

# Innovative Scientific Computing by Integration of (Simulation+Data+Learning)



**Wisteria  
BDEC-01**



**SC22**  
Dallas, TX | hpc  
accelerates.

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



2001-2005	2006-2010	2011-2015	2016-2020	2021-2025	2026-2030
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**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**  
200+ 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

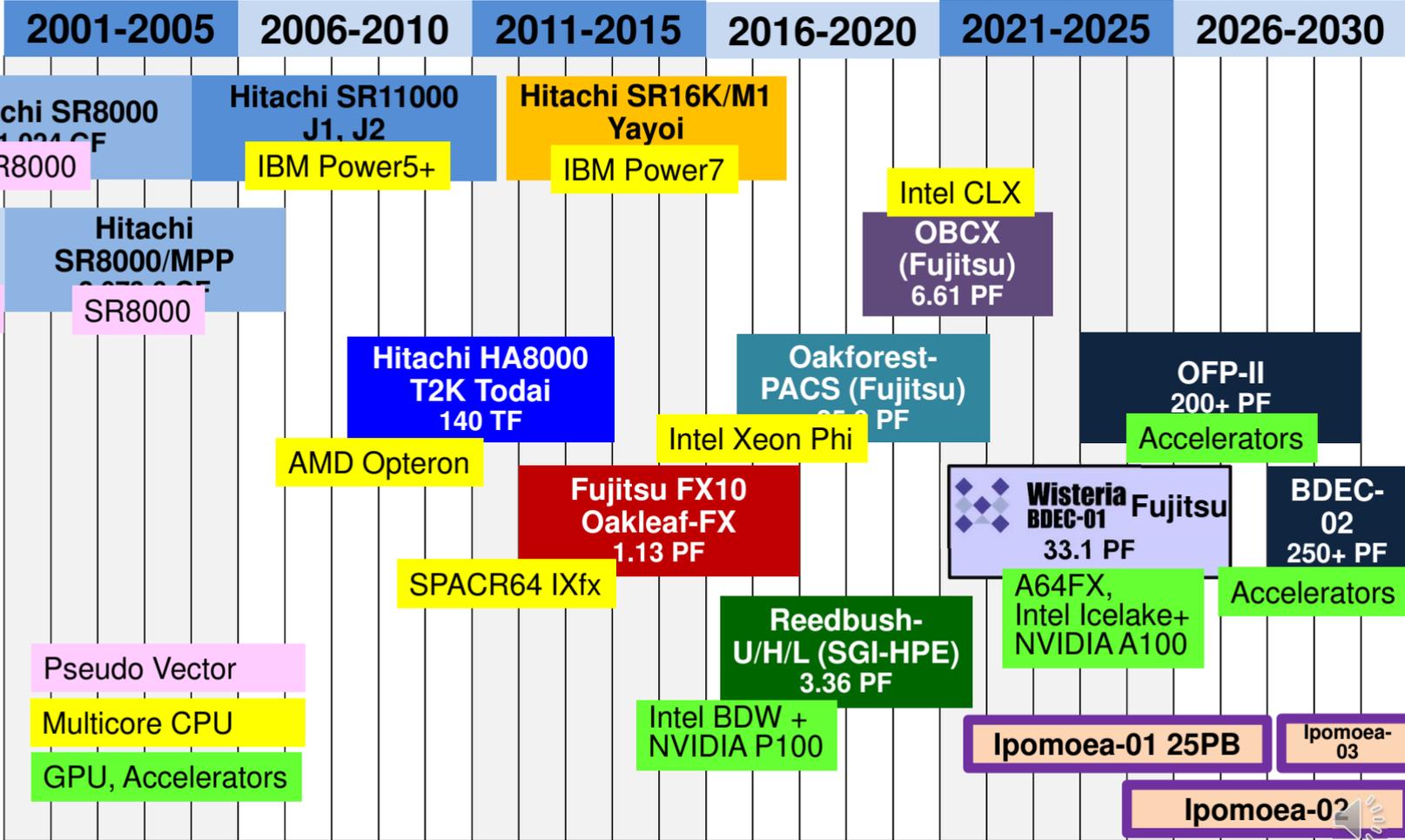
**Reedbush-U/H/L (SGI-HPE)**  
3.36 PF

**Ipomoea-01 25PB**

**Ipomoea-03**

**Ipomoea-02**





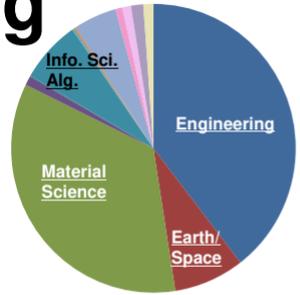
Pseudo Vector  
 Multicore CPU  
 GPU, Accelerators

Ipomoea-02

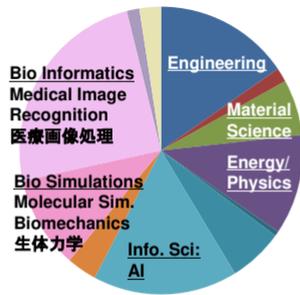
# Future of Supercomputing

- Various Types of Workloads

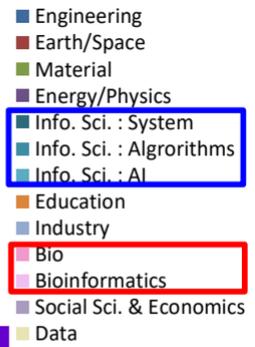
- Computational Science & Engineering: Simulations
- Big Data Analytics
- AI, Machine Learning ...



**Multicore Cluster**  
Intel BDW Only  
(Reedbush-U)



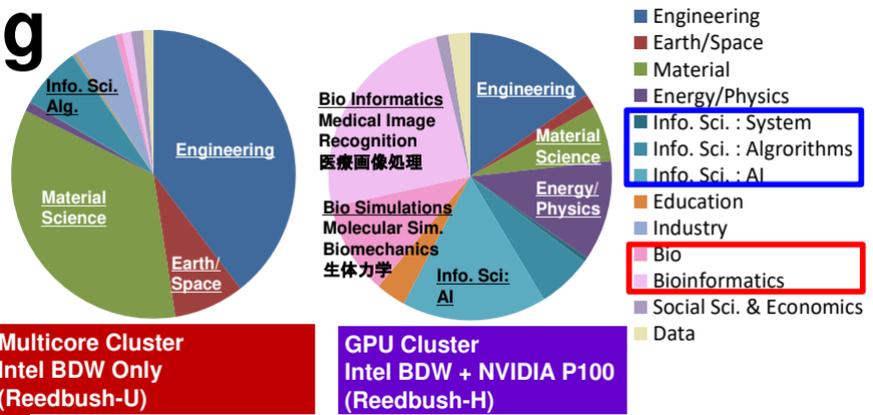
**GPU Cluster**  
Intel BDW + NVIDIA P100  
(Reedbush-H)



# Future of Supercomputing

## • Various Types of Workloads

- Computational Science & Engineering: Simulations
- Big Data Analytics
- AI, Machine Learning ...



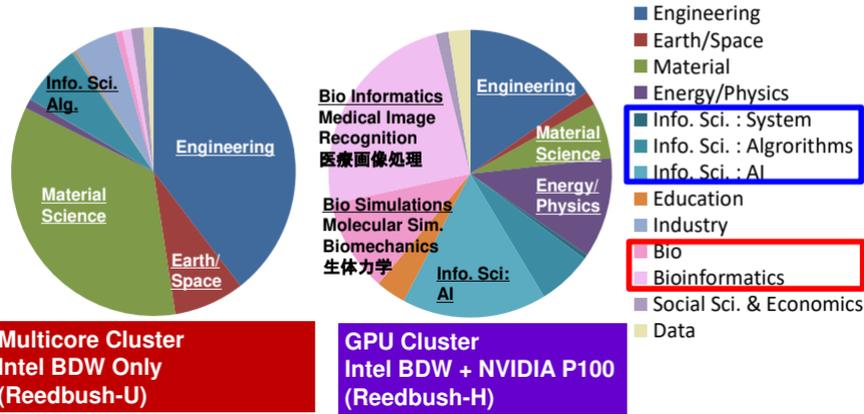
## • Integration/Convergence of (Simulation + Data + Learning) (S+D+L) is important towards Society 5.0

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



# 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, AI for Science, Digital Twins
  - Planning started in 2015

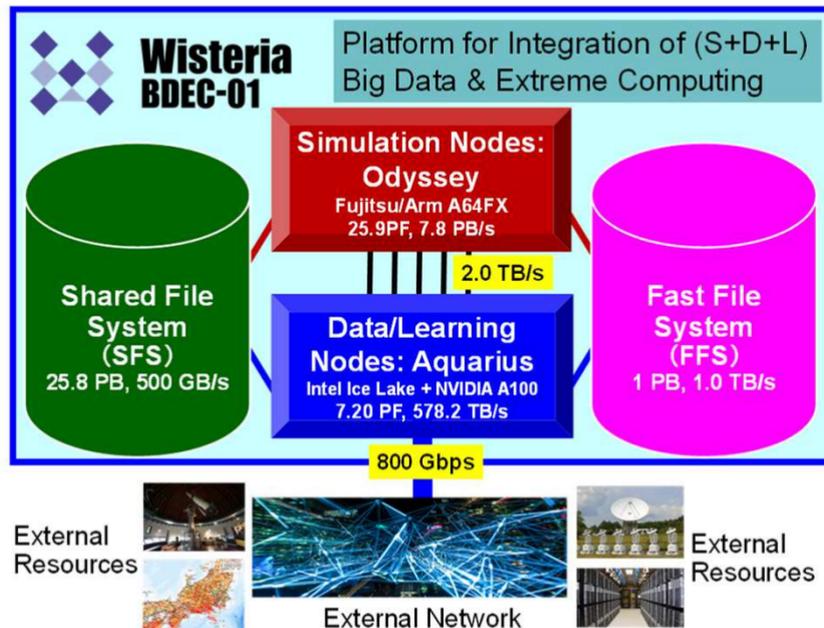
**BDEC (Big Data & Extreme Computing)**

**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, ~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)

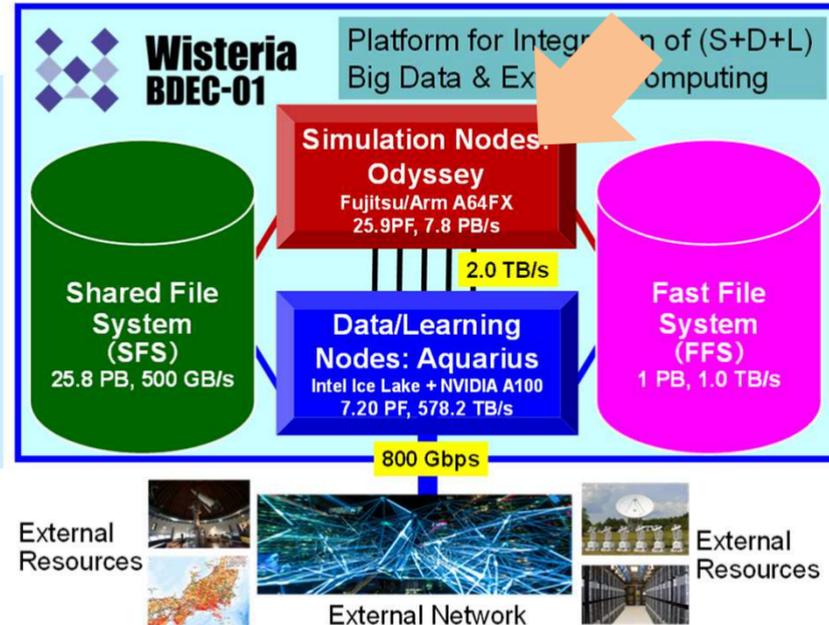
## The 1<sup>st</sup> BDEC System (Big Data & Extreme Computing) Platform for Integration of (S+D+L)



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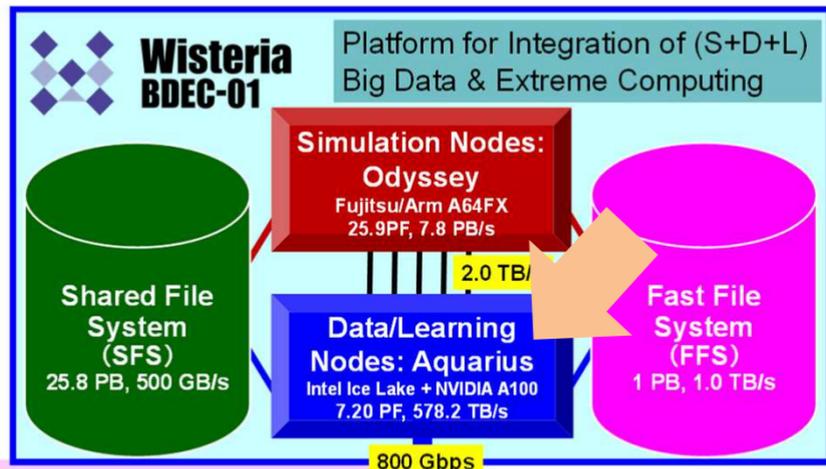
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# Rankings@ISC 2022

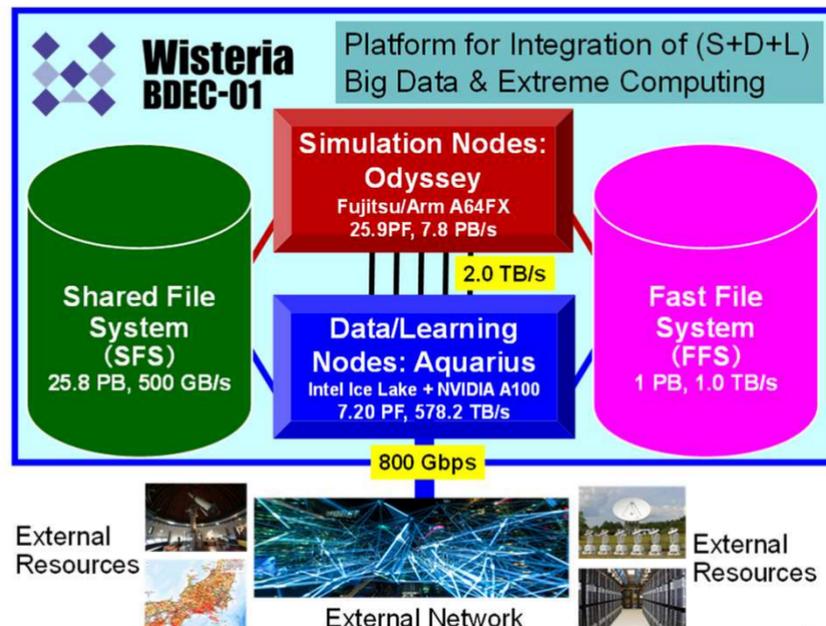
## June 2022



ISC HIGH  
PERFORMANCE  
2021 DIGITAL

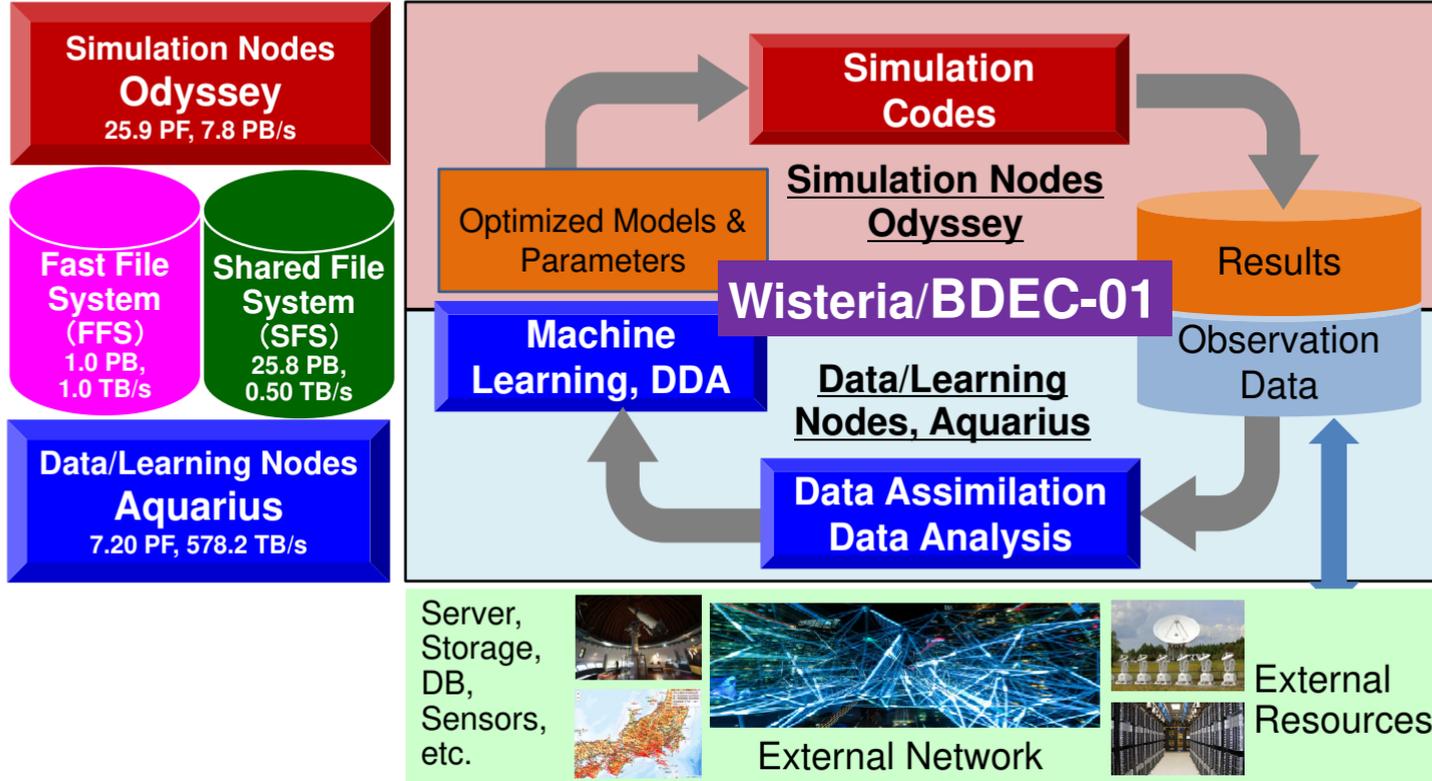
JUNE 24 - JULY 2, 2021  
ISC-HPC.COM

	Odyssey	Aquarius
TOP 500	20	115
Green 500	34	21
HPCG	10	62
Graph 500 BFS	3	-
HPL-AI	10	-



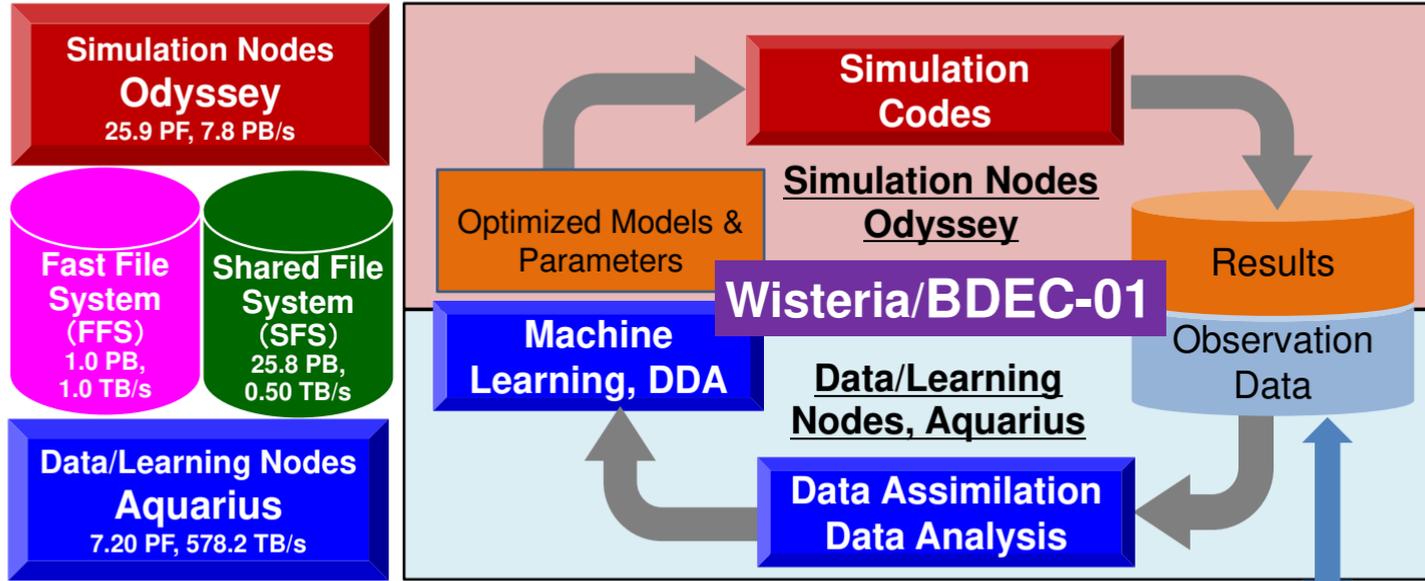
# Wisteria/BDEC-01

Platform for Integration of (Simulation+Data+Learning) (S+D+L)



# Wisteria/BDEC-01

Platform for Integration of (Simulation+Data+Learning) (S+D+L)



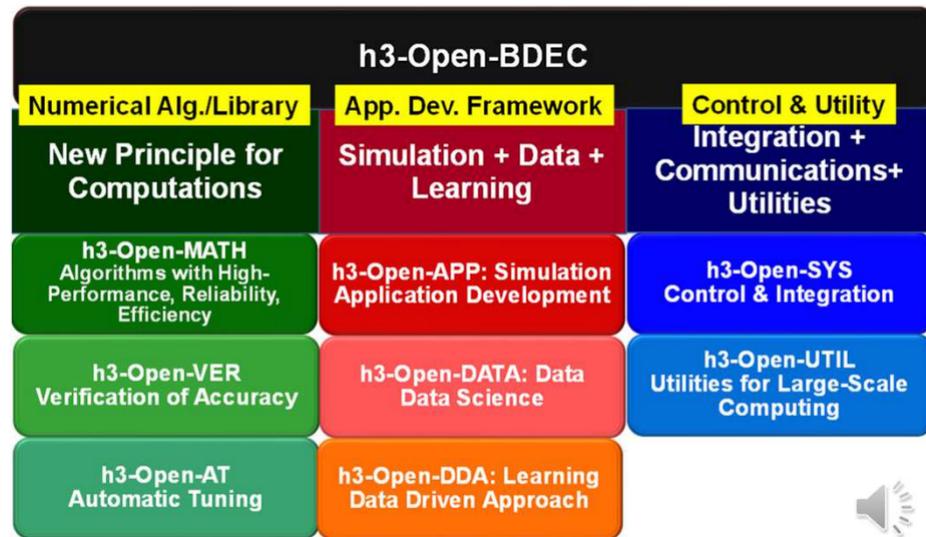
**Optimization of Models/Parameters for Simulations by Data Analytics & Machine Learning (S+D+L)**



# 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 (JSPS) since 2019
- Leading-PI: Kengo Nakajima (The University of Tokyo)
- Total Budget: 1.41M USD

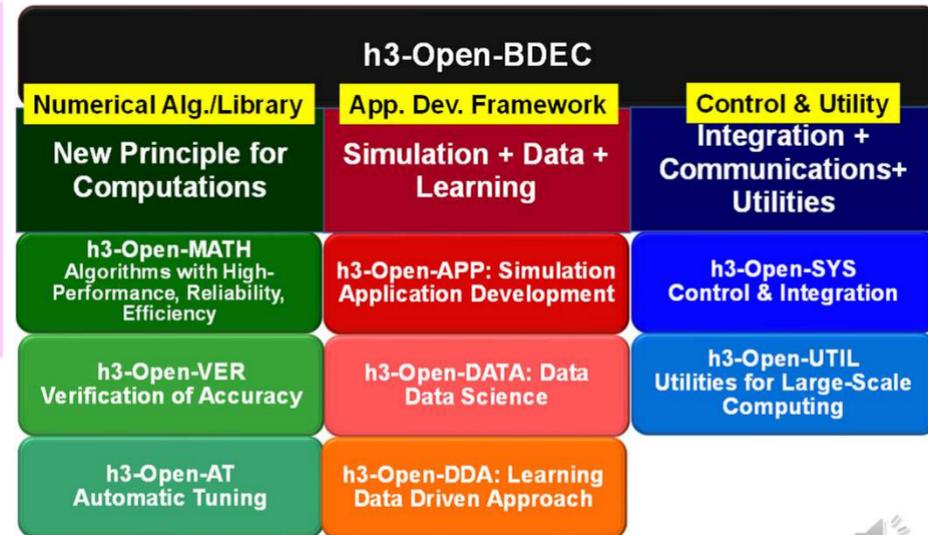


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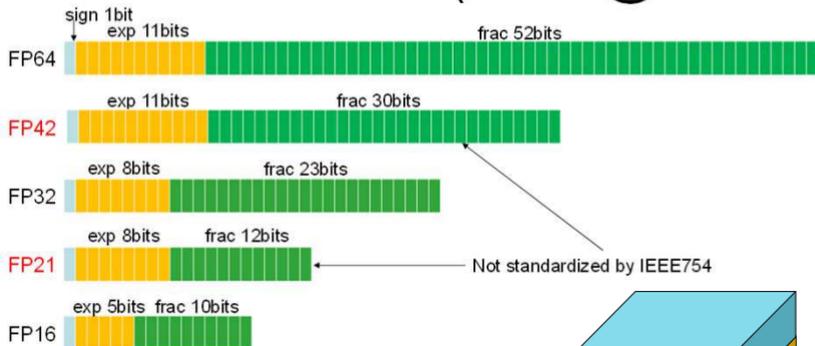
- “Three” Innovations

- New Principles for Numerical Analysis by Adaptive Precision, Automatic Tuning & Accuracy Verification
- Hierarchical Data Driven Approach (*hDDA*) based on Machine Learning
- Software & Utilities for Heterogeneous Environment, such as Wisteria/BDEC-01

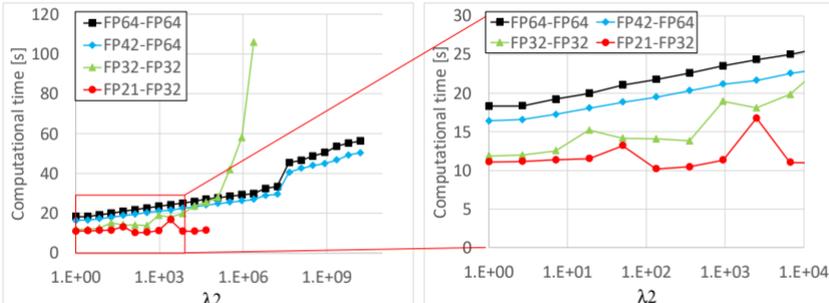
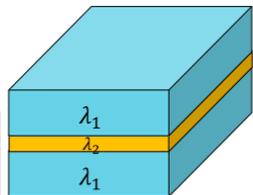


# Adaptive Precision Computing with FP42/FP21

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



Heat Conduction with Heterogeneous Material Property



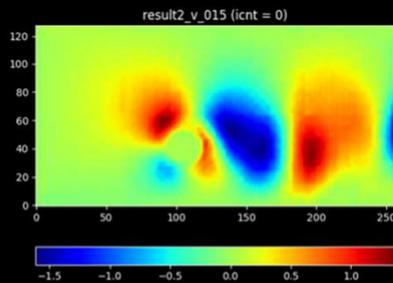
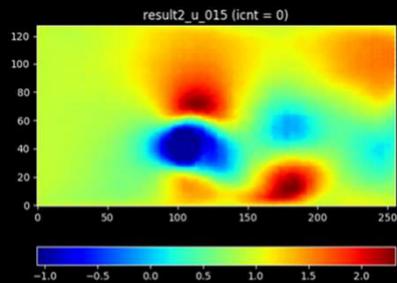
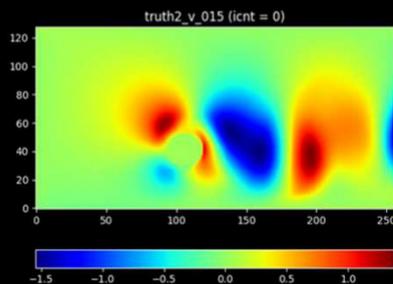
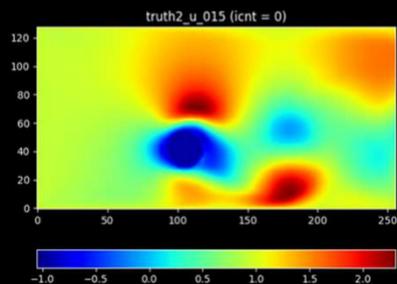
Computation Time for ICCG Solver  
Various Types of Precisions on Intel Xeon Cascadelake

In recent years, the usefulness of low-precision floating-point representation has been studied 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 an application with a memory bandwidth bottleneck, the effect of reducing 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 strongly 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 ( $\lambda_2$  is larger), FP21-FP32 provides the best performance if  $\lambda_2$  is up to  $10^4$ . (“FP21-FP32” means “matrices are in FP21, and vectors are in FP32”).

# Prediction of CFD Simulation by Deep Learning

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



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 calculation results by CFD simulation approximately at high speed. We are working on a project to develop a parallelization method to make it possible to apply the surrogate method based on the deep learning to large scale geometry. Unlike the model parallel computing, the method we are currently developing predicts large-scale steady flow simulation results by dividing the input geometry into multiple parts and applying a single 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 divided 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.

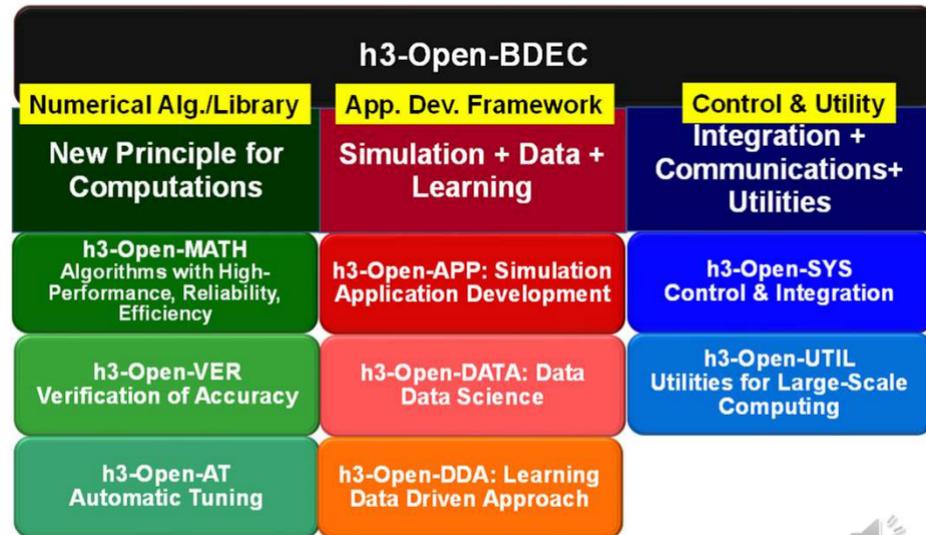
Comparison of the flow velocity results obtained by the conventional simulation (upper) and the prediction of these results by deep learning (lower)

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

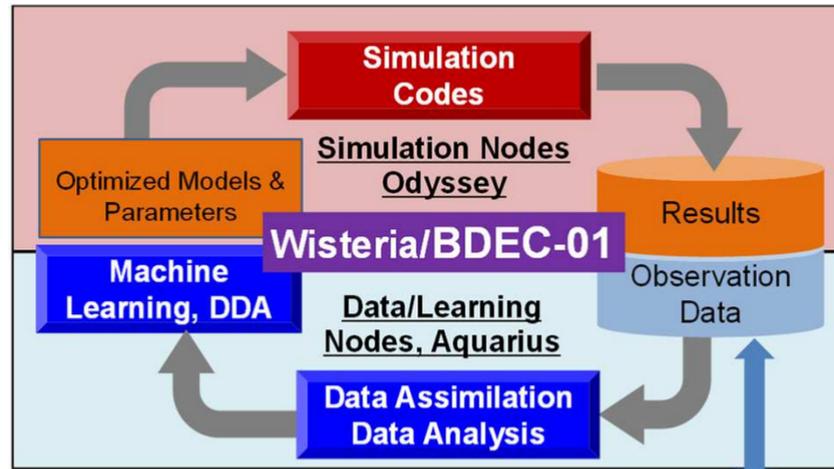
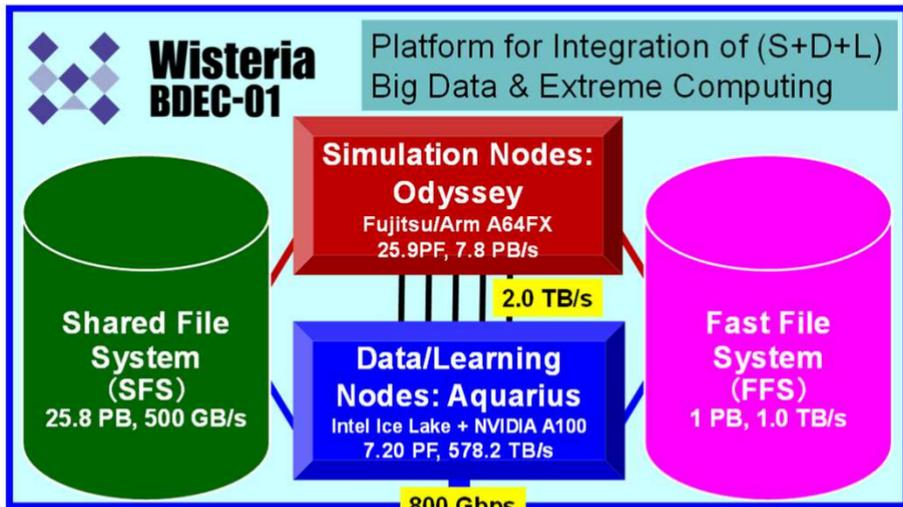


- “Three” Innovations

- New Principles for Numerical Analysis by Adaptive Precision, Automatic Tuning & Accuracy Verification
- Hierarchical Data Driven Approach (*hDDA*) based on Machine Learning
- Software & Utilities for Heterogeneous Environment, such as Wisteria/BDEC-01



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



Server,  
Storage,  
DB,  
Sensors,  
etc.



External  
Resources

External Network

External  
Resources



External Network



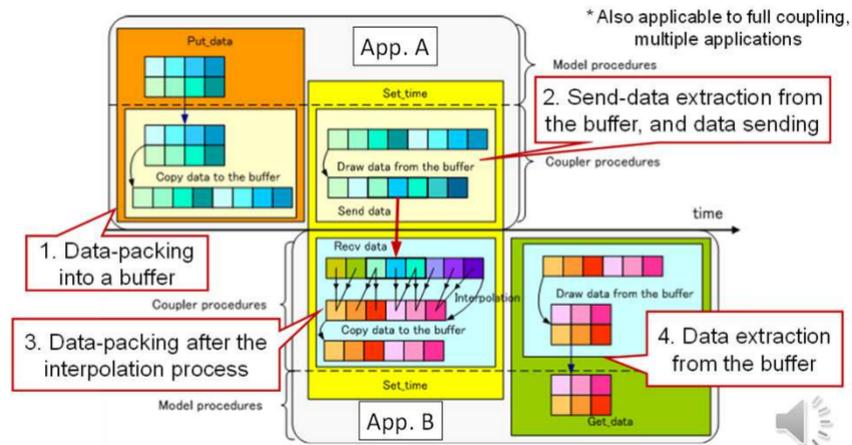
External  
Resources



# h3-Open-UTIL/MP

## Multilevel Coupler/Data Assimilation

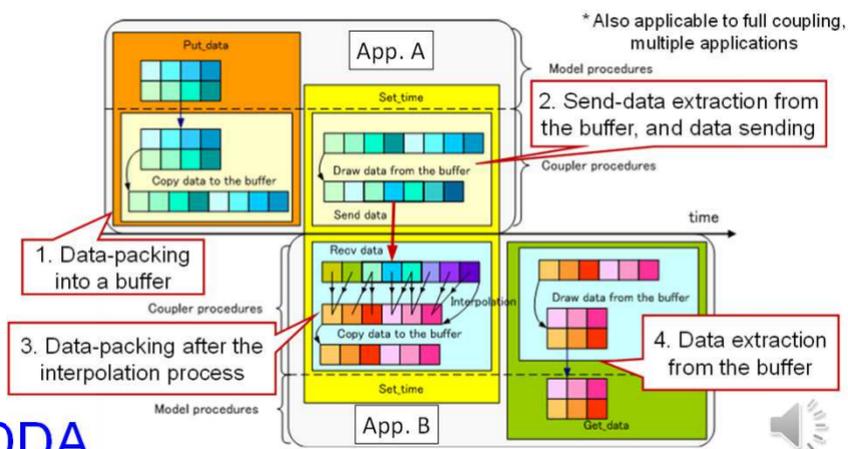
- Current Coupler: ppOpen-MATH/MP
  - Weak-Coupling of Multiple (usually two) Applications
    - Each application does a single computation



# h3-Open-UTIL/MP

## Multilevel Coupler/Data Assimilation

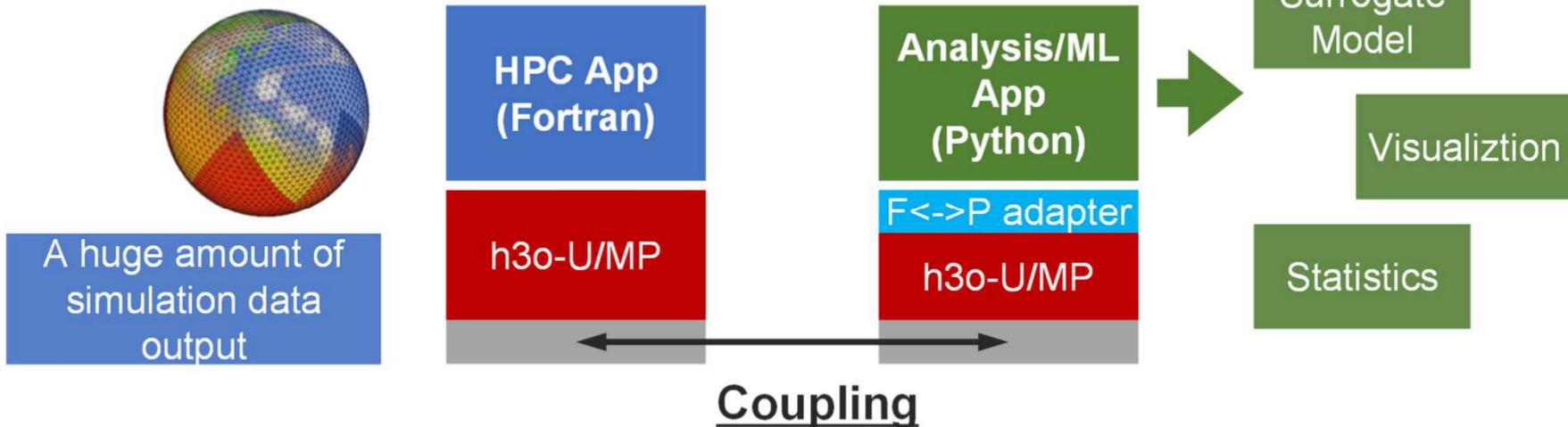
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- h3-Open-UTIL/MP
  - Data Assimilation (Multiple Computations: Ensemble)
  - Assimilation of Computations with Different Resolutions
    - h3-Open-DATA, h3-Open-APP
  - Data Assimilation by Coupled Codes
    - e.g. Atmosphere-Ocean
- Data Assimilation: 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

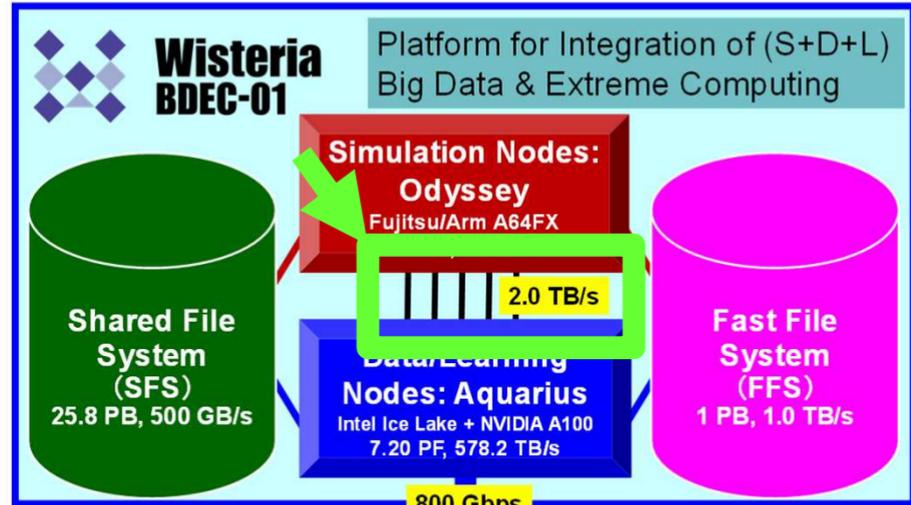
[Dr. H. Yashiro, NIES]



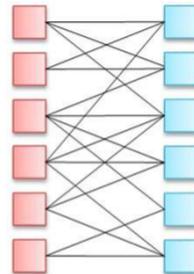
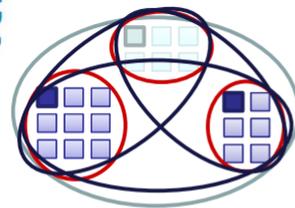
- Providing on-the-fly input/output/training data to the Analysis/ML tools
  - Easy to apply to existing HPC applications
  - Easy access to existing Python-based tools for AI/ML

# Computing on Wisteria/BDEC-01

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



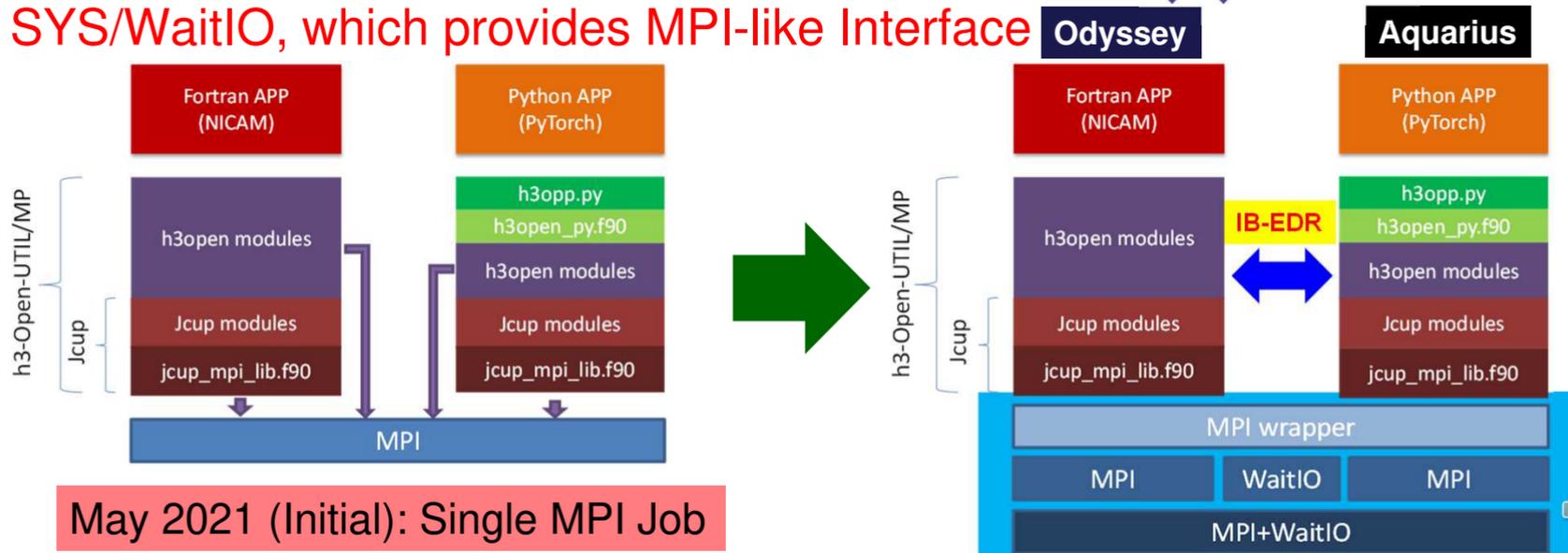
# h3-Open-UTIL/MP + h3-Open-SYS/WaitIO-Socket



- Single MPI Job (May 2021)
- Direct Communication between Odyssey-Aquarius through IB-EDR by h3-Open-SYS/WaitIO, which provides MPI-like Interface



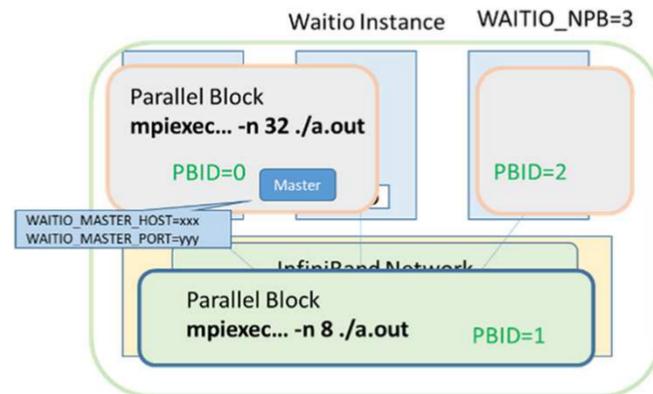
**Wisteria  
BDEC-01**



May 2021 (Initial): Single MPI Job

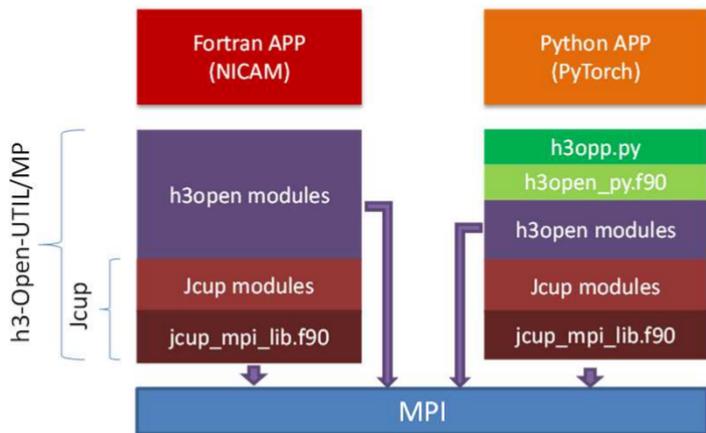
# API of h3-Open-SYS/WaitIO-Socket PB (Parallel Block): Each Application

WaitIO API	Description
<code>waitio_isend</code>	Non-Blocking Send
<code>waitio_irecv</code>	Non-Blocking Receive
<code>waitio_wait</code>	Termination of <code>waitio_isend/irecv</code>
<code>waitio_init</code>	Initialization of WaitIO
<code>waitio_get_nprocs</code>	Process # for each PB (Parallel Block)
<code>waitio_create_group</code> <code>waitio_create_group_wranks</code>	Creating communication groups among PB's
<code>waitio_group_rank</code>	Rank ID in the Group
<code>waitio_group_size</code>	Size of Each Group
<code>waitio_pb_size</code>	Size of the Entire PB
<code>waitio_pb_rank</code>	Rank ID of the Entire PB

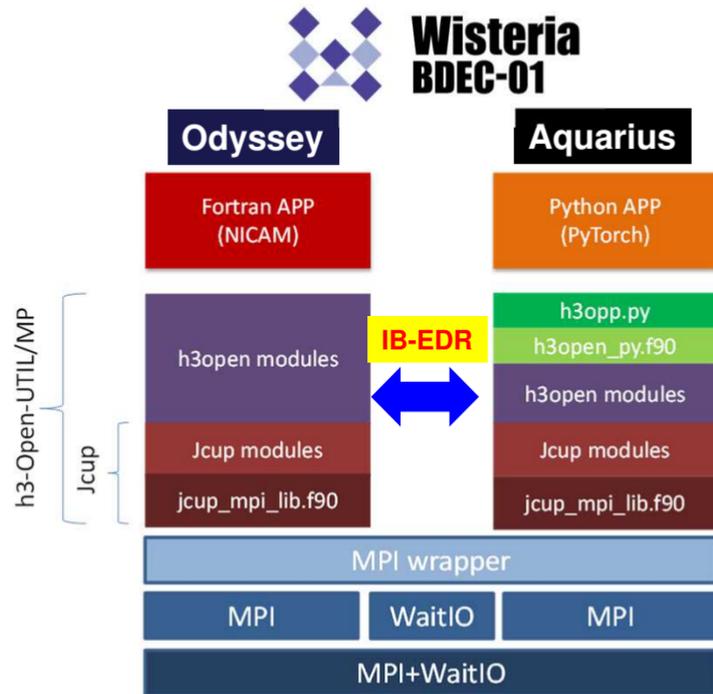
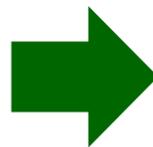


# h3-Open-UTIL/MP + h3-Open-SYS/WaitIO-Socket

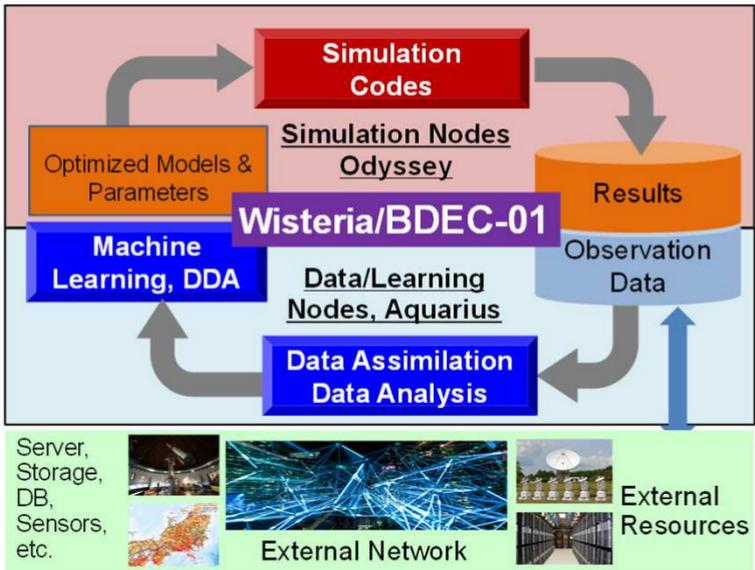
## Available in June 2022



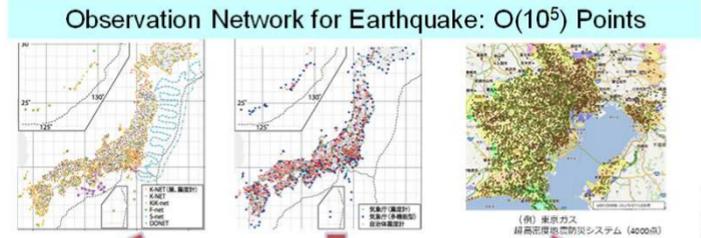
May 2021: MPI Only



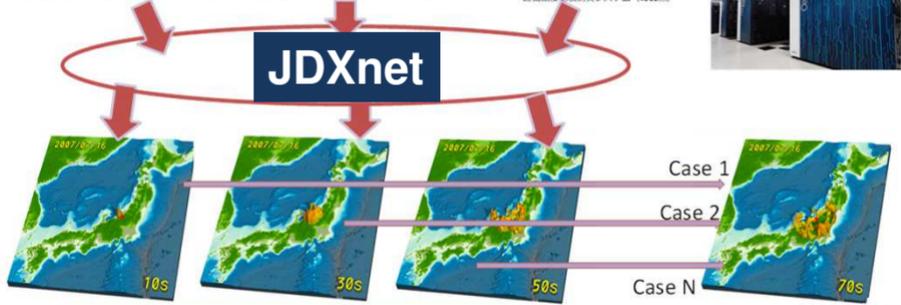
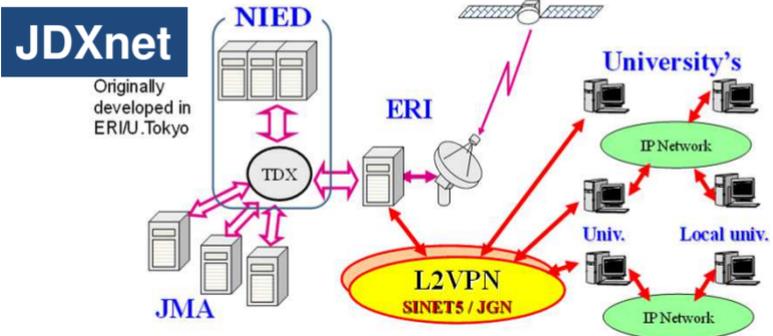
June 2022: Coupler + WaitIO



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



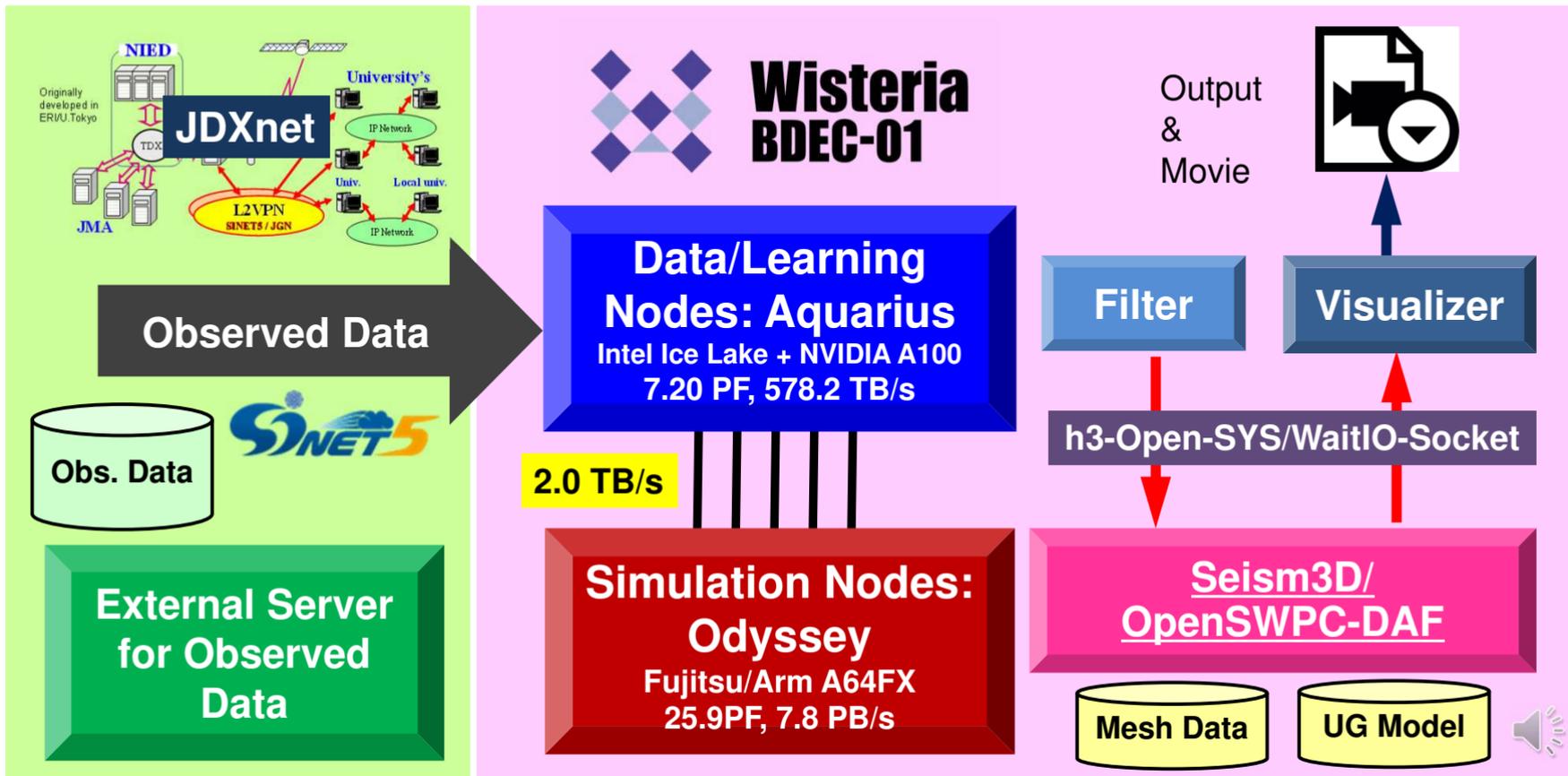
[c/o Furumura]



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

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

# System on Wisteria/BDEC-01 using WaitIO



# Communications by WaitIO-Socket

[Kasai et al. 2021]

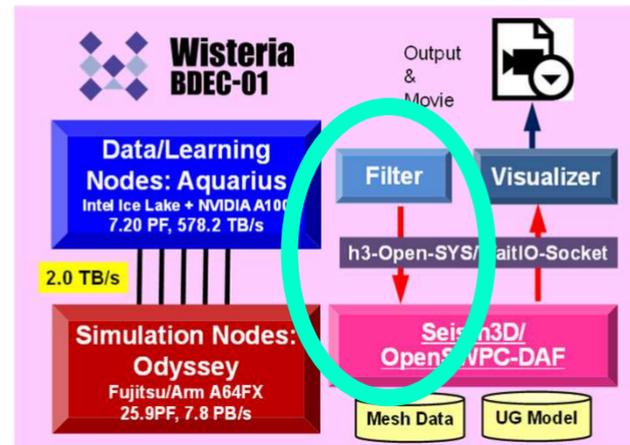
## Aquarius: SEND

```
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)

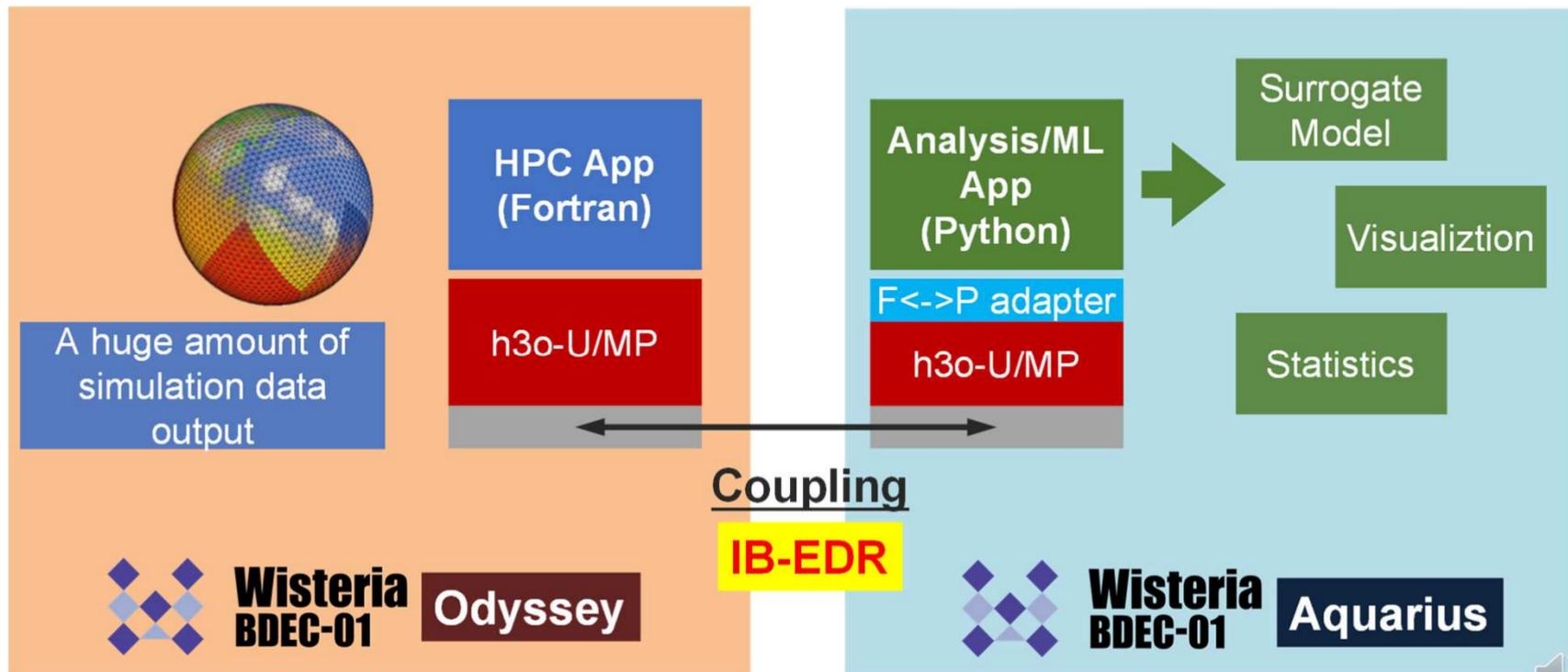
if (myrank==0) then
open(100,file='./obsfile_list.txt', form='formatted', status='old', iostat=ierr)
do i=1,300
<省略: obsデータ読み込み処理>
print *, "Send obs data ....."
call WAITIO_MPI_ISEND (NTMAX1_o, 1, WAITIO_MPI_INTEGER, 2,1, WAITIO_COMM_UNIVERSE, req(1,1), ierr)
call WAITIO_MPI_ISEND (DT_o, 1, WAITIO_MPI_FLOAT, 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_INTEGER, 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_INTEGER, 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, ...)
```



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



# 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!

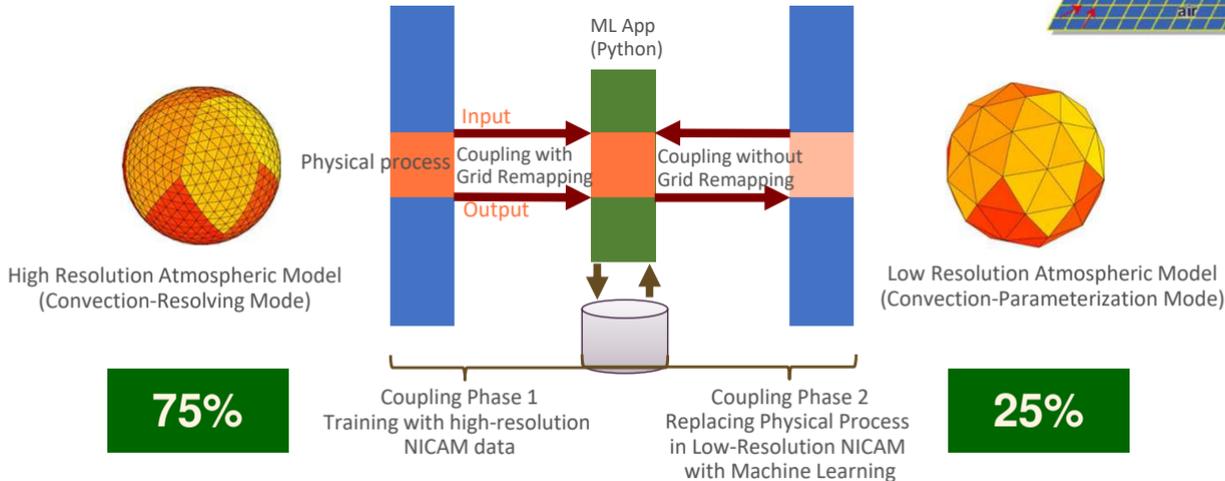
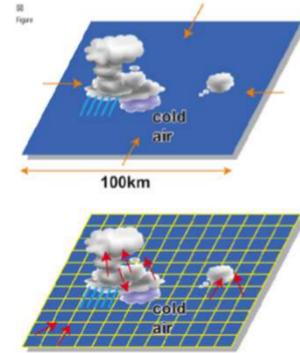
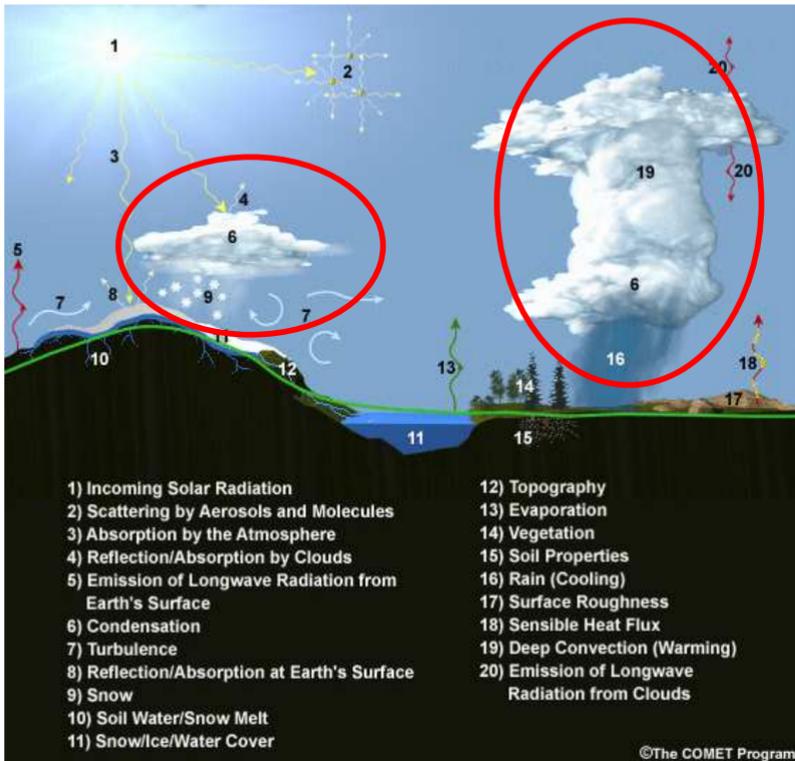


Diagram of applying ML to an atmospheric model



# Atmosphere-ML Coupling



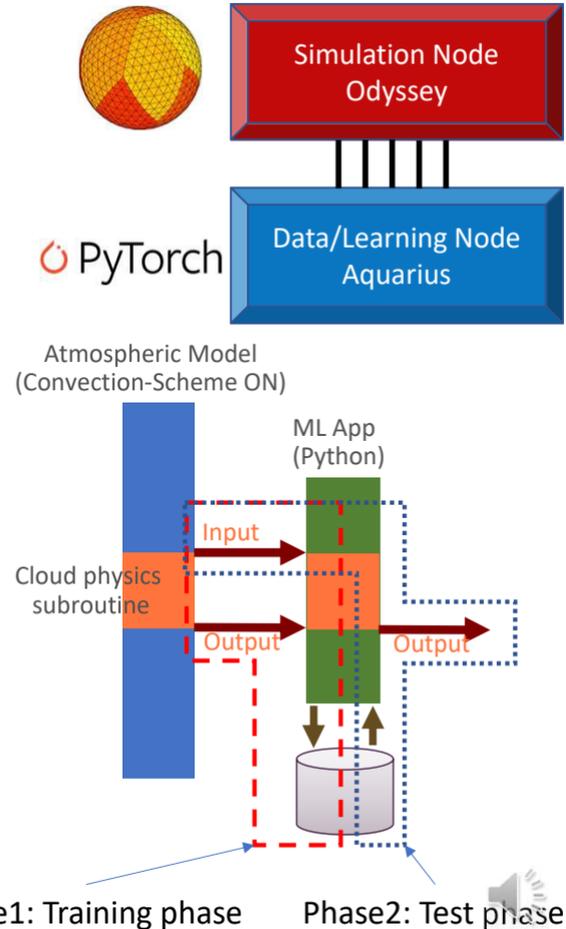
- Model component emulation (surrogation)
  - The emulation target in this study is cloud microphysical processes (phase changes, collision, coagulation, and precipitation)
  - Atmospheric pressure, temperature, and vertical distribution of water will change between before and after computing the cloud microphysical processes
  - The data-driven cloud model predicts atmospheric state changes per unit of time



# Experimental Design

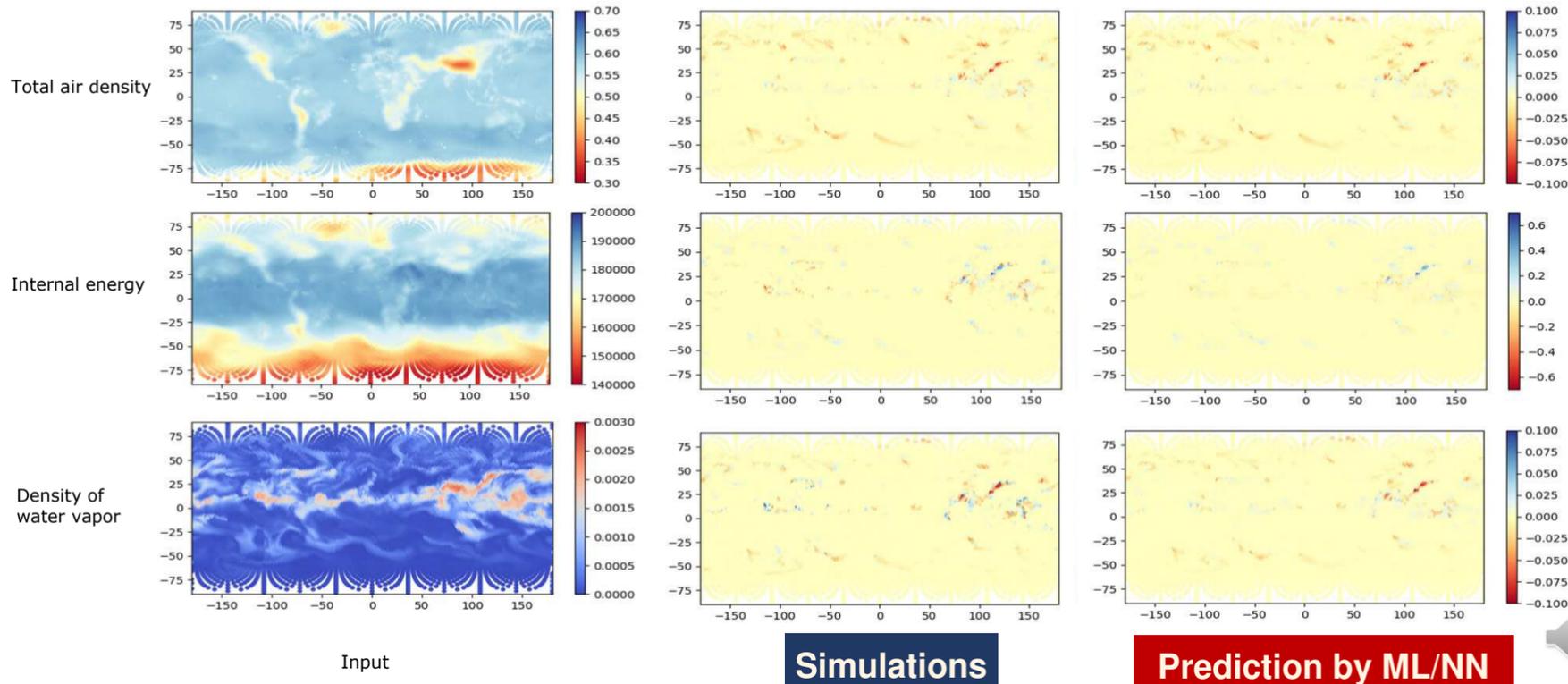
- Atmospheric model on Odyssey
  - NICAM : global non-hydrostatic model with an icosahedral grid
  - Resolution : horizontal : 10240, vertical : 78
- ML on Aquarius
  - Framework : PyTorch
  - Method : Three-Layer MLP
  - Resolution : horizontal : 10240, vertical : 78
- Experimental design
  - Phase1: PyTorch is trained to reproduce output variables from input variables of cloud physics subroutine.
  - Phase2: Reproduce the output variables from Input variables and training results
- Training data
  - Input : total air density ( $\rho$ ), internal energy ( $e_{in}$ ), density of water vapor ( $\rho_q$ )
  - Output : tendencies of input variables computed within the cloud physics subroutine

$\frac{\Delta \rho}{\Delta T}$	$\frac{\Delta e_{in}}{\Delta T}$	$\frac{\Delta \rho_q}{\Delta T}$
--------------------------------	----------------------------------	----------------------------------



# Test calculation

- Compute output variables from input variables and PyTorch
  - The rough distribution of all variables is well reproduced
  - The reproduction of extreme values is no good



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  
200+ 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

Mercury

Ipomoea-01 25PB

Ipomoea-  
03

Ipomoea-02

2021

# Near Future Plan: Shifting to GPUs

- U.Tokyo is shifting to GPUs/Accelerators in next 10 years
  - Maximum performance under constraint of power consumption
- **Wisteria-Mercury (October 2023)**
  - GPU Cluster, for supporting “Aquarius”
  - Prototype of OFP-II (128+ GPU’s, 32+ nodes)
- **OFP-II (April 2024)**
  - Successor of OFP (JCAHPC, U.Tsukuba & U.Tokyo), 200+PF
  - Group-A (CPU+GPU), Group-B (Only CPU)
    - Same GPUs as those of Mercury
    - CPUs in Group-A and Group-B could be different
- Porting codes of 3,000+ users of OFP to GPU is the most critical issue
  - Starting this Fall



**Wisteria  
BDEC-01**



**JCAHPC**



筑波大学  
University of Tsukuba



東京大学  
THE UNIVERSITY OF TOKYO



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Ipomoea-01 25PB

Ipomoea-  
03

Ipomoea-02



# BDEC-02 (Fall 2027-Spring 2028)

- Platform for “Digital Twin”, “S+D+L”
- GPU Cluster + CPU Cluster: GPU-Focused
- We are thinking about introducing DPU, IPU, Quantum-Inspired Devices etc. for supporting workloads for (D+L)
  - ✓ We are also considering the introduction of multiple types of GPUs
- We have been using Fujitsu’s Digital Annealer since 2019: Combinatorial Optimization
- Programming Environment & Communication Library for Integration of HPC and Such Devices are needed.
  - ✓ We can extend the idea of h3-Open/SYS-WaitIO

