

# 【Grant-in-Aid for Scientific Research (S)】

## Broad Section J



### Title of Project : Innovative Methods for Scientific Computing in the Exascale Era by Integrations of (Simulation+Data+ Learning)

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Keyword : Supercomputing, Data Assimilation, Machine Learning, Integration of (Simulation+Data+Learning)

#### 【Purpose and Background of the Research】

The performance of the fastest supercomputer will reach Exa-FLOPS ( $10^{18}$  Floating point Operations Per Second) in 2021. Towards the end of Moore's law, we need to develop not only new hardware, but also new algorithms and applications. In this study, we propose an innovative method for computational science 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.

#### 【Research Methods】

The BDEC system (Big Data & Extreme Computing), which is scheduled to be introduced to the Information Technology Center, the Tokyo University in 2021, is a Hierarchical, Hybrid, Heterogeneous (h3) system, which consists of computing nodes for computational science and those for data science/machine learning. In this study, we consider the BDEC as the platform for integration of (S+D+L), develop an innovative software platform “h3-Open-BDEC” for integration of (S+D+L), and evaluate the effects of integration of (S+D+L) on the BDEC. The h3-Open-BDEC (Figure 1) is designed for extracting the maximum performance of the supercomputers with minimum energy consumption focusing on (1) innovative method for numerical analysis with high-performance/high-reliability/power-saving based on the new principle of computing by adaptive precision, accuracy verification and automatic tuning, and (2) Hierarchical Data Driven Approach (hDDA) based on machine learning.

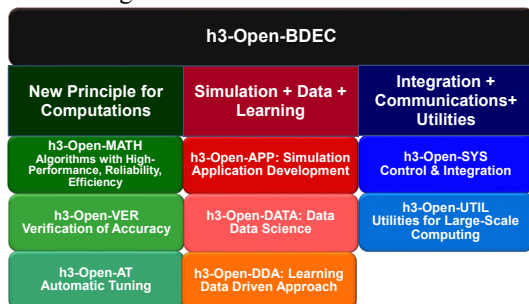


Figure 1 Overview of h3-Open-BDEC

In Data Driven Approach (DDA), technique of machine learning is introduced for predicting the results of simulations with different parameters. DDA generally requires a lot of simulations for generation of teaching data. We propose the hDDA, where simplified models for generating teaching data are constructed automatically by

machine learning with Feature Detection, MOR, UQ, Sparse Modeling and AMR (Figure 2)

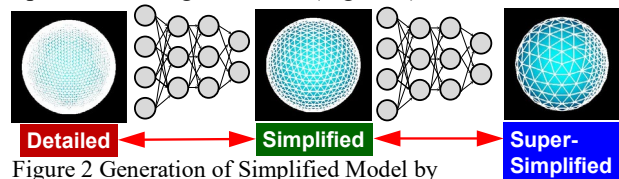


Figure 2 Generation of Simplified Model by Hierarchical DDA (hDDA)

#### 【Expected Research Achievements and Scientific Significance】

The h3-Open-BDEC is the first innovative software platform to realize integration of (S+D+L) on supercomputers in the Exascale Era, where computational scientists can achieve such integration without supports by other experts. Source codes and documents are open to public for various kinds of computational environments. This integration by h3-Open-BDEC enables significant reduction of computations and power consumptions, compared to those by conventional simulations.

#### 【Publications Relevant to the Project】

- K. Nakajima, T. Furumura, T. Iwashita, T. Katagiri et al., ppOpen-HPC: Open Source Infrastructure for Development and Execution of Large-Scale Scientific Applications on Post-Peta-Scale Supercomputers with Automatic Tuning (AT), Mathematics for Industry 13, 15-35, Springer, 2015
- K. Fujita, T. Ichimura, K. Nakajima et al., Wave propagation simulation of complex multi-material problems with fast low-order unstructured finite-element meshing and analysis, ACM Proceedings of HPC Asia 2018, 2018 (Best Paper Award)

#### 【Term of Project】 FY2019-2023

#### 【Budget Allocation】 152,700 Thousand Yen

#### 【Homepage Address and Other Contact Information】

<http://nkl.cc.u-tokyo.ac.jp/h3-Open-BDEC>  
<https://github.com/Post-Peta-Crest/ppOpenHPC>