC+Python)
  - October 2021 on Odyssey only (Single MPI)
- h3-Open-UTIL/MP+h3-Open-SYS/WaitIO via IB-EDR
  - January-April 2022



# h3-Open-BDEC: Summary

<https://h3-open-bdec.cc.u-tokyo.ac.jp/>



- By Integration of (S+D+L) using **h3-Open-BDEC (Adaptive Precision + hDDA)**, total energy consumption (=total computation time) for simulations will be 10% of that by the conventional methods for simulations with parameter studies
- h3-Open-BDEC is the 1st innovative software platform for integration of (S+D+L) on Exascale systems, where computational scientists can achieve such integration without supports by other experts in data analytics and AI/ML.
- Source codes and documents (in English) are open to public for various kinds of computational environments.