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

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

Wisteria
BDEC-01

Overview of h3-Open-BDEC:
Innovative Software Infrastructure for Scientific Computing in the Exascale Era by Integrations of (Simulation + Data + Learning)

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

Kengo Nakajima
Information Technology Center
The University of Tokyo

International Workshop on the Integration of (Simulation + Data + Learning) : Towards Society h3-Open-BDEC, November 30 & December 3, 2021 (Online)

International Workshop on the Integration of (Simulation + Data + Learning): Towards Society 5.0 by h3-Open-BDEC (1/2)

- ✓ Towards the end of Moore's law, we need to develop new algorithms and applications.
- ✓ We are developing h3-Open-BDEC, which is innovative software for sustainable promotion of scientific discovery by supercomputers in the Exascale Era by combining (Simulation + Data + Learning (S+D+L)), where ideas of data science and machine learning are introduced to computational science.
- ✓ Integration of (S+D+L) is also important for realization of Society 5.0, which is a “Super Smart and Human-centered Society” by digital innovation, such as IoT, Big Data, AI etc., and by integration of cyber-space (digital/virtual space) and physical-space (real space).

International Workshop on the Integration of (Simulation + Data + Learning): Towards Society 5.0 by h3-Open-BDEC (2/2)

- ✓ The h3-Open-BDEC project is funded by Japanese Government via JSPS Grant-in-Aid for Scientific Research（S）(Leading PI: Kengo Nakajima, the University of Tokyo, 19H05662) since 2019.
- ✓ In this workshop, we would like to report our progress of research and development in recent 2.5 years.
- ✓ While there are talks by Co-PI's and members of the project, we have 6 excellent invited talks from Japan, Taiwan, USA and Germany.

Invited Speakers
Thank you very much for your excellent contributions !!

- ✓ Gerhard Wellein (FAU Erlangen-Nuremberg, Germany)
- ✓ Kento Sato (RIKEN Center for Computational Science, Japan)
- ✓ Osni Marques (Laurence Berkley National Laboratory, USA)
- ✓ Rich Vuduc (Georgia Institute of Technology, USA)
- ✓ Takeshi Fukaya (Hokkaido University/JST PRESTO, Japan)
- ✓ Weichung Wang (National Taiwan University, Taiwan)

International Workshop on the Integration of (Simulation + Data + Learning): Towards Society 5.0 by h3-Open-BDEC (2/2)

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- ✓ While there are talks by Co-PI's and members of the project, we have 6 excellent invited talks from Japan, Taiwan, USA and Germany.
- ✓ All members of the project are happy to welcome all participants, and would like to discuss on various aspects of integration of (S+D+L). Please enjoy this two-day online event.

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International Workshop on the Integration of (Simulation + Data + Learning) : Towards Society h3-Open-BDEC, November 30 & December 3, 2021 (Online)

3 Systems in April 2021 (ITC/U.Tokyo)

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 56th 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 56th TOP 500, July 2019-June 2023
  - SSD's are installed to 128 nodes (out of 1,368)

3 Systems at the end of March 2021

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

- Reedbush (HPE, Intel BDW + NVIDIA P100 (Pascal))
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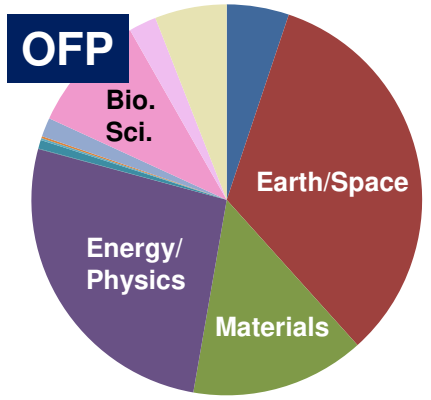
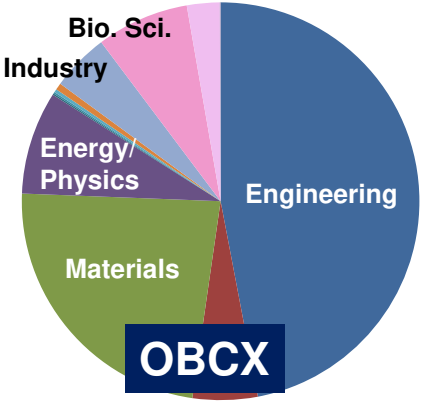
Research Area based on CPU Hours (FY.2020)



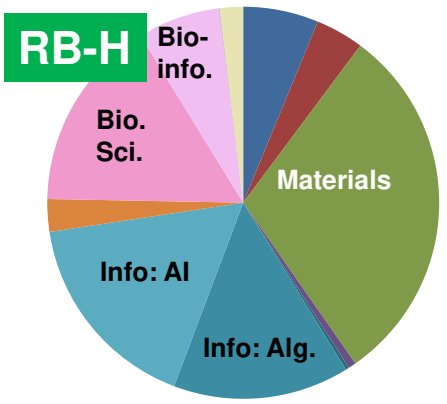
- Engineering
- Earth/Space
- Material
- Energy/Physics
- Info. Sci. : System
- Info. Sci. : Algrorithms
- Info. Sci. : AI
- Education
- Industry
- Bio
- Bioinformatics
- Social Sci. & Economics
- Data

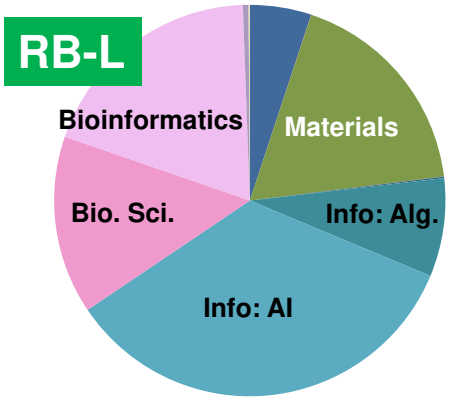


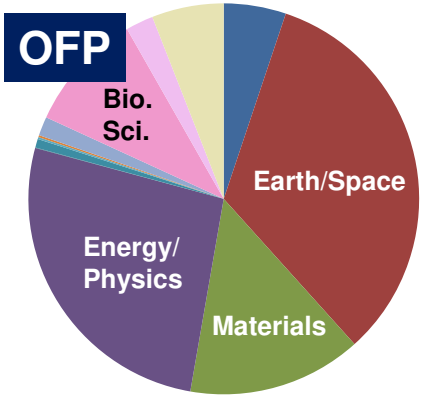
CPU

GPU

Research Area based on CPU Hours (FY.2020)







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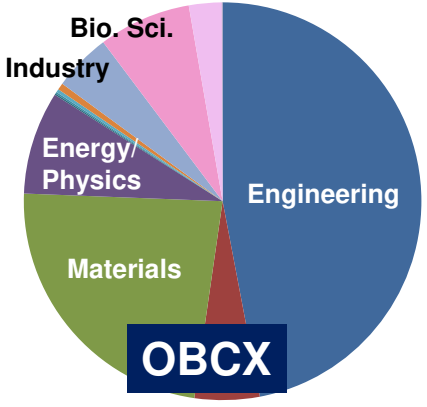
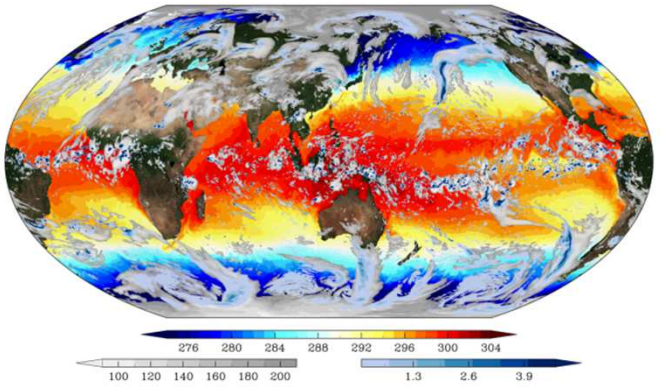
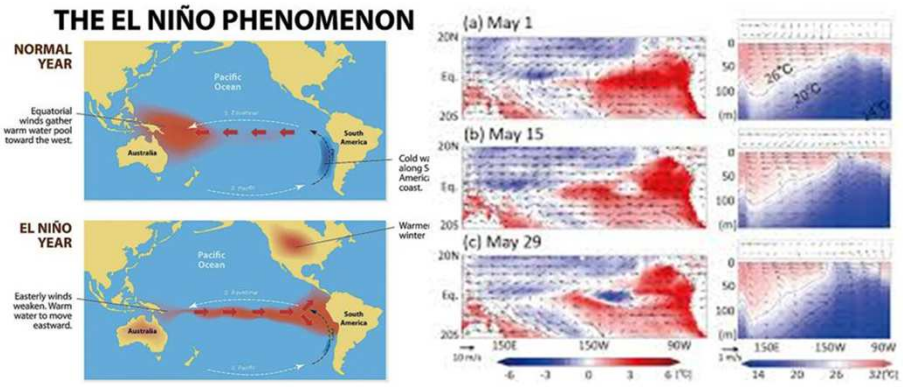


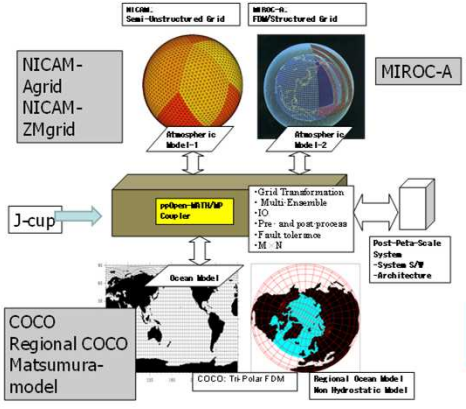
CPU

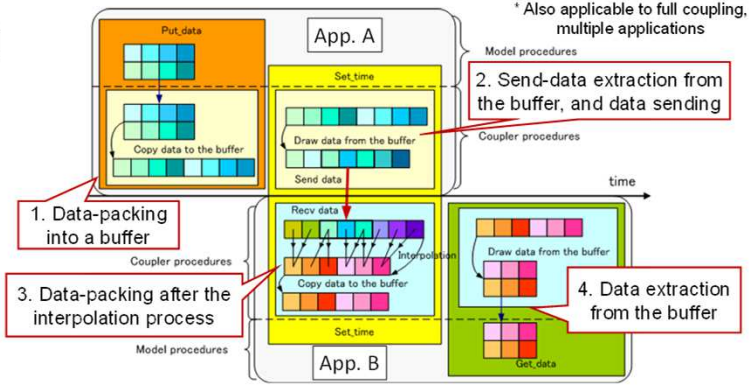
GPU

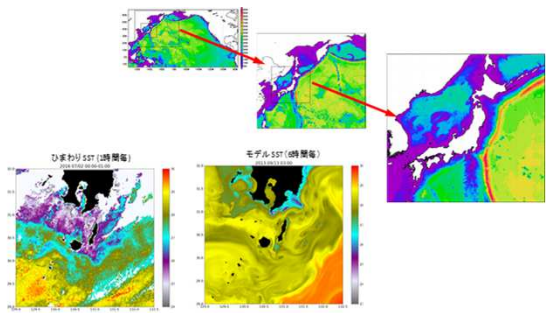
Global Atmosphere-Ocean Coupled Simulations







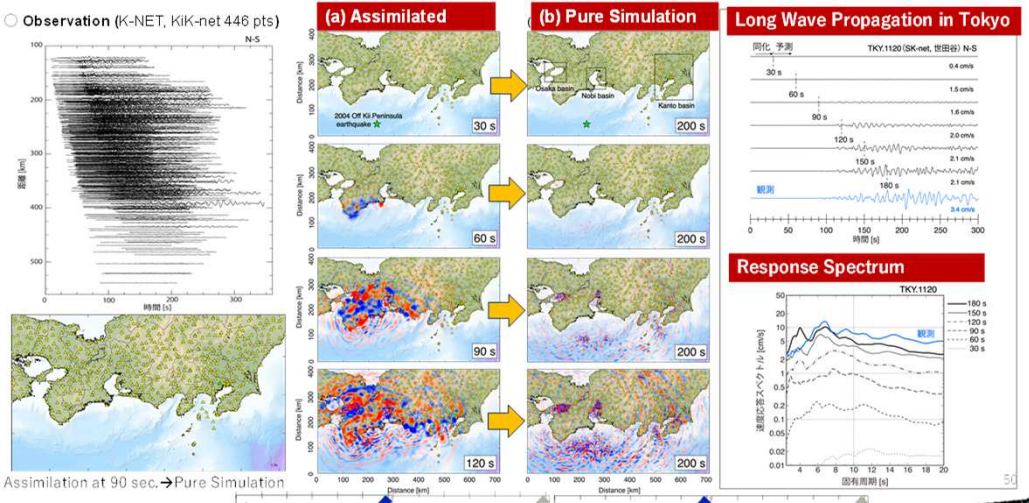


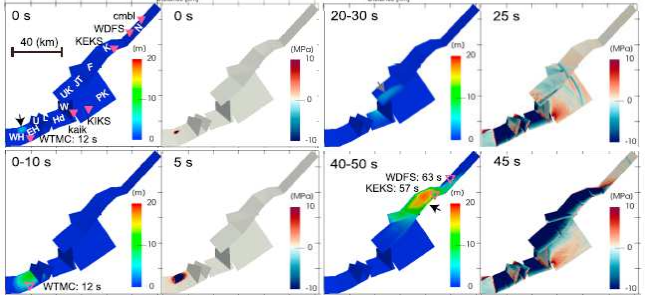


[c/o Prof. M. Sato, Prof. H. Hasumi (AORI/U.Tokyo)]

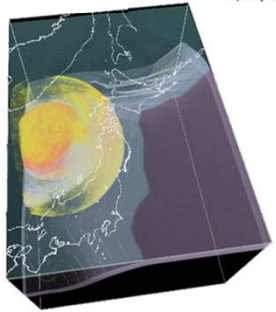
Solid Earth & Earthquake Simulations

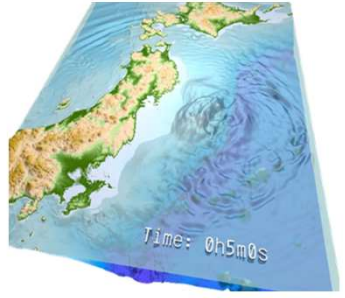
[c/o Prof. T. Furumura, Prof. T. Ichimura (ERI/U.Tokyo)]

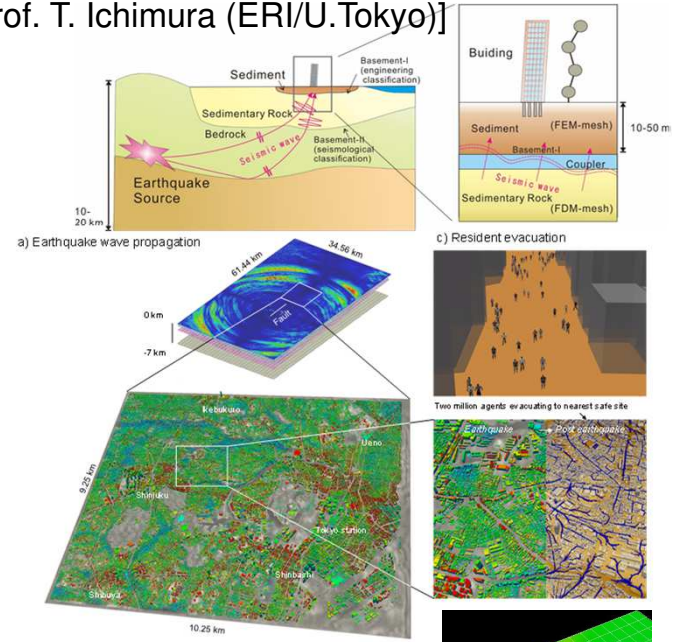


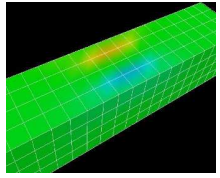


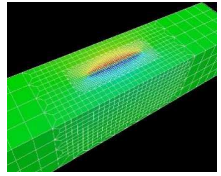
[c/o Prof. R. Ando (U.Tokyo)]





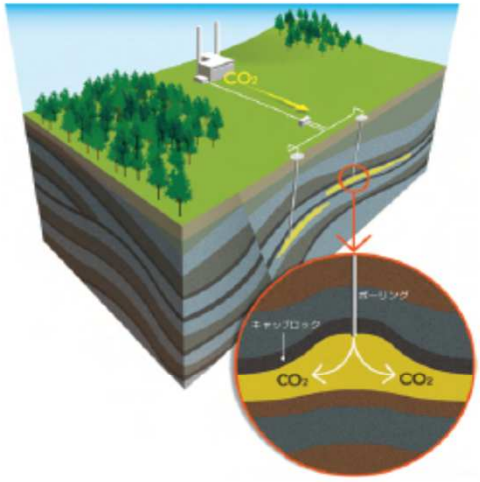






Simulation of Geologic CO_2 Storage

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



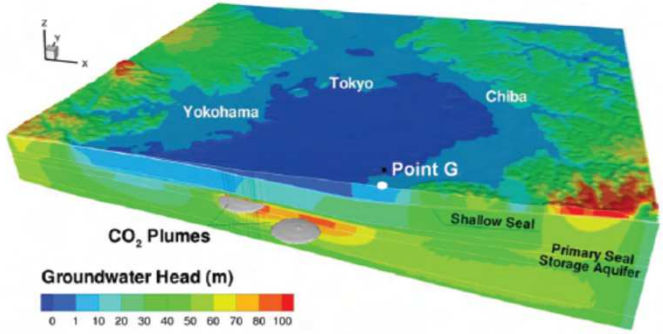
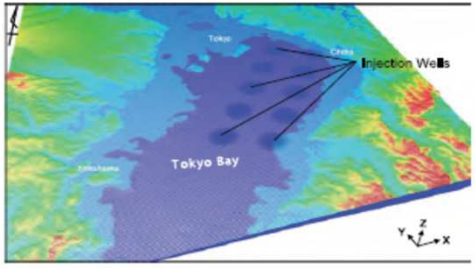
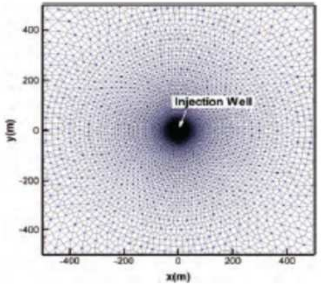
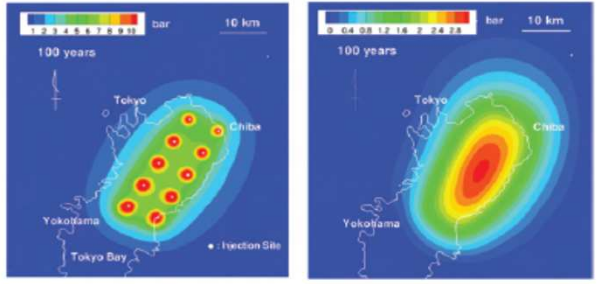


図 -4　CO_2 圧入後の地下水圧（全水頭換算）の分布（100 年後）

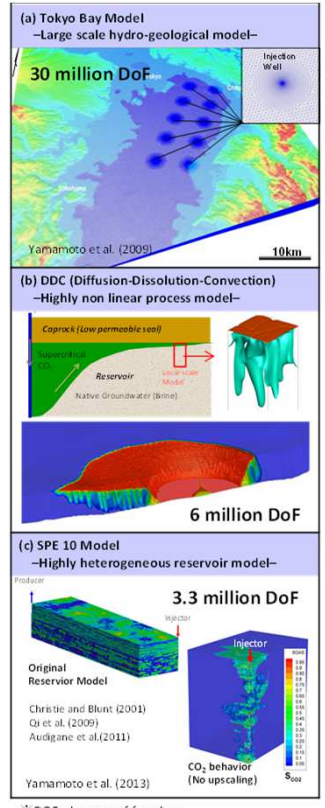






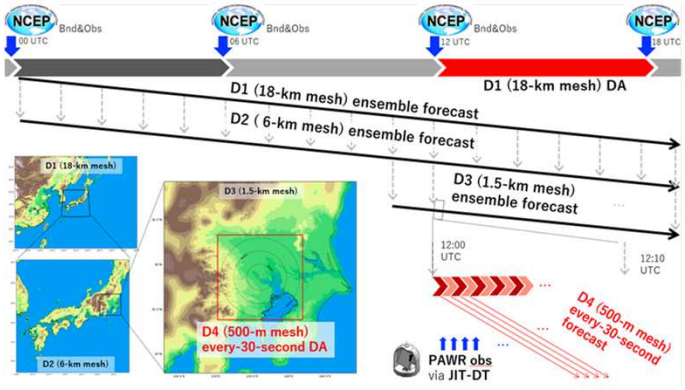
(a) 深部遮蔽層下面　　(b) 浅部遮蔽層下面

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）

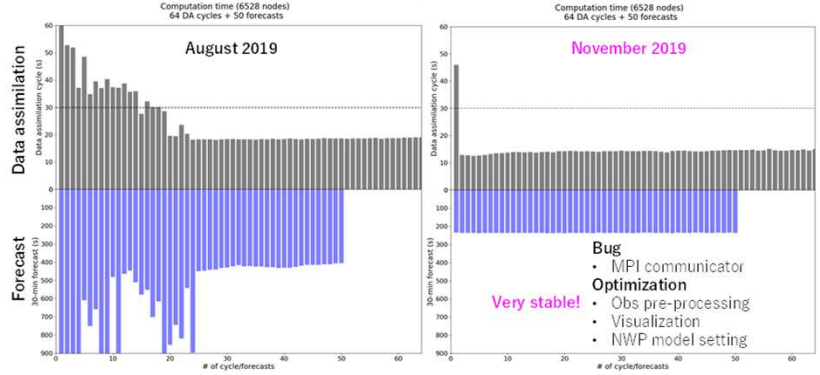


※DOF: degrees of freedom

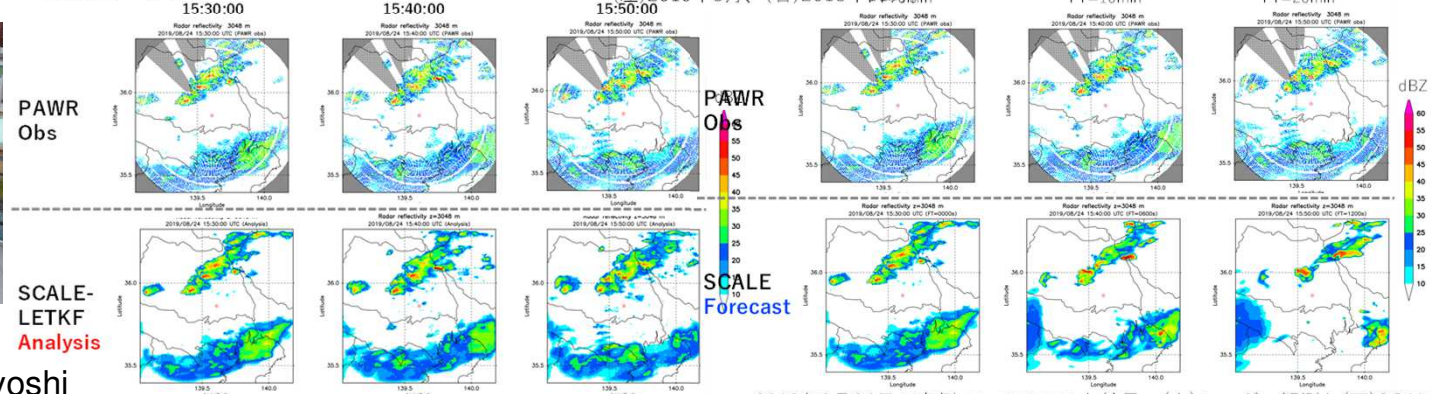
Real-Time Prediction of Severe Rainstorm by OFP



全体のワークフロー



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。



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

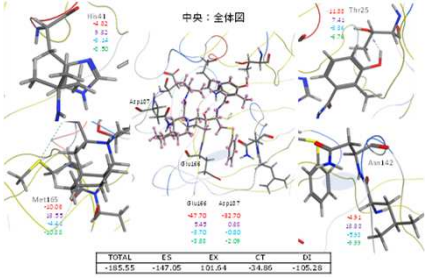
2019年8月24日の事例ついてのテスト結果。(上)レーダー観測と(下)SCALE-LETKFによる解析で得られたレーダー反射強度(dBZ)を示す。

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

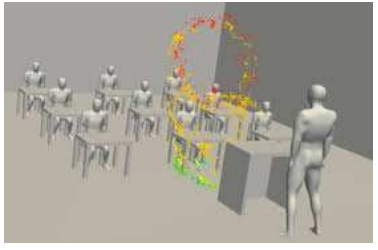
HPCI Urgent Call for Fighting against COVID-19 in Japan (FY.2020)

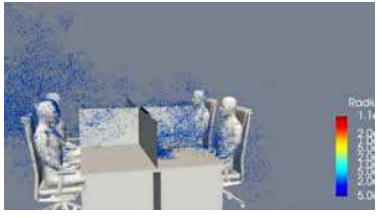
by 8 SC Centers of Natl. Univ., AIST etc.
6 of 14 accepted projects use U.Tokyo's Systems

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 (Rikkto U.)]





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

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

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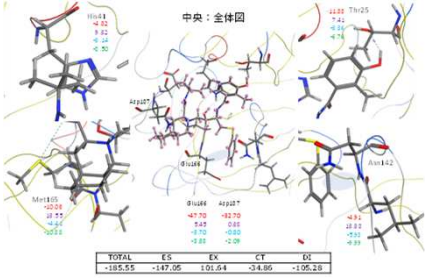
6

turbulent puff of saturated exhaled air

(OIST)

COVID-19
HPCI COVID-19 Urgent Call



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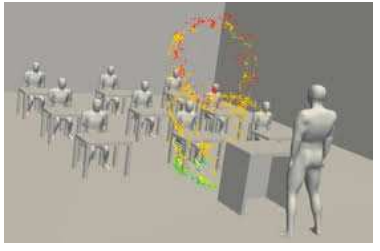
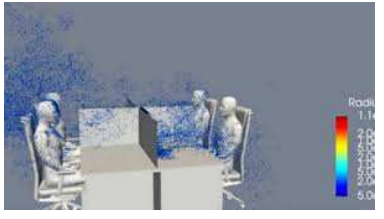




[c/o Prof. M.Tsubokura (Kobe U.)]

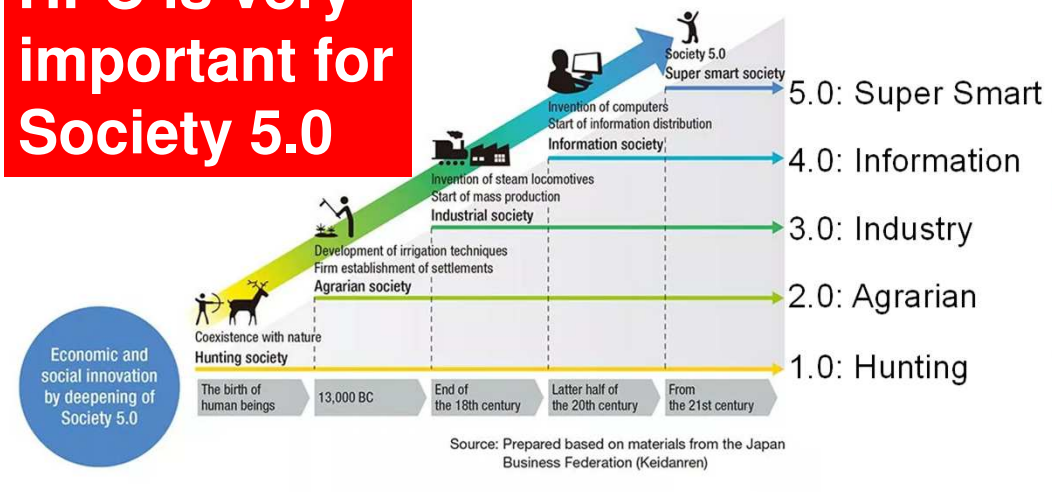
Society 5.0 & BDEC System

- 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

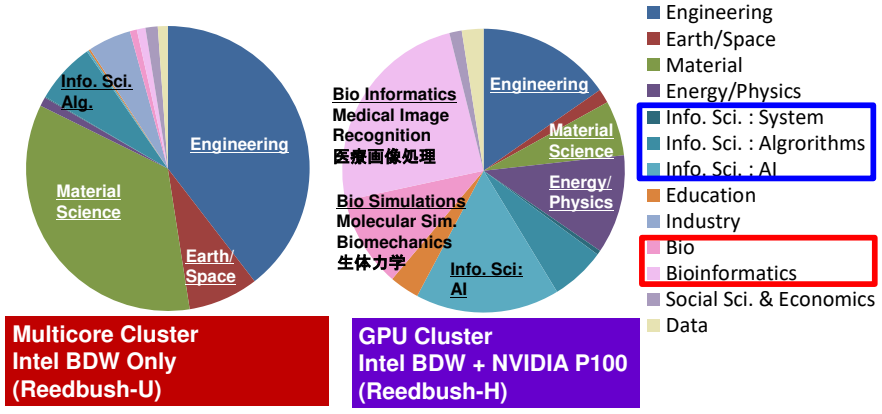
- Super Smart & Human-centered Society by Digital Innovation (IoT, Big Data, AI etc.) and by **Integration of Cyber Space & Physical Space**

HPC is very important for Society 5.0



Future of Supercomputing

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



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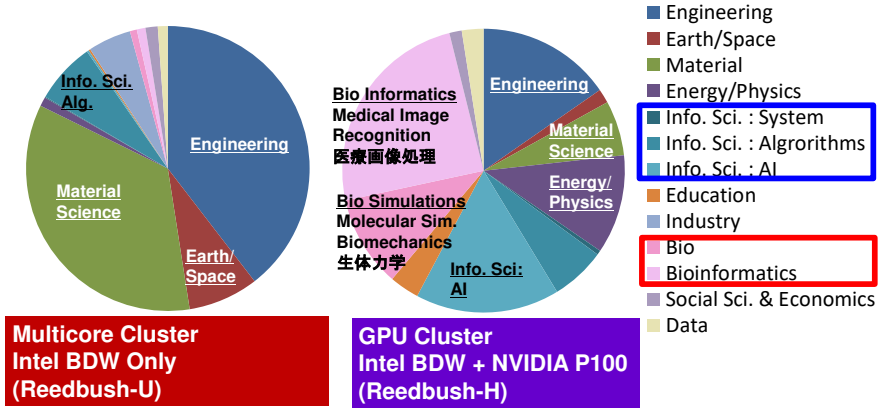

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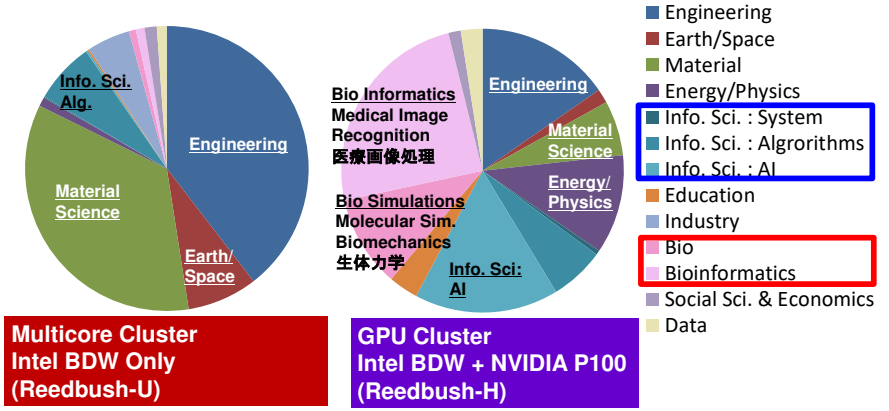
- **Integration/Convergence of (Simulation + Data + Learning) (S+D+L) is important towards Society 5.0**
- **BDEC (Big Data & Extreme Computing)**
  - **Platform for Integration of (S+D+L)**
  - **Focusing on S (Simulation)**
    - **AI for HPC, Sophisticated Simulation**
  - **Planning started in 2015**



BDEC (Big Data & Extreme Computing)

S + D + L

Society 5.0 & BDEC System

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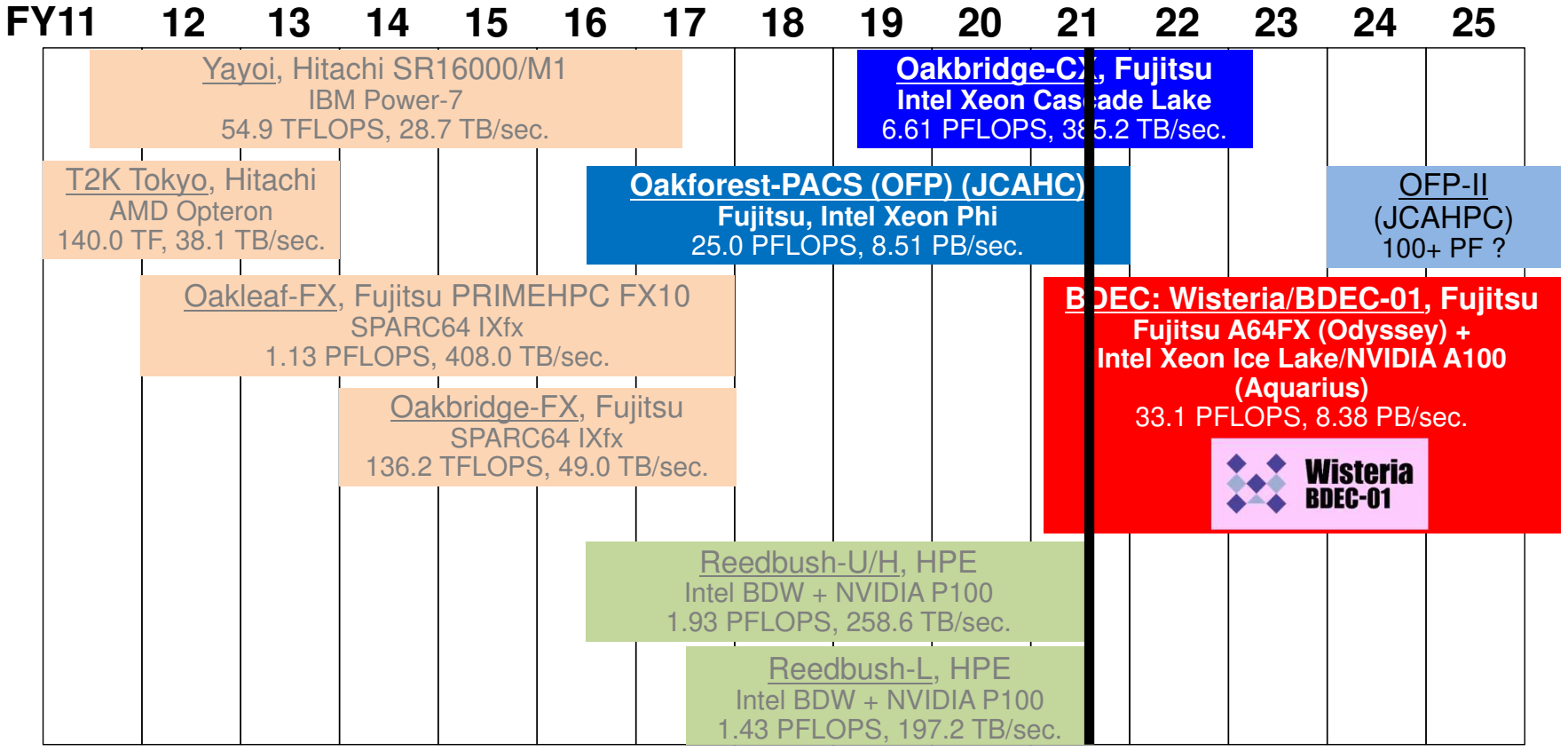
- **We have been operating 3 systems, and are now introducing the BDEC (Big Data & Extreme Computing) System as the Platform for Integration of (S+D+L)**
  - **Wisteria/BDEC-01 with 33.1 PF**

Supercomputers in ITC/U.Tokyo

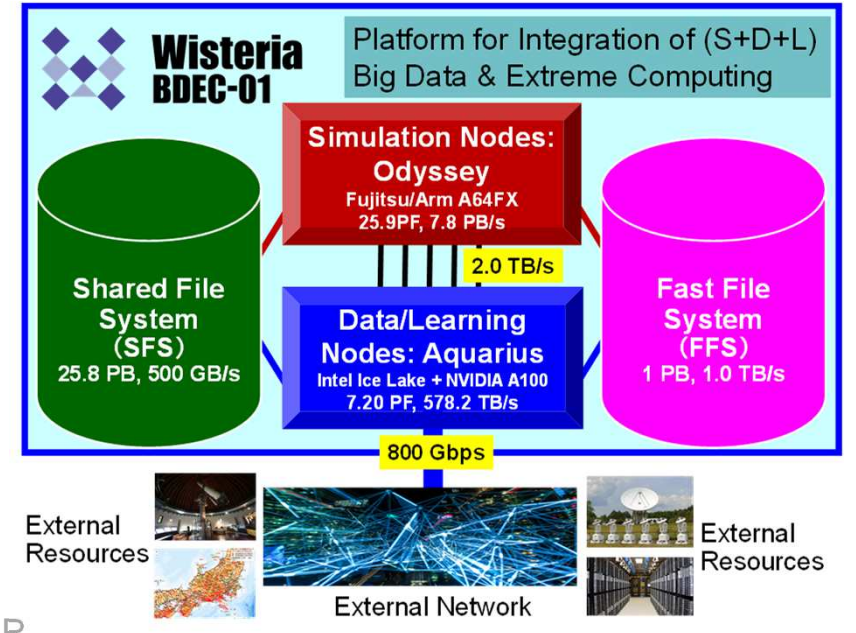
Information Technology Center, The University of Tokyo



Wisteria/BDEC-01

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

- Operation starts on May 14, 2021
- 33.1 PF, 8.38 PB/sec by **Fujitsu**
  - ~4.5 MVA with Cooling, ~360m^2
- 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)



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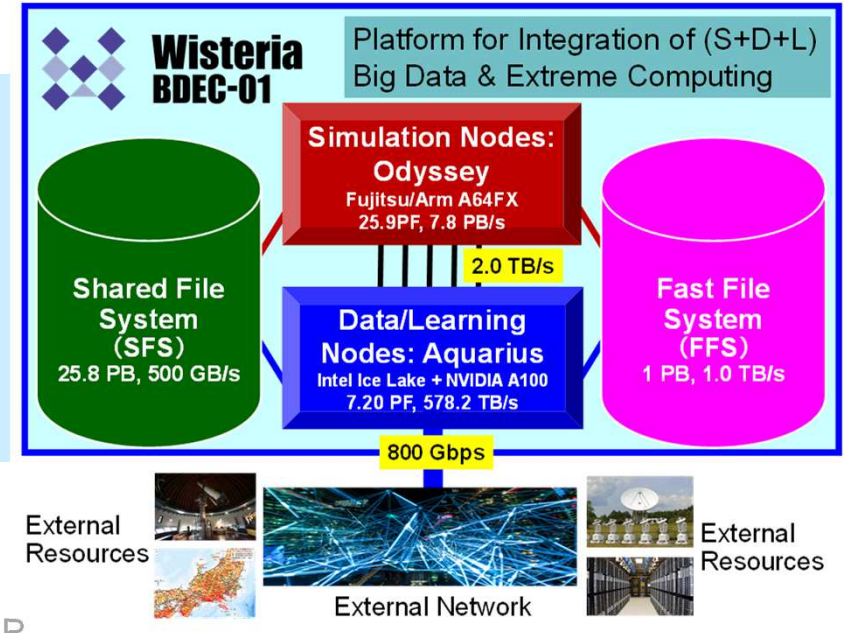

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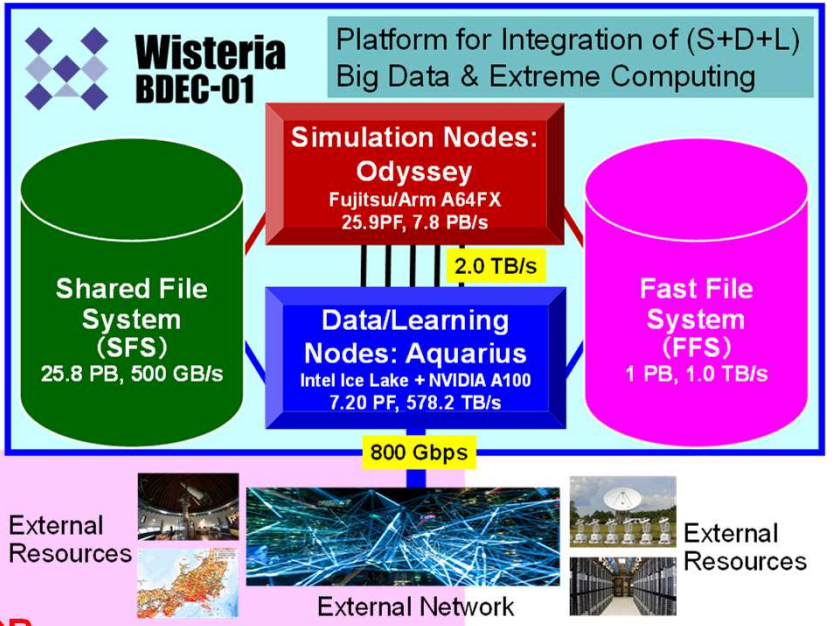
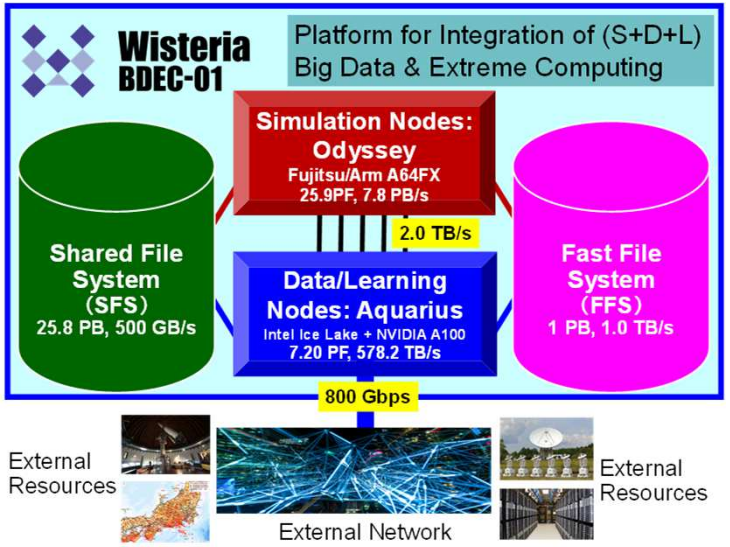




Simulation Nodes (Odyssey)

Data/Learning Nodes (Aquarius)

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

Reedbush (HPE, Intel BDW + NVIDIA P100 (Pascal))

- Prototype of "Wisteria/BDEC-01" for Integration of (S+D+L)
- July 2016 – November 2021 (Retired)
- Our First GPU Cluster, 3.36 PF

Oakforest-PACS (OFP) (Fujitsu, Intel Xeon Phi (KNL))

- JCAHPC (U.Tsukuba, U.Tokyo), October 2016 – March 2022
- 25 PF, #39 in 58th TOP 500 (November 2021)

Oakbridge-CX (OBCX) (Fujitsu, Intel Xeon CLX)

- July 2019 – June 2023
- 6.61 PF, #110 in 58th TOP500

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

Wisteria/BDEC-01 (Fujitsu)

- **Simulation Nodes (Oddysey): A64FX (#17)**
- **Data/Learning Nodes (Aquarius) (#106)**
- 33.1 PF, Operation started on May 14, 2021
- Platform for Integration of "Simulation+Data+Learning (S+D+L)"
- Innovative Software Platform "h3-Open-BDEC" supported by Janapese Government (JSPS Grant-in-Aid for Scientific Res. (S) FY.2019-2023)

Reedbush

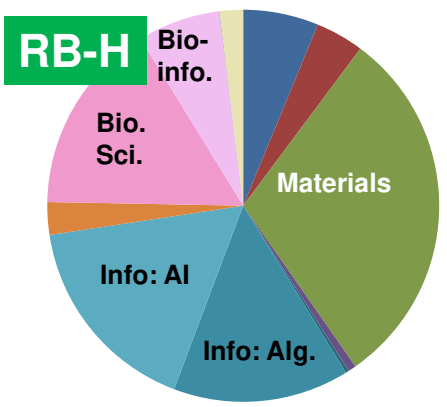
Oakforest-PACS

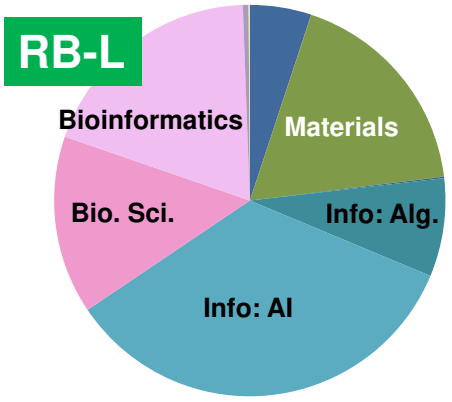
Oakbridge-CX

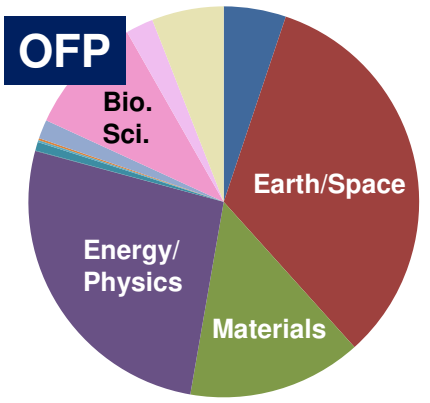
Rankings@SC21
November 2021

System	TOP500	Green500	HPCG	Graph500	HPL-AI
Oakforest-PACS	39	65	23	-	-
Oakbridge-CX	110	62	71	-	-
Wisteria/BDEC-01 (Odyssey)	**17**	**27**	**9**	**3**	**9**
Wisteria/BDEC-01 (Aquarius)	**106**	**15**	**58**	**-**	**-**

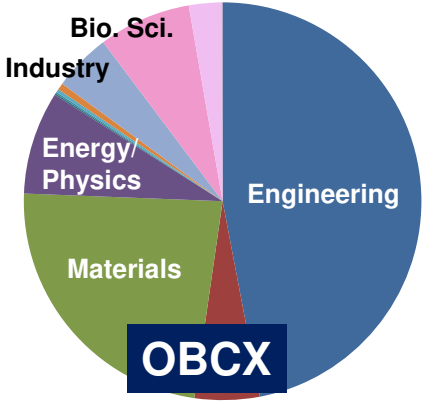
Research Area based on CPU Hours (FY.2020)







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

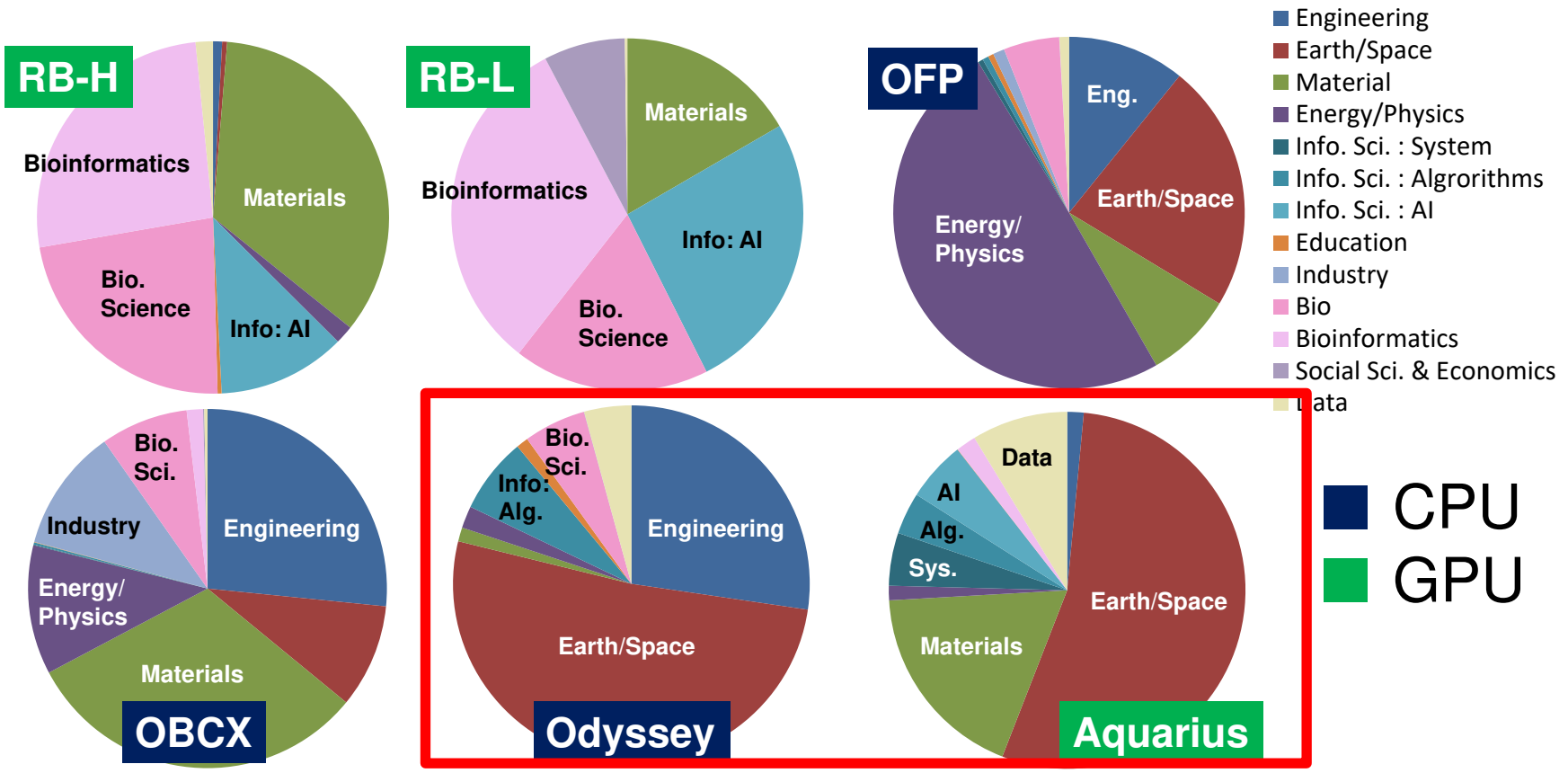


CPU

GPU

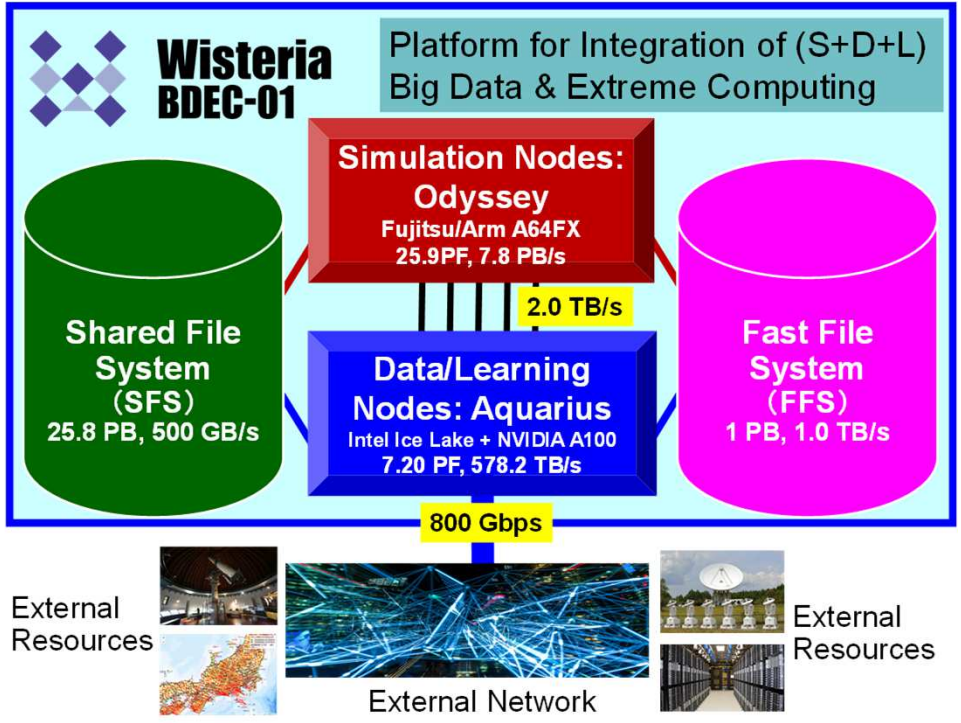
Research Area based on CPU Hours (FY.2021)

Apr.2021-Sep.2021, Only Aug./Sep. for Odyssey & Aquarius

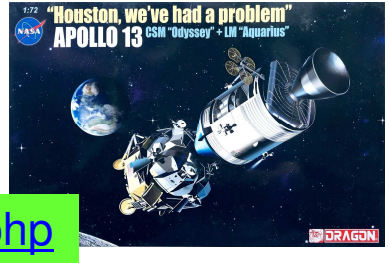


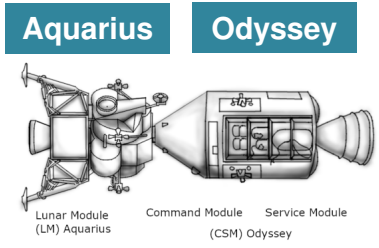
Wisteria/BDEC-01

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)





https://www.cc.u-tokyo.ac.jp/public/pr/pr-wisteria.php

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

Simulation Codes

Optimized Models & Parameters

Simulation Nodes Odyssey

Results

Wisteria/BDEC-01

Machine Learning, DDA

Observation Data

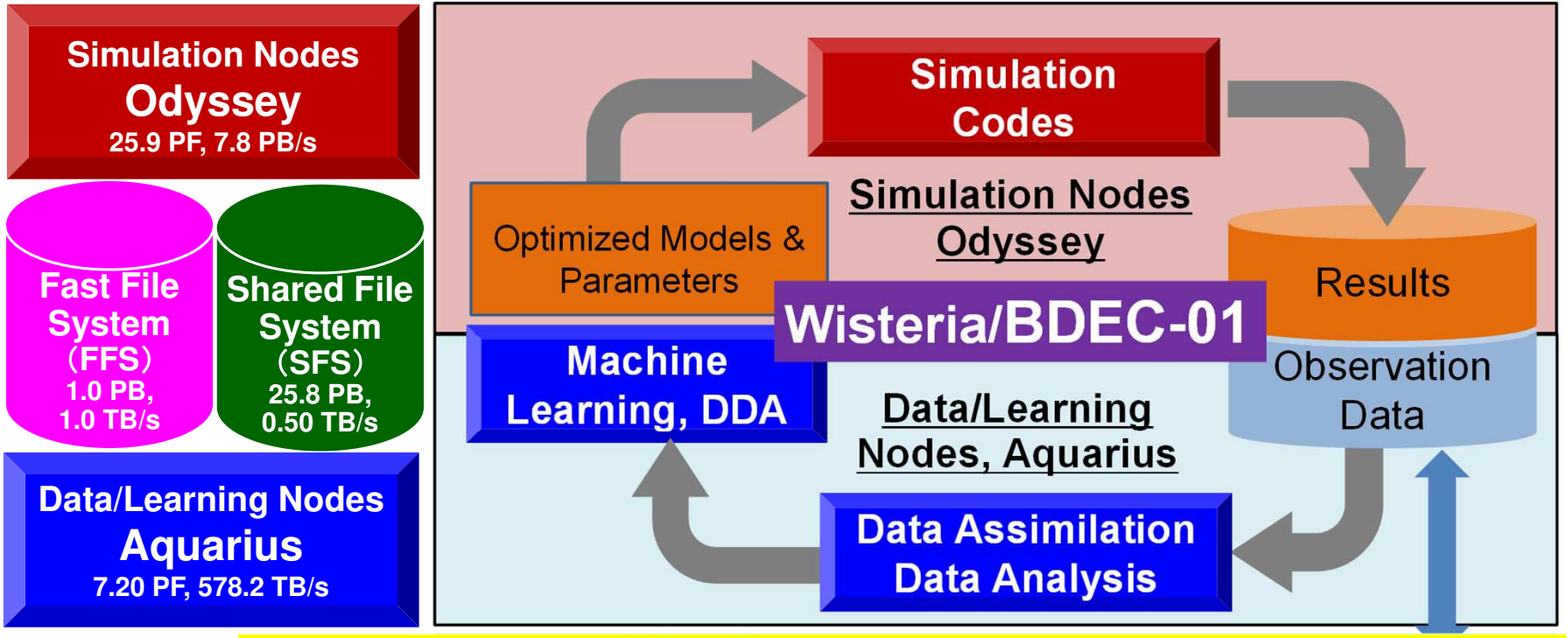
Data/Learning Nodes, Aquarius

Data Assimilation Data Analysis

Server, Storage, DB, Sensors, etc.

External Network

External Resources



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 Assimilatic
- 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

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

東京大学
THE UNIVERSITY OF TOKYO

北海道大学
HOKKAIDO UNIVERSITY

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

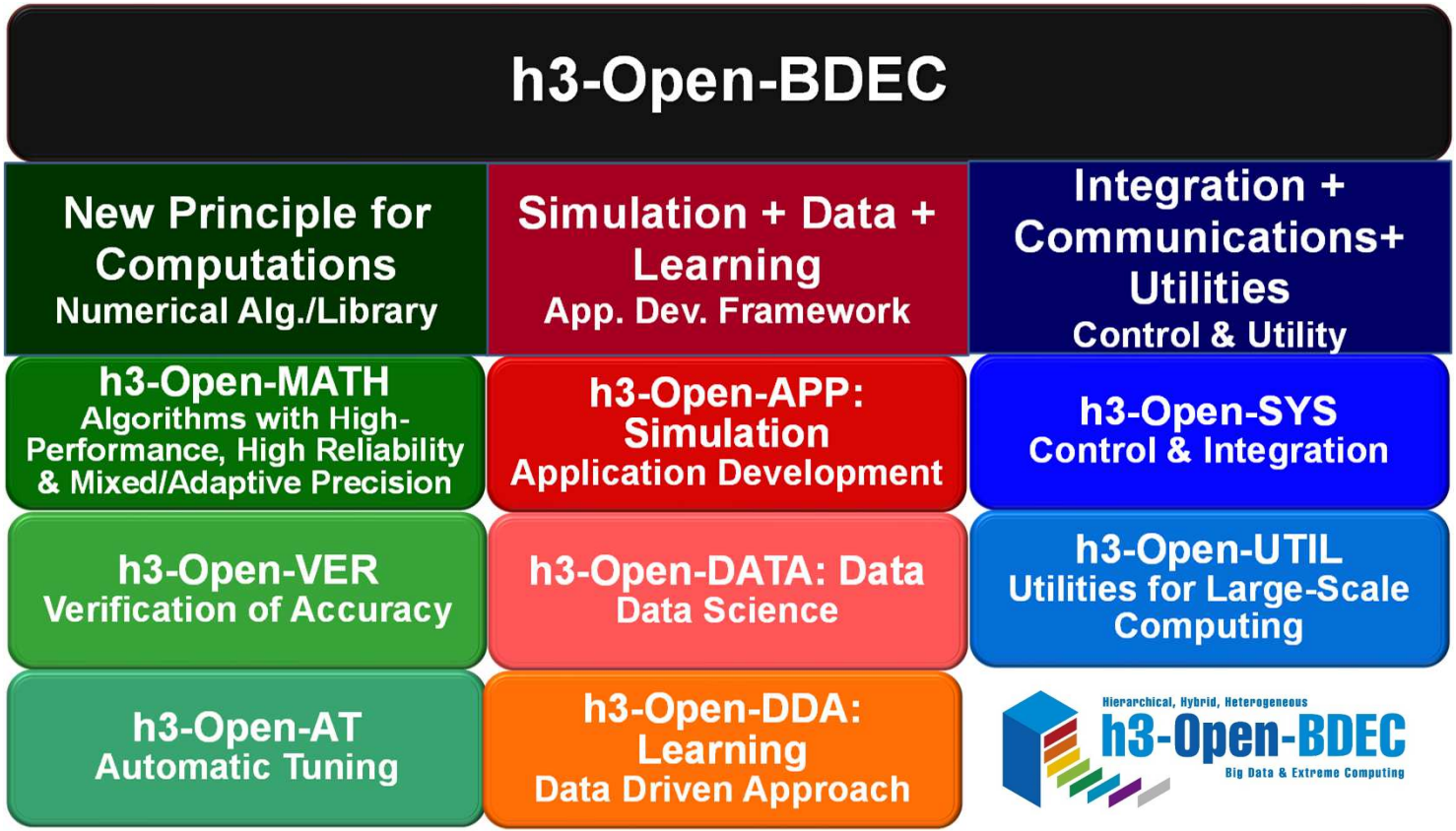
Tokyo Woman's Christian University
東京女子大学

名古屋大学
NAGOYA UNIVERSITY

RIKEN
R-CCS

h3-Open-BDEC

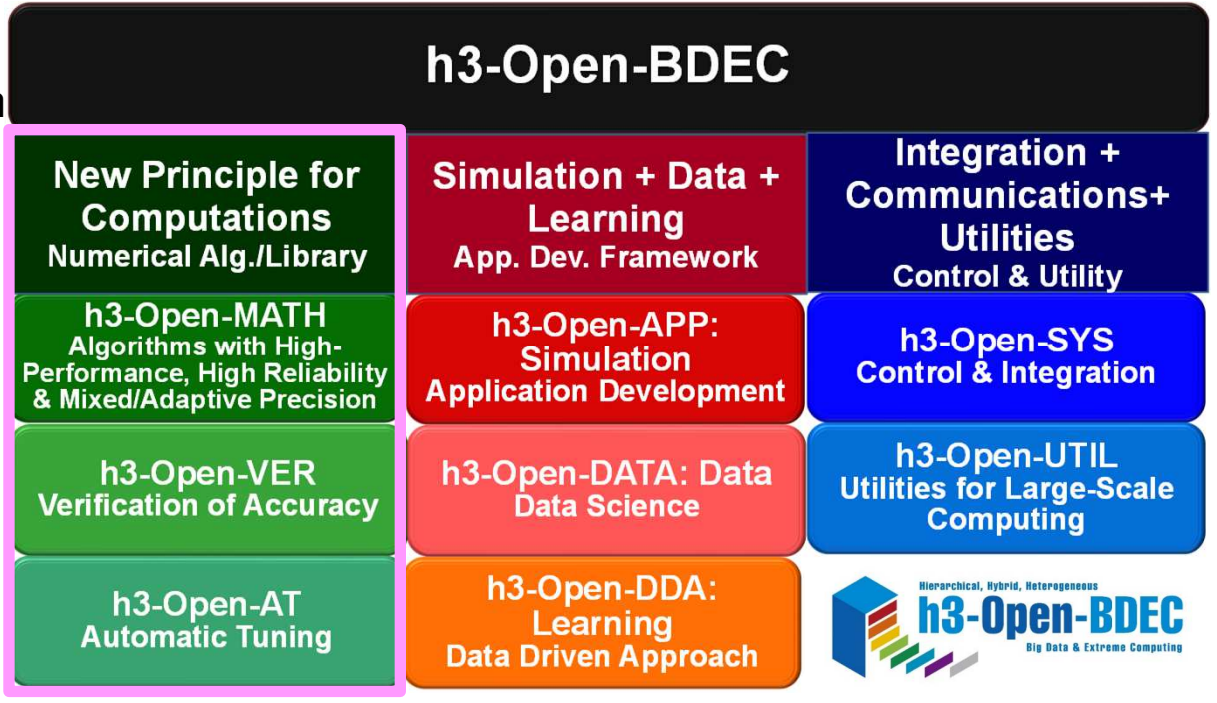
Innovative Software Platform for Integration of (S+D+L) on BDEC



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**

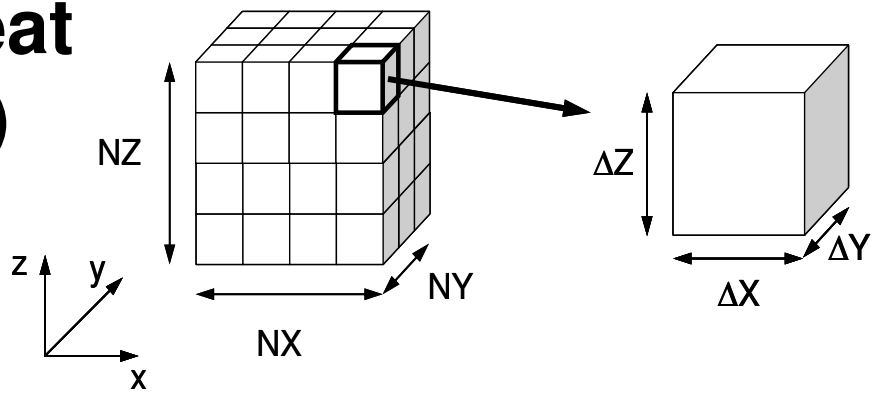
Approximate Computing with Low/Adaptive/Trans Precision

- 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**

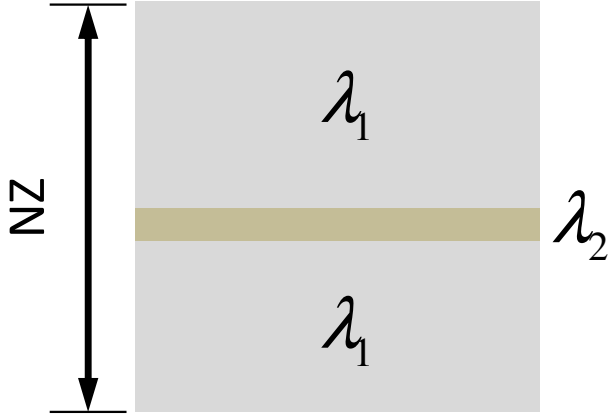
P3D: Steady State 3D Heat Conduction by FVM (1/2)

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

- 7-point Stencil
- Heterogenous Material Property



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



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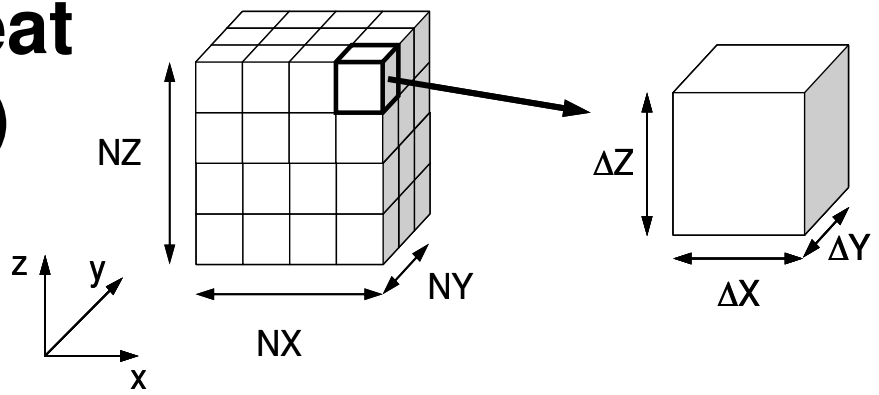
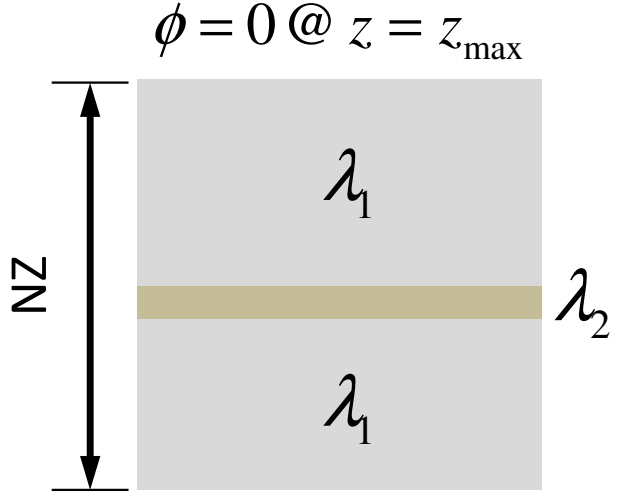


- 7-point Stencil
- **Heterogenous Material Property**
  - **λ_1/λ_2 is proportional to the condition number of coefficient matrices**
- **Coefficient Matrix**
  - **Sparse, SPD**
- **ICCG Solver**
- **Fortran 90 + OpenMP**
- **CM-RCM Reordering**



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

- Various Configurations
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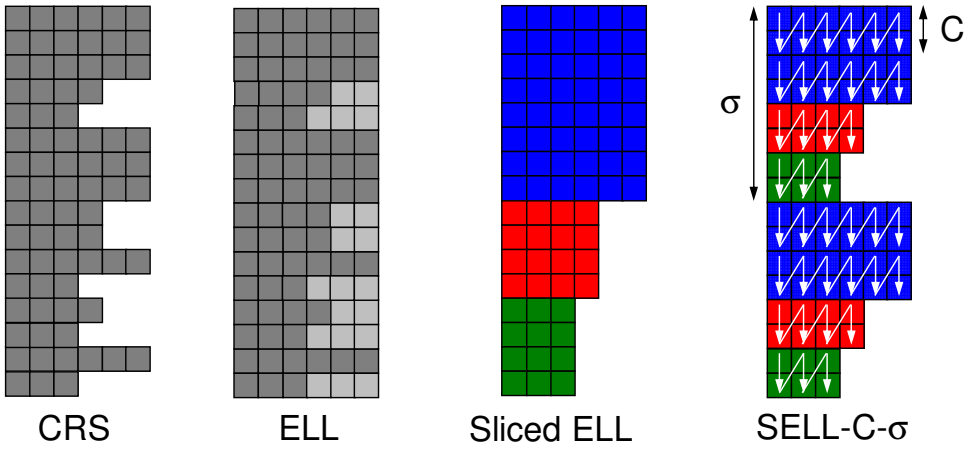
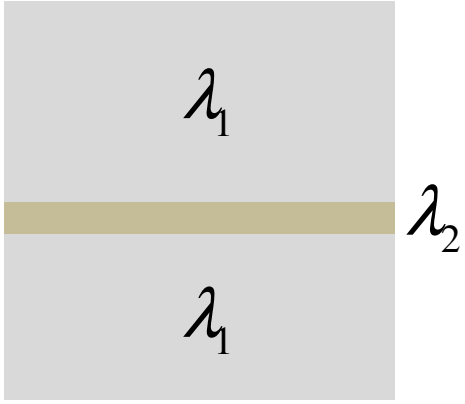
  - Matrix Storage Format (CRS, ELL, SELL-C-σ etc.)



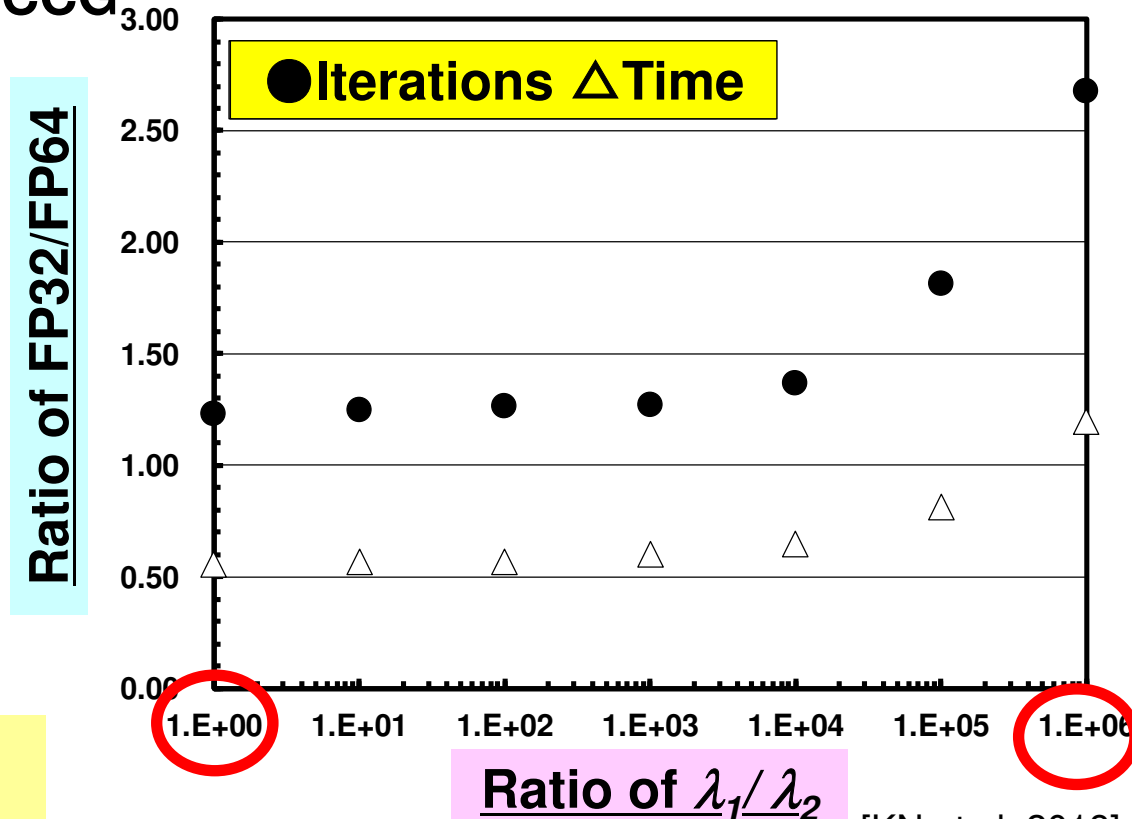
Ratio of FP32(SP)/FP64(DP): CRS

Iterations● & Time△ for ICCG
λ_1/λ_2, 128^3 DOF, CRS
Ratio<1 ⇒ FP32 is faster



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

Intel Xeon BDW
1 Node: 18 cores x 2 soc's



[KN et al. 2018]

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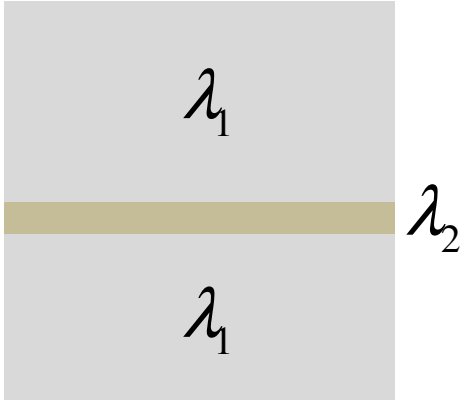

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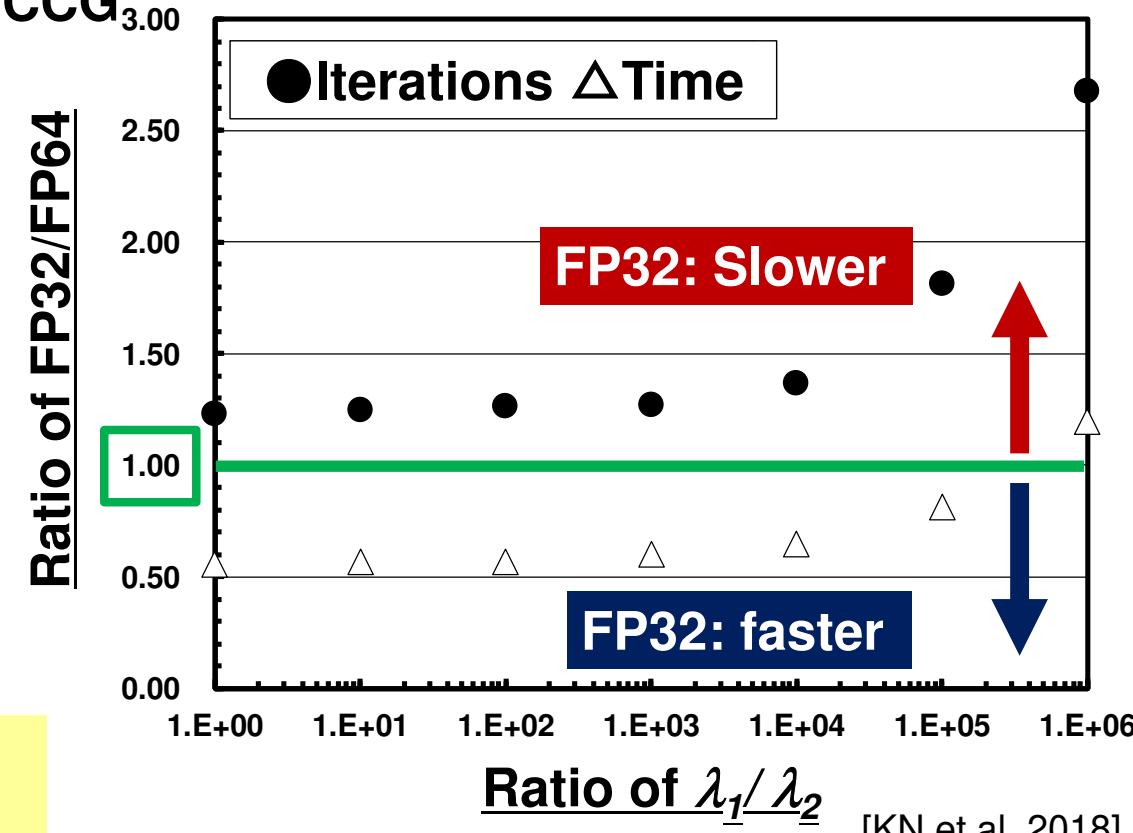

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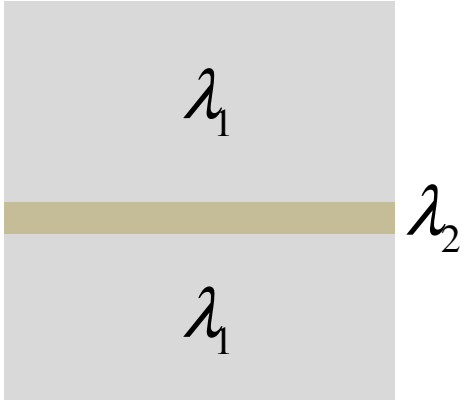

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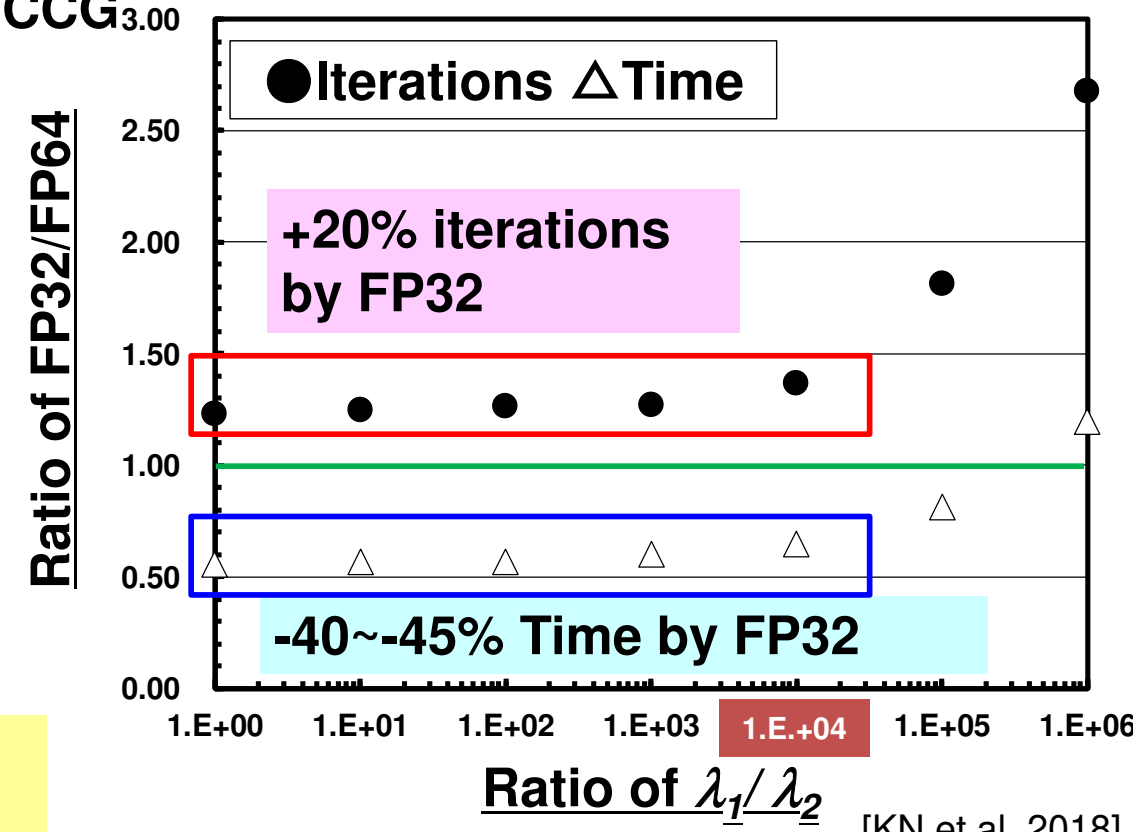

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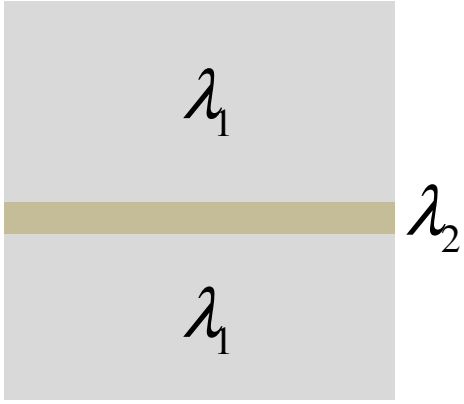

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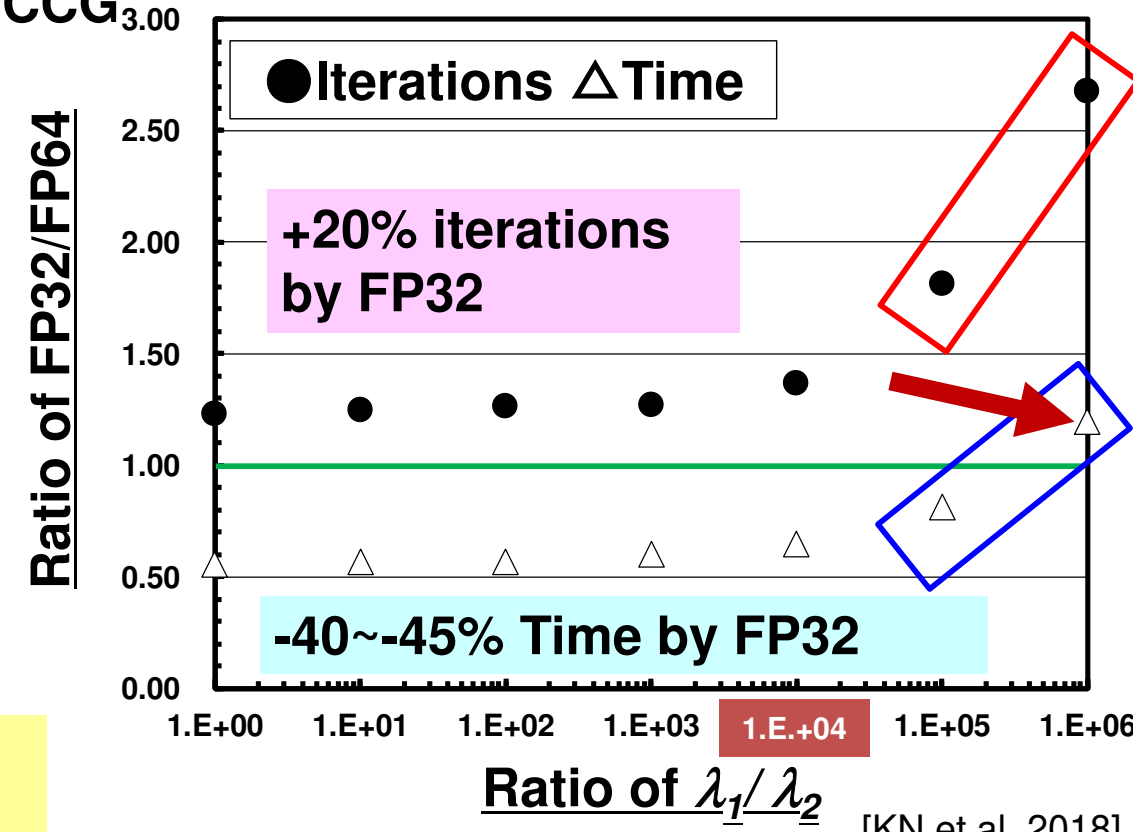
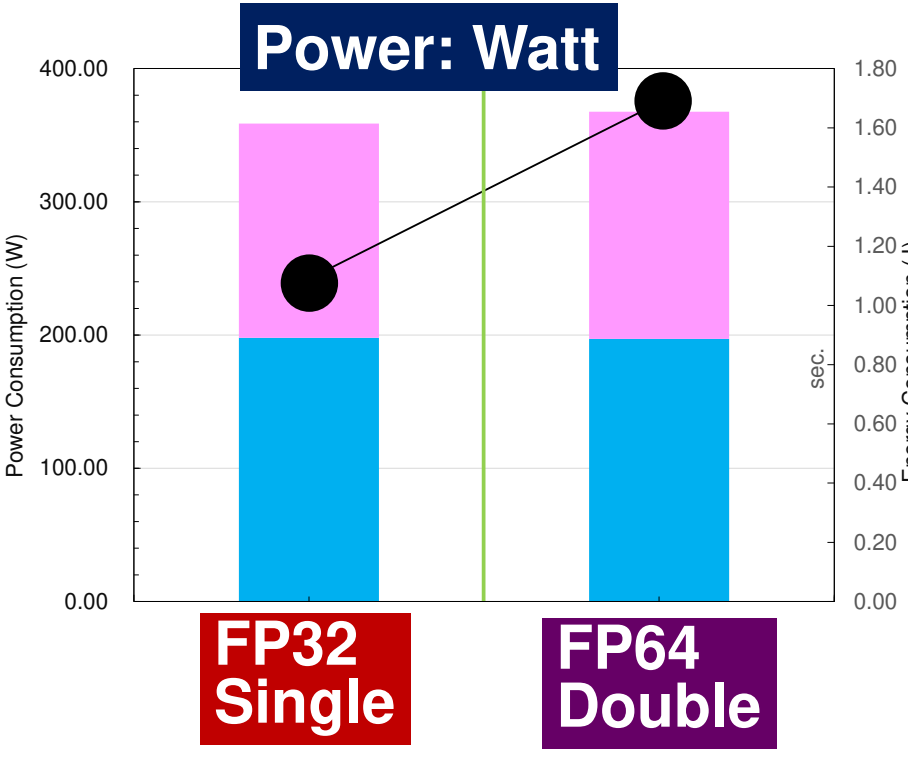


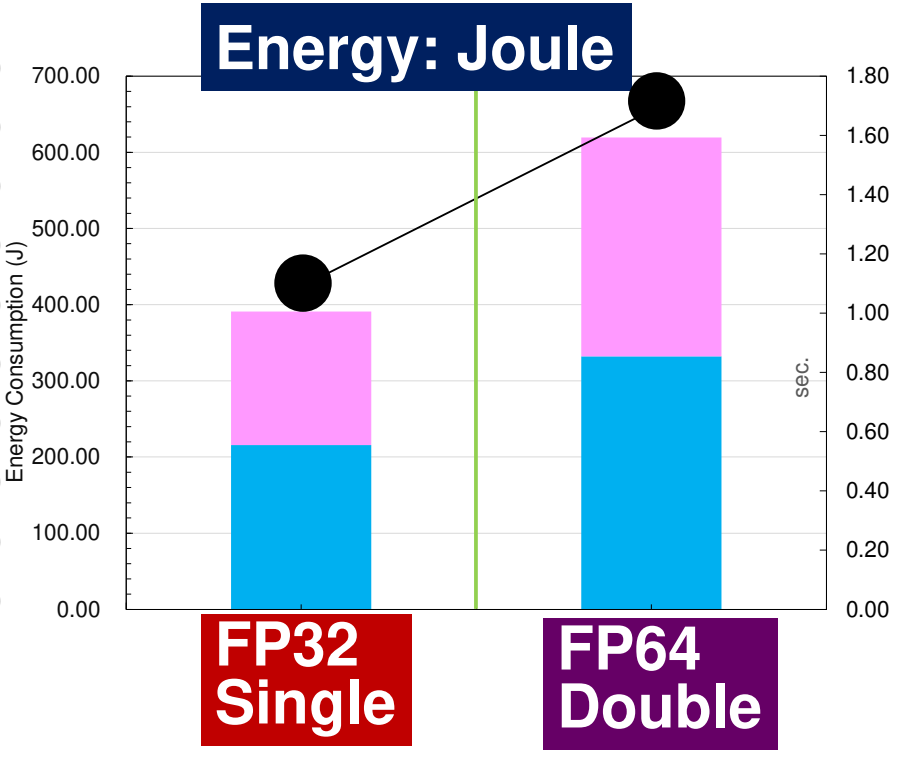
[KN et al. 2018]

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

[Sakamoto et al. 2020]

N=128³, : CPU, : Memory, : Time





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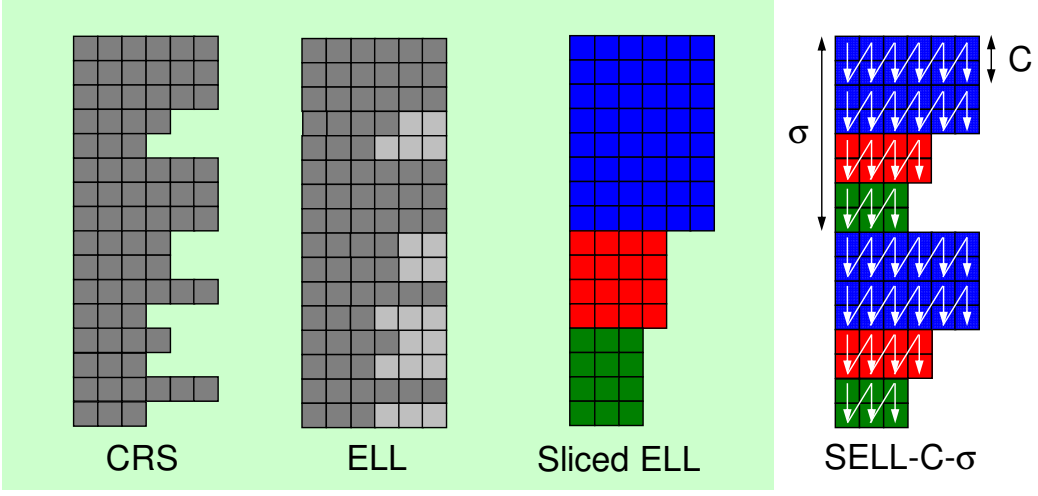
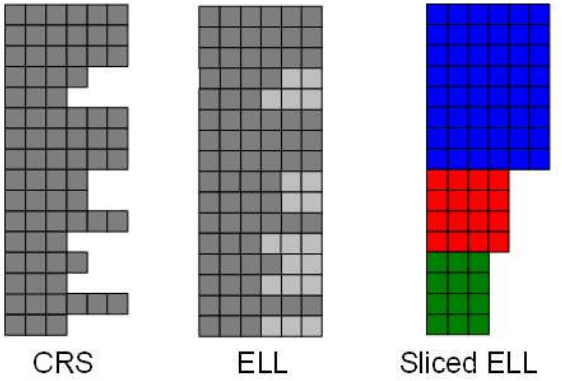


System	Oakforet-PACS	Oakbridge-CX	Oakleaf-7 (FX700)
Abbreviation	OFP	OBCX	OL7
Architecture of CPU	Intel Xeon Phi 7250 (Knights Landing, KNL)	Intel Xeon Platinum 8280 (Cascade Lake, CLX)	Fujitsu A64FX（1.8GHz）
Core#/Socket	68	28	48
Socket#/Node	1	2	1
Peak Performance (DP) (GFLOPS)/Node	3,046	4,838	2,765
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

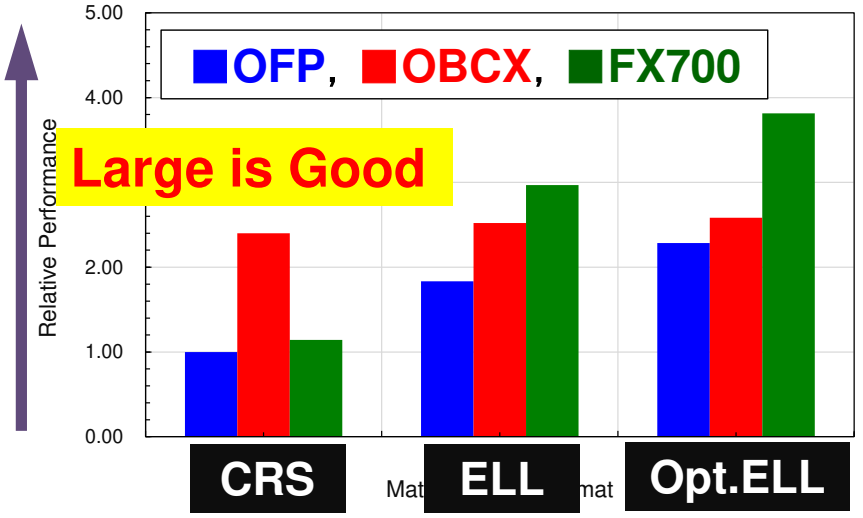
Ratio of Performance

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

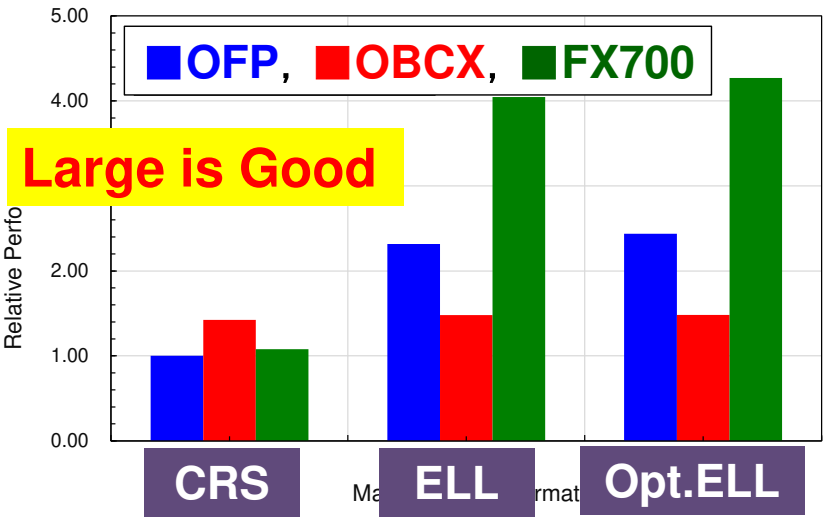
[KN et al. SWoPP 2020]



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

[KN et al. SWoPP 2020]

Mixed Precision Computing for P3D on FX700 Implementation of Forward Substitution (CRS) in ICCG

[KN et al. SWoPP 2020]

FP64
FP32
FP16

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 -  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
```

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)= Ws(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
```

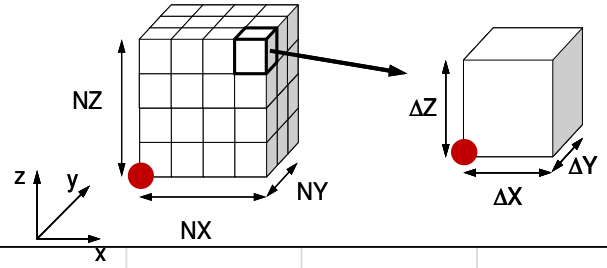
D-H

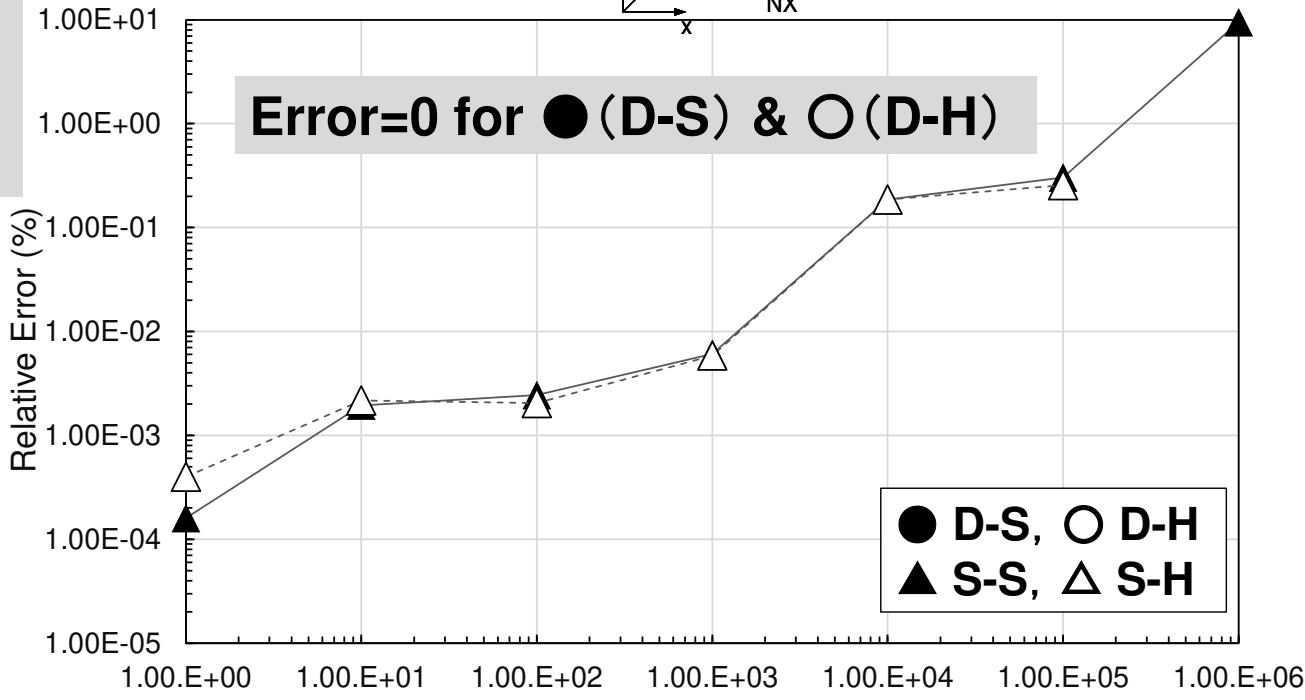
```
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
        Ws(i,Z)= W(i,R)
      enddo
      enddo

!$omp parallel private(ic,ip,ip1,i,WVALs,k)
      do ic= 1, NCOLORtot
!$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

(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
```

Mixed Precision Computation

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

Relative Error (%) compared to D-D @●





[KN et al. SWoPP 2020]

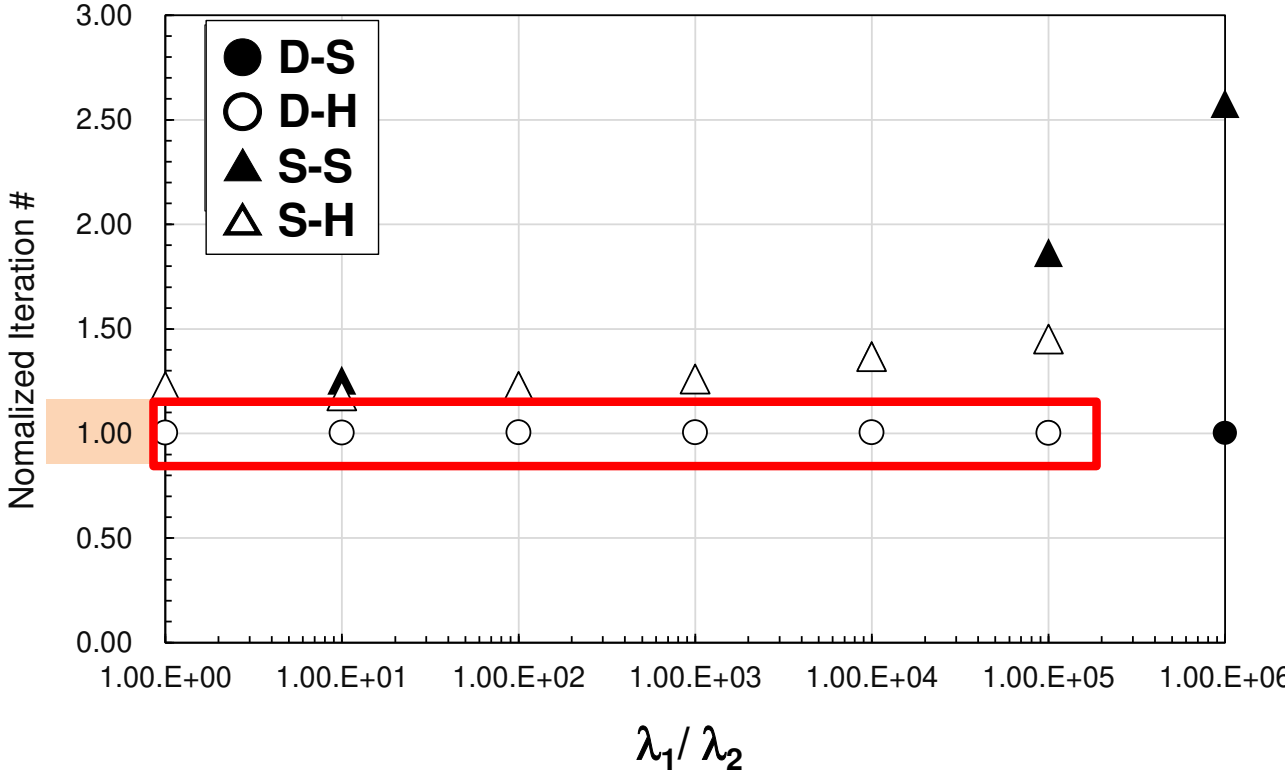
Mixed Precision Computation

[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 $\lambda_1/\lambda_2 \leqq 10^5$)



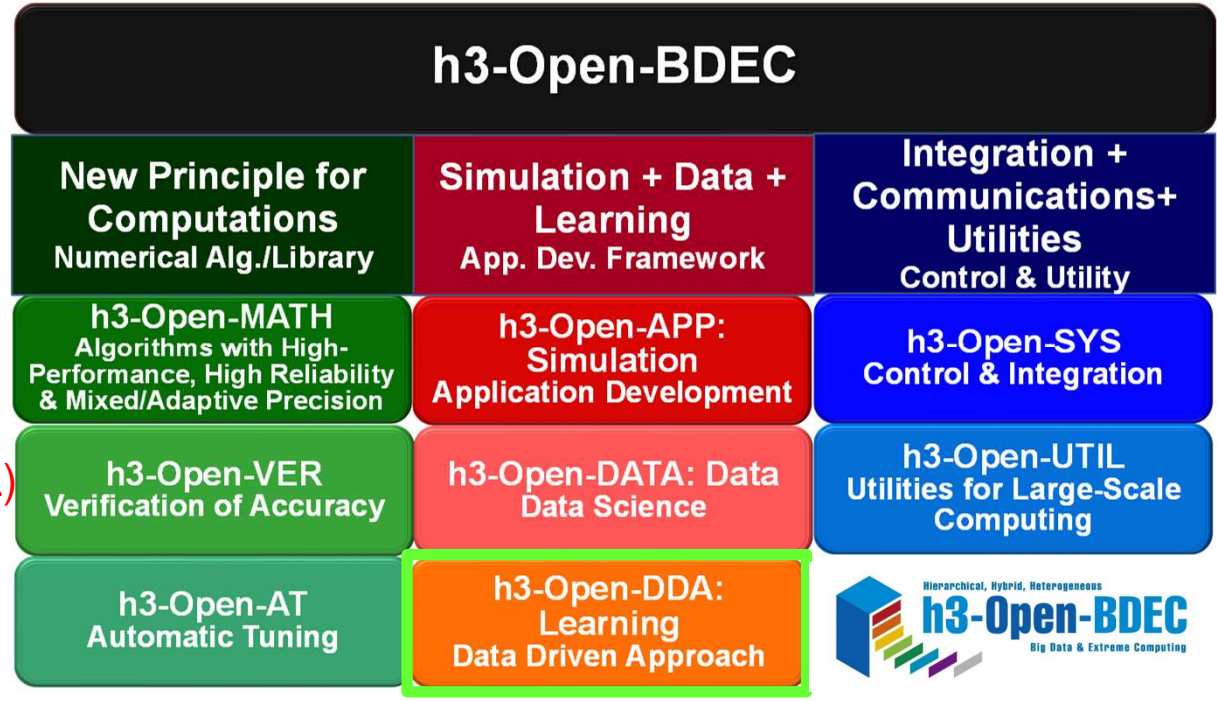
h3-Open-BDEC: Two Significant Innovations

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 (*h*DDA) 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

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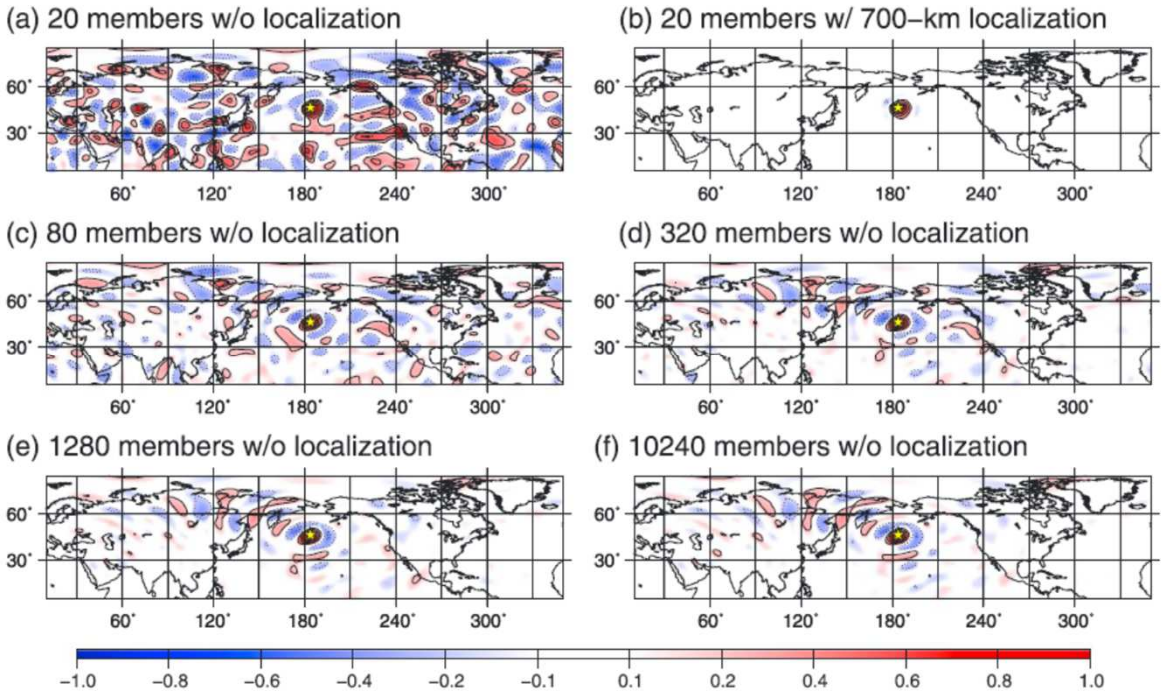
- Non-Linear: Huge Number of Parameter Studies needed
  - ✓ Reduction of cases is very crucial

[Miyoshi et al. 2014]

- 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),



Hierarchical Data Driven Approach: *h*DDA

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

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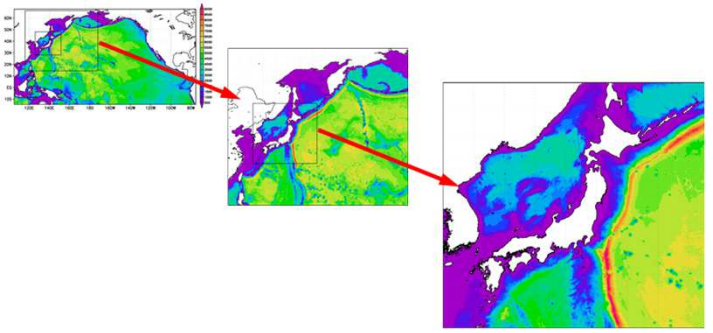
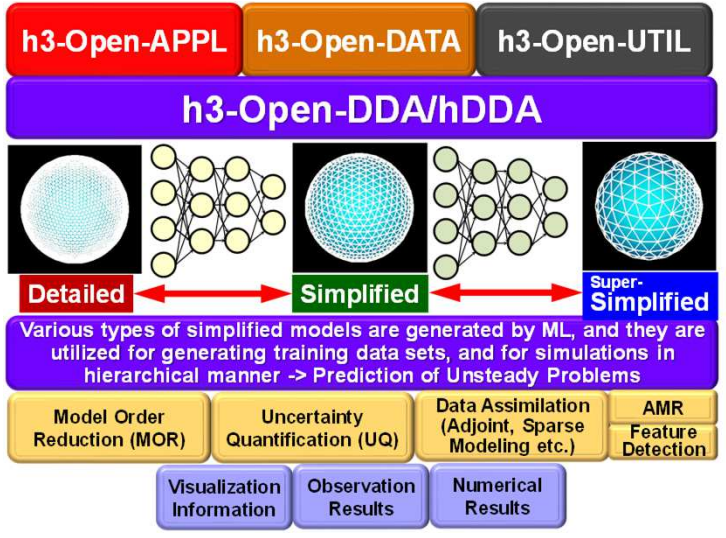
- ***h*DDA (Hierarchical DDA)**
  - Simplified models with coarser meshes (but preserving original features of physics) for efficient training are constructed automatically by Machine Learning using:
    - Feature Detection, AMR
    - MOR (Model Order Reduction)
    - UQ (Uncertainty Quantification)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





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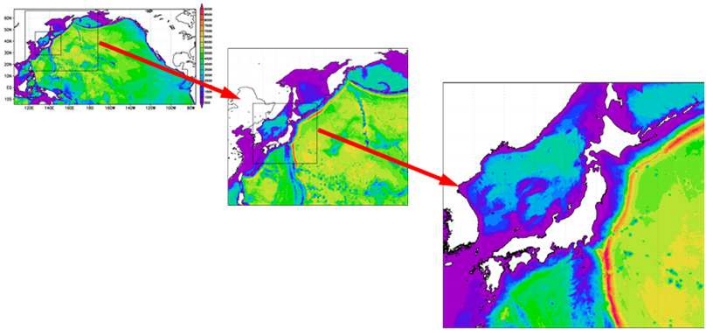
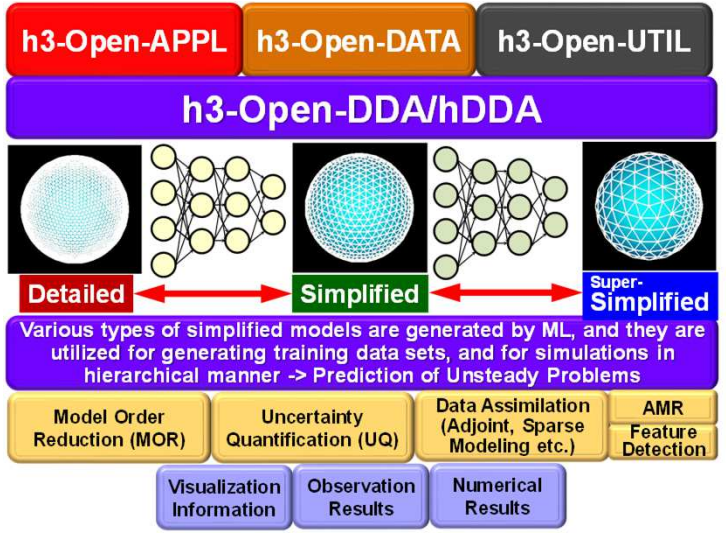
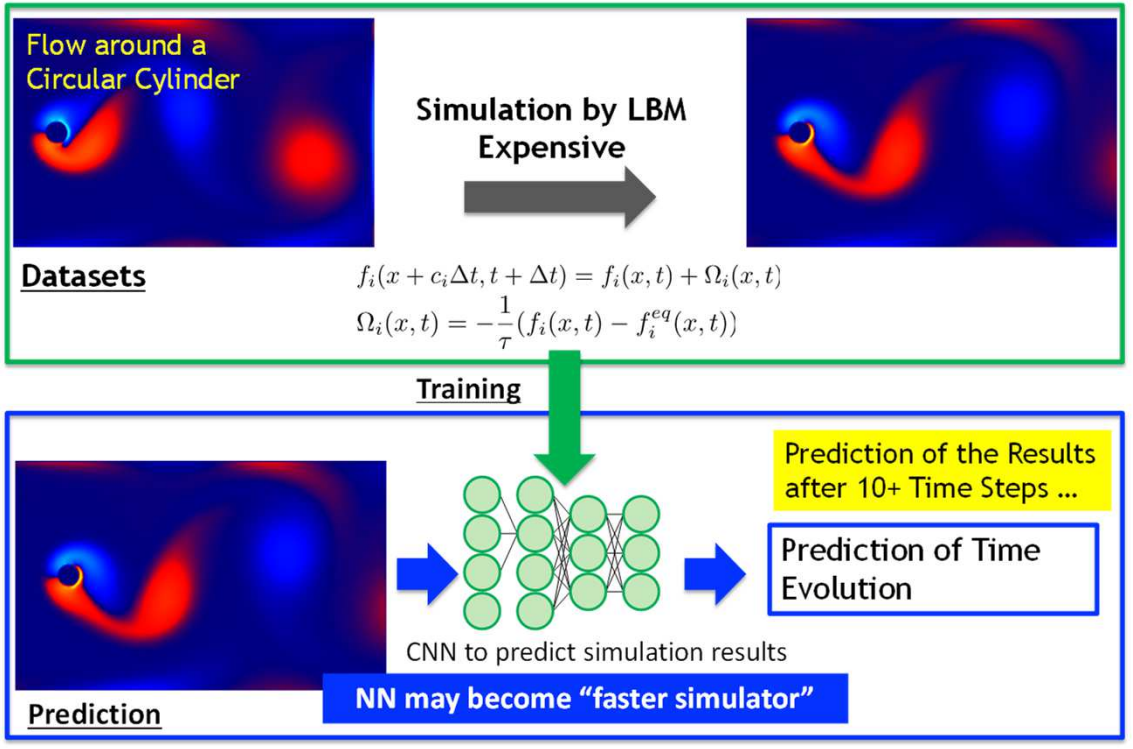
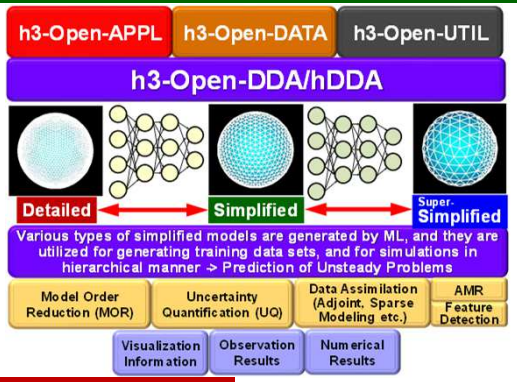




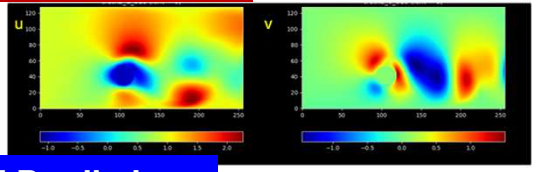
Acceleration of Transient CFD Simulations using ML/CNN Integration of (S+D+L), AI for HPC



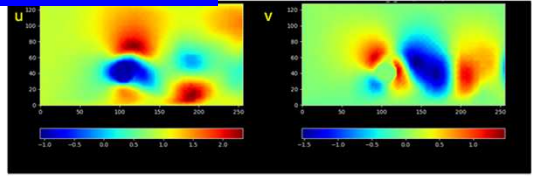
[c/o Takashi Shimokawabe (ITC/U.Tokyo)]



Simulations: LBM

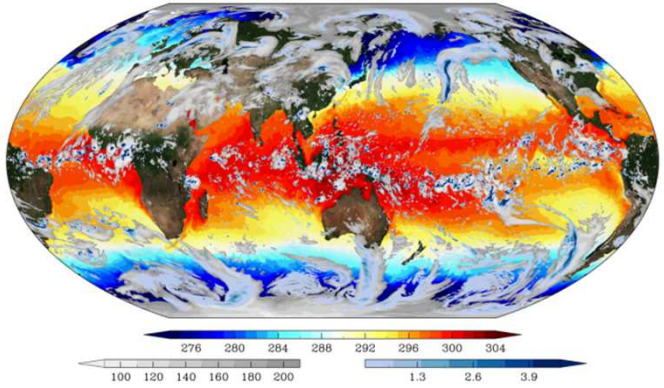


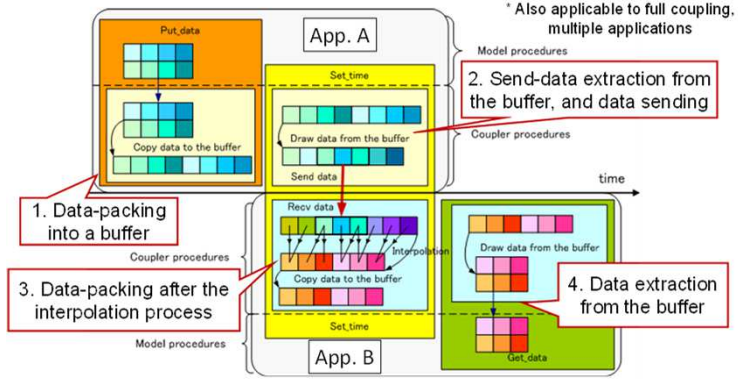
CNN Predictions



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





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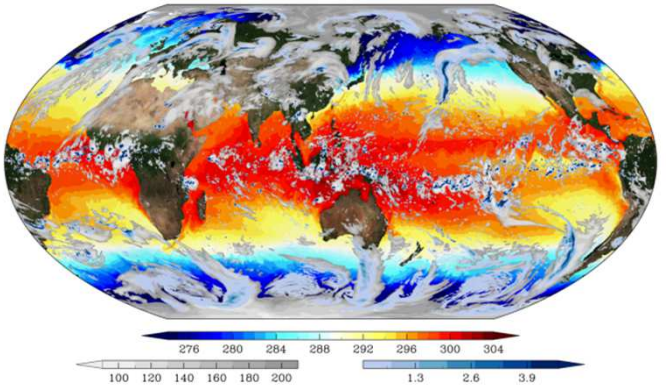
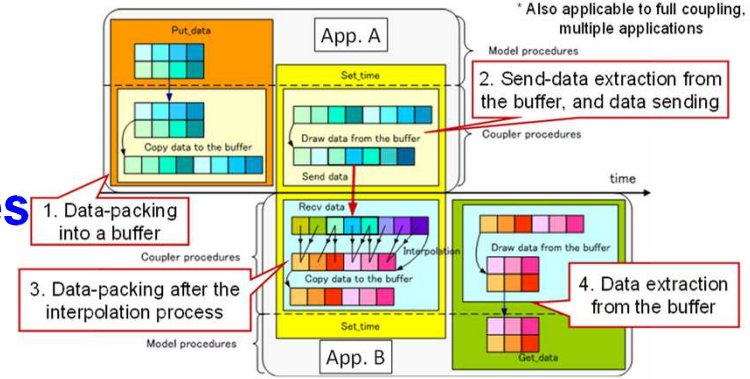
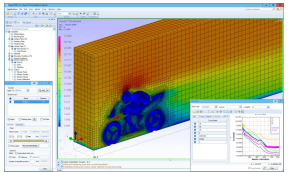
  - AORI/U.Tokyo, RIKEN R-CCS, NIES
- **Earthquake Simulations with Real-Time Data Assimilation (My Talk on Friday)**
  - **ERI/U. Tokyo**
- **Real-Time Disaster Simulations**
  - **Flood, Tsunami**
- **(S+D+L) for Existing Simulation Codes (Open Source SW**
  - **OpenFOAM**

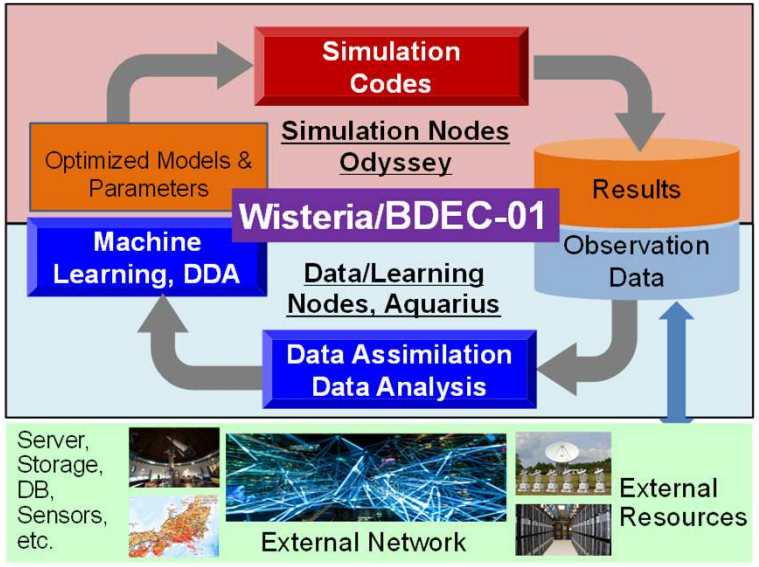


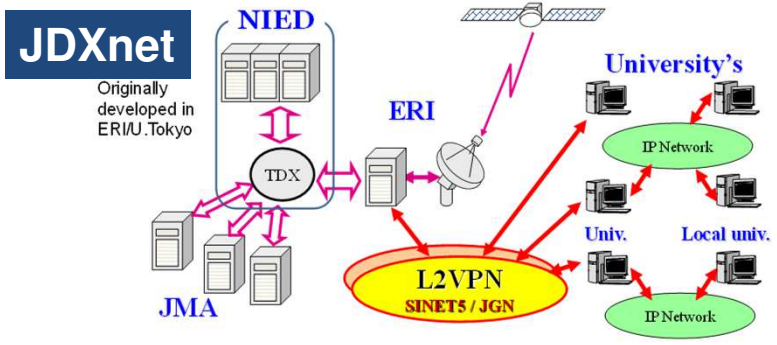


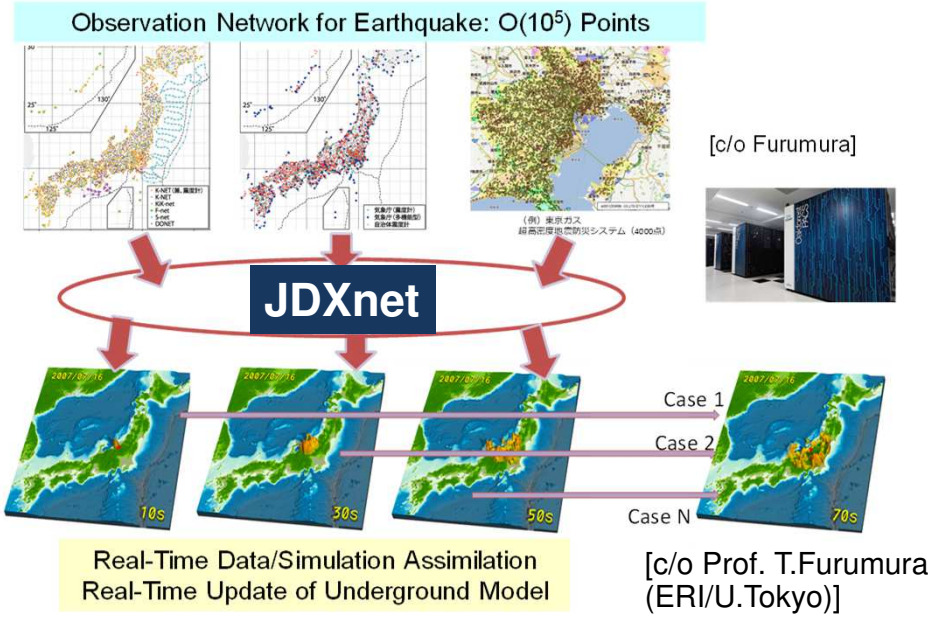


3D Earthquake Simulation with Real-Time Data Observation/Assimilation

Simulation of Strong Motion (Wave Propagation) by 3D FDM







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

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 + *h*DDA)**, total energy consumption (=total computation time) for simulations will be 10% of that by the conventional methods for simulations with parameter studies

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- By Integration of (S+D+L) using h3-Open-BDEC (Adaptive Precision + *h*DDA), 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 experts in data analytics and AI/ML.**
- **Source codes and documents (in English) are open to public for various kinds of computational environments.**

International Workshop on the Integration of (Simulation + Data + Learning): Towards Society 5.0 by h3-Open-BDEC

Towards the end of Moore's law, we need to develop new algorithms and applications. We are developing h3-Open-BDEC, which is innovative software for sustainable promotion of scientific discovery by supercomputers in the Exascale Era by combining (Simulation + Data + Learning (S+D+L)), where ideas of data science and machine learning are introduced to computational science. Integration of (S+D+L) is also important for realization of Society 5.0, which is a “Super Smart and Human-centered Society” by digital innovation, such as IoT, Big Data, AI etc., and by integration of cyber-space (digital/virtual space) and physical-space (real space). The h3-Open-BDEC project is funded by Japanese Government via JSPS Grant-in-Aid for Scientific Research（S）(Leading PI: Kengo Nakajima, the University of Tokyo, 19H05662) since 2019. In this workshop, we would like to report our progress of research and development in recent 2.5 years. While there are talks by Co-PI’s and members of the project, we have 6 excellent invited talks from Japan, Taiwan, USA and Germany. All members of the project are happy to welcome all participants, and would like to discuss on various aspects of integration of (S+D+L). Please enjoy this two-day online event.

	JST: Japan	CTT: Taiwan	CET: Germany	EST: Atlanta	PST: Berkeley	Speaker
Session-1 **Adaptive Precision, AT & Verification (I)**	0800-0830, Nov30	0700-0730, Nov30	0000-0030, Nov30	1800-1830, Nov29	1500-1530, Nov29	Kengo Nakajima (U.Tokyo): Overview
	0830-0850	0730-0750	0030-0050	1830-1850	1530-1550	Takeshi Iwashita (Hokkaido U.)
	0850-0910	0750-0810	0050-0110	1850-1910	1650-1710	Masatoshi Kawai (U.Tokyo)
	0910-0950	**0810-0850**	**0110-0150**	**1910-1950**	**1710-1750**	**Rich Vuduc (Georgia Tech)**
Session-2 **Integration of (S+D+L) (I)**	**1600-1640, Nov30**	**1500-1540, Nov30**	**0800-0840, Nov30**	**0200-0240, Nov30**	**2300-2340, Nov29**	**Kento Sato (RIKEN)**
	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Takashi Shimokawabe (U.Tokyo)
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hayato Shiba (U.Tokyo)
	1720-1800	**1620-1700**	**0920-1000**	**0320-0400**	**2420-2500**	**Weichung Wang (National Taiwan U)**

	JST: Japan	CTT: Taiwan	CET: Germany	EST: Atlanta	PST: Berkeley	Speaker
Session-3 **Adaptive Precision, AT & Verification (II)**	**0800-0840, Dec03**	**0700-0740, Dec03**	**0000-0040, Dec03**	**1800-1840, Dec02**	**1500-1540, Dec02**	**Osni Marques (LBNL)**
	0840-0900	0740-0800	0040-0100	1840-1900	1540-1600	Takahiro Katagiri (Nagoya U.)
	0900-0920	0800-0820	0100-0120	1900-1920	1600-1620	Takeshi Ogita (TWCU)
	0920-0940	**0820-0840**	**0120-0140**	**1920-1940**	**1620-1640**	**Takeshi Fukaya (Hokkaido U.)**
	0940-1020	**0840-0920**	**0140-0220**	**1940-2020**	**1640-1720**	**Discussions on Computing by Low/Adaptive Precision**
Session-4 **Integration of (S+D+L) (II)**	**1600-1640, Dec03**	**1500-1540, Dec03**	**0800-0840, Dec03**	**0200-0240, Dec03**	**2300-0340, Dec02**	**Gerhard Wellein (FAU Erlangen)**
	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Kengo Nakajima (U.Tokyo): Earthquake
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hiromichi Nagao (U.Tokyo)
	1720-1740	1620-1640	0920-0940	0320-0340	2420-2440	Hisashi Yashiro (NIES, Japan)
	1740-1800	1640-1700	0940-1000	0340-0400	2440-2500	Hiroya Matsuba (U.Tokyo)
	1800-1810	1700-1710	1000-1010	0400-0410	2500-2510	Closing

	JST: Japan	CTT: Taiwan	CET: Germany	EST: Atlanta	PST: Berkeley	Speaker
Session-1 **Adaptive Precision, AT & Verification (I)**	0800-0830, Nov30	0700-0730, Nov30	0000-0030, Nov30	1800-1830, Nov29	1500-1530, Nov29	Kengo Nakajima (U.Tokyo): Overview
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	0850-0910	0750-0810	0050-0110	1850-1910	1650-1710	Masatoshi Kawai (U.Tokyo)
	0910-0950	0810-0850	0110-0150	1910-1950	1710-1750	Rich Vuduc (Georgia Tech)
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	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Takashi Shimokawabe (U.Tokyo)
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hayato Shiba (U.Tokyo)
	1720-1800	1620-1700	0920-1000	0320-0400	2420-2500	Weichung Wang (National Taiwan U)
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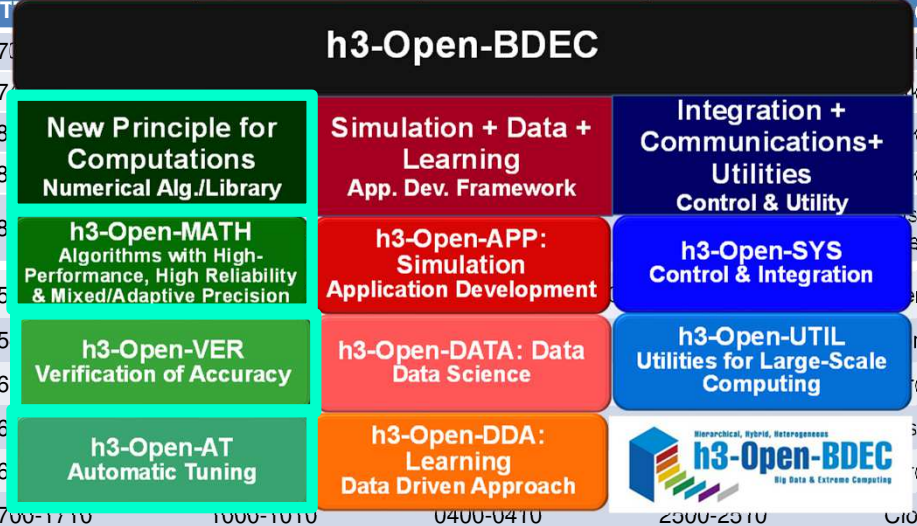
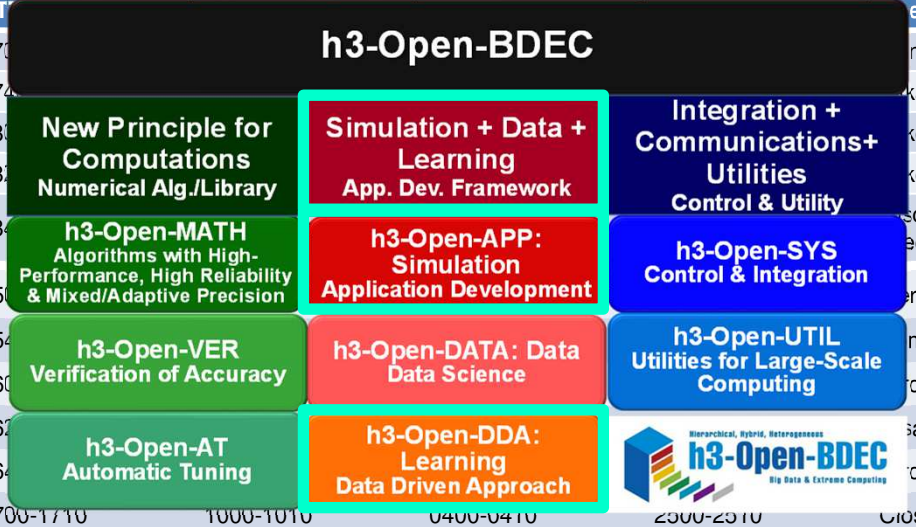
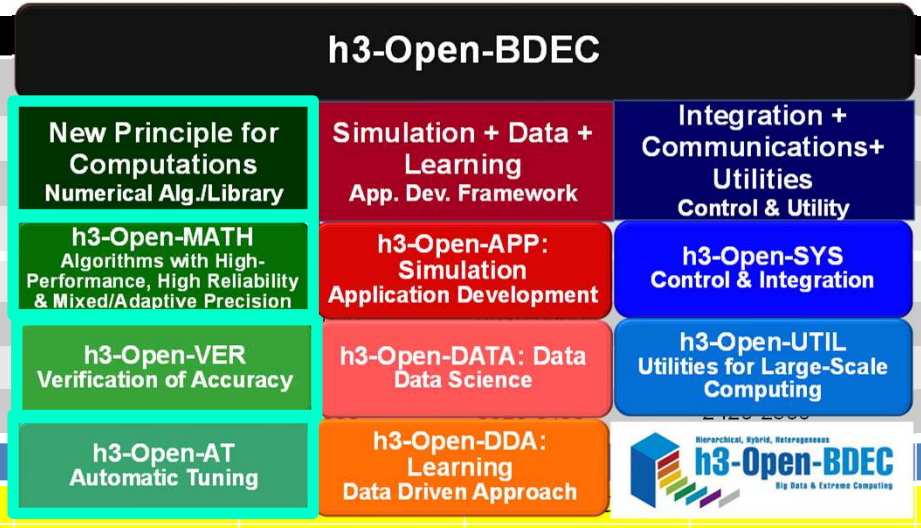
	0800-0840, Dec03	07				ni Marques (LBNL)
	0840-0900	07				kahiro Katagiri (Nagoya U.)
	0900-0920	08				keshi Ogita (TWCU)
	0920-0940	08				keshi Fukaya (Hokkaido U.)
	0940-1020	08				scussions on Computing by Low/Adaptive ecision
Session-4 **Integration of (S+D+L) (II)**	1600-1640, Dec03	15				rhard Wellein (FAU Erlangen)
	1640-1700	15				ngo Nakajima (U.Tokyo): Earthquake
	1700-1720	16				omichi Nagao (U.Tokyo)
	1720-1740	16				sashi Yashiro (NIES, Japan)
	1740-1800	16				oya Matsuba (U.Tokyo)
	1800-1810	1700-1710	1000-1010	0400-0410	2300-2310	Closing

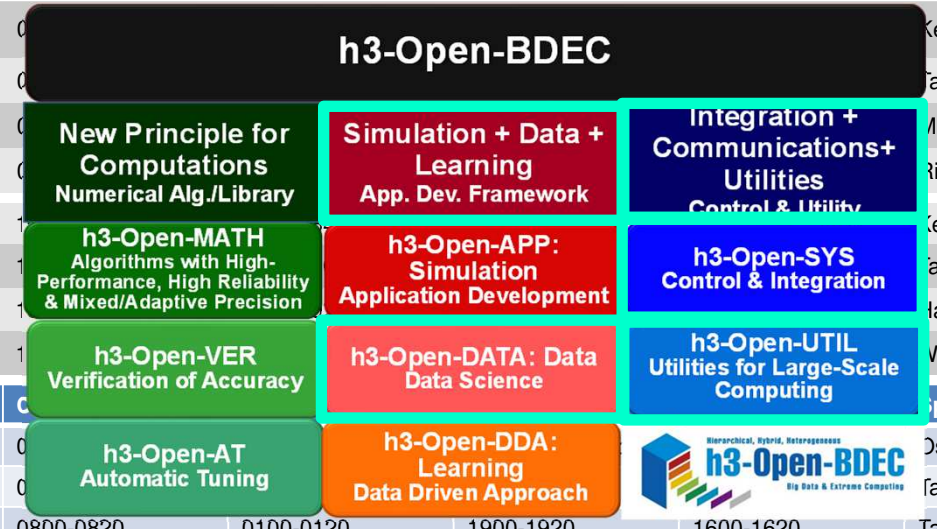


	JST: Japan	CTT: Taiwan	CET: Germany	EST: Atlanta	PST: Berkeley	Speaker
Session-1 **Adaptive Precision, AT & Verification (I)**	0800-0830, Nov30	0700-0730, Nov30	0000-0030, Nov30	1800-1830, Nov29	1500-1530, Nov29	Kengo Nakajima (U.Tokyo): Overview
	0830-0850	0730-0750	0030-0050	1830-1850	1530-1550	Takeshi Iwashita (Hokkaido U.)
	0850-0910	0750-0810	0050-0110	1850-1910	1650-1710	Masatoshi Kawai (U.Tokyo)
	0910-0950	0810-0850	0110-0150	1910-1950	1710-1750	Rich Vuduc (Georgia Tech)
Session-2 **Integration of (S+D+L) (I)**	1600-1640, Nov30	1500-1540, Nov30	0800-0840, Nov30	0200-0240, Nov30	2300-2340, Nov29	Kento Sato (RIKEN)
	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Takashi Shimokawabe (U.Tokyo)
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hayato Shiba (U.Tokyo)
	1720-1800	1620-1700	0920-1000	0320-0400	2420-2500	Weichung Wang (National Taiwan U)
Session-3 **Adaptive Precision, AT & Verification (II)**	JST: Japan	CT				eaker
	0800-0840, Dec03	07				ni Marques (LBNL)
	0840-0900	07				kahiro Katagiri (Nagoya U.)
	0900-0920	08				keshi Ogita (TWCU)
	0920-0940	08				keshi Fukaya (Hokkaido U.)
	0940-1020	08				scussions on Computing by Low/Adaptive ecision
Session-4 **Integration of (S+D+L) (II)**	1600-1640, Dec03	15				rhard Wellein (FAU Erlangen)
	1640-1700	15				ngo Nakajima (U.Tokyo): Earthquake
	1700-1720	16				omichi Nagao (U.Tokyo)
	1720-1740	16				sashi Yashiro (NIES, Japan)
	1740-1800	16				oya Matsuba (U.Tokyo)
	1800-1810	1700-1710	1000-1010	0400-0410	2300-2310	Closing





	JST: Japan					Speaker
Session-1 Adaptive Precision, AT & Verification (I)	0800-0830, Nov30					Kengo Nakajima (U.Tokyo): Overview
	0830-0850					Takeshi Iwashita (Hokkaido U.)
	0850-0910					Masatoshi Kawai (U.Tokyo)
	0910-0950					Rich Vuduc (Georgia Tech)
Session-2 Integration of (S+D+L) (I)	1600-1640, Nov30					Kento Sato (RIKEN)
	1640-1700					Takashi Shimokawabe (U.Tokyo)
	1700-1720					Hayato Shiba (U.Tokyo)
	1720-1800					Weichung Wang (National Taiwan U)
Session-3 Adaptive Precision, AT & Verification (II)	JST: Japan					Speaker
	0800-0840, Dec03					Osni Marques (LBNL)
	0840-0900	0740-0800	0040-0100	1840-1900	1540-1600	Takahiro Katagiri (Nagoya U.)
	0900-0920	0800-0820	0100-0120	1900-1920	1600-1620	Takeshi Ogita (TWCU)
	0920-0940	0820-0840	0120-0140	1920-1940	1620-1640	Takeshi Fukaya (Hokkaido U.)
	0940-1020	**0840-0920**	**0140-0220**	**1940-2020**	**1640-1720**	**Discussions on Computing by Low/Adaptive Precision**
Session-4 Integration of (S+D+L) (II)	1600-1640, Dec03	1500-1540, Dec03	0800-0840, Dec03	0200-0240, Dec03	2300-0340, Dec02	Gerhard Wellein (FAU Erlangen)
	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Kengo Nakajima (U.Tokyo): Earthquake
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hiromichi Nagao (U.Tokyo)
	1720-1740	1620-1640	0920-0940	0320-0340	2420-2440	Hisashi Yashiro (NIES, Japan)
	1740-1800	1640-1700	0940-1000	0340-0400	2440-2500	Hiroya Matsuba (U.Tokyo)
	1800-1810	1700-1710	1000-1010	0400-0410	2500-2510	Closing



	JST: Japan	CTT: Taiwan	CET: Germany	EST: Atlanta	PST: Berkeley	Speaker
Session-1 Adaptive Precision, AT & Verification (I)	0800-0830, Nov30	0				Kengo Nakajima (U.Tokyo): Overview
	0830-0850	0				Takeshi Iwashita (Hokkaido U.)
	0850-0910	0				Masatoshi Kawai (U.Tokyo)
	0910-0950	0				Rich Vuduc (Georgia Tech)
Session-2 Integration of (S+D+L) (I)	1600-1640, Nov30	1				Kento Sato (RIKEN)
	1640-1700	1				Takashi Shimokawabe (U.Tokyo)
	1700-1720	1				Hayato Shiba (U.Tokyo)
	1720-1800	1				Weichung Wang (National Taiwan U)
Session-3 Adaptive Precision, AT & Verification (II)	JST: Japan	C				Speaker
	0800-0840, Dec03	0				Osni Marques (LBNL)
	0840-0900	0				Takahiro Katagiri (Nagoya U.)
	0900-0920	0800-0820	0100-0120	1900-1920	1600-1620	Takeshi Ogita (TWCU)
	0920-0940	0820-0840	0120-0140	1920-1940	1620-1640	Takeshi Fukaya (Hokkaido U.)
	0940-1020	0840-0920	0140-0220	1940-2020	1640-1720	Discussions on Computing by Low/Adaptive Precision
Session-4 Integration of (S+D+L) (II)	1600-1640, Dec03	1500-1540, Dec03	0800-0840, Dec03	0200-0240, Dec03	2300-0340, Dec02	Gerhard Wellein (FAU Erlangen)
	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Kengo Nakajima (U.Tokyo): Earthquake
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hiromichi Nagao (U.Tokyo)
	1720-1740	1620-1640	0920-0940	0320-0340	2420-2440	Hisashi Yashiro (NIES, Japan)
	1740-1800	1640-1700	0940-1000	0340-0400	2440-2500	Hiroya Matsuba (U.Tokyo)
	1800-1810	1700-1710	1000-1010	0400-0410	2500-2510	Closing

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	0830-0850	0730-0750	0030-0050	1830-1850	1530-1550	Takeshi Iwashita (Hokkaido U.)
	0850-0910	0750-0810	0050-0110	1850-1910	1650-1710	Masatoshi Kawai (U.Tokyo)
	0910-0950	0810-0850	0110-0150	1910-1950	1710-1750	Rich Vuduc (Georgia Tech)
Session-2 **Integration of (S+D+L) (I)**	1600-1640, Nov30	1500-1540, Nov30	0800-0840, Nov30	0200-0240, Nov30	2300-2340, Nov29	Kento Sato (RIKEN)
	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Takashi Shimokawabe (U.Tokyo)
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hayato Shiba (U.Tokyo)
	1720-1800	1620-1700	0920-1000	0320-0400	2420-2500	Weichung Wang (National Taiwan U)
Session-3 **Adaptive Precision, AT & Verification (II)**	**JST: Japan**	**CTT: Taiwan**	**CET: Germany**	**EST: Atlanta**	**PST: Berkeley**	**Speaker**
	0800-0840, Dec03	0700-0740, Dec03	0000-0040, Dec03	1800-1840, Dec02	1500-1540, Dec02	Osni Marques (LBNL)
	0840-0900	0740-0800	0040-0100	1840-1900	1540-1600	Takahiro Katagiri (Nagoya U.)
	0900-0920	0800-0820	0100-0120	1900-1920	1600-1620	Takeshi Ogita (TWCU)
	0920-0940	0820-0840	0120-0140	1920-1940	1620-1640	Takeshi Fukaya (Hokkaido U.)
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	1640-1700	1540-1600	0840-0900	0240-0300	2340-2400	Kengo Nakajima (U.Tokyo): Earthquake
	1700-1720	1600-1620	0900-0920	0300-0320	2400-2420	Hiromichi Nagao (U.Tokyo)
	1720-1740	1620-1640	0920-0940	0320-0340	2420-2440	Hisashi Yashiro (NIES, Japan)
	1740-1800	1640-1700	0940-1000	0340-0400	2440-2500	Hiroya Matsuba (U.Tokyo)
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