jh170058-NAHI

Takeo Hoshi (Tottori University)

Development of next-generation quantum material research platform

Overview

- The present project aims an international collaboration, mainly between Japan and USA, for developing the next-generation quantum material research 'platform'.
- The platform contains several scalable quantum material simulators and data scientific analyzers.
- We will concentrate on developing software components that can be used commonly with simulators.
- The platform will be built on Oakforest-PACS.
- An international workshop is planned on 4. Dec. at U Tokyo.

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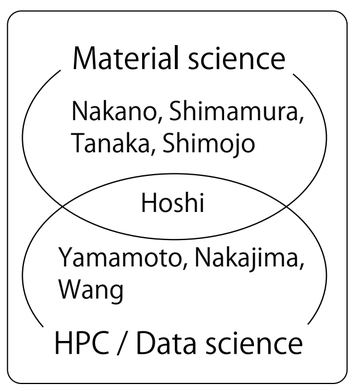
Members

→interdisciplinary among material science and HPC/data science

Leader
Takeo Hoshi (Tottori U)
Deputy Leaders
Aiichiro Nakano
(U South California)
Yusaku Yamamoto
(U Elec. Comm.)
Other members (except students)
Kengo Nakajima (U Tokyo)
Kohei Shimamura (Kobe U)
Shigenori Tanaka (Kobe U)
Fuyuki Shimojo (Kumamoto U)
Weichung Wang
(National Taiwan U)



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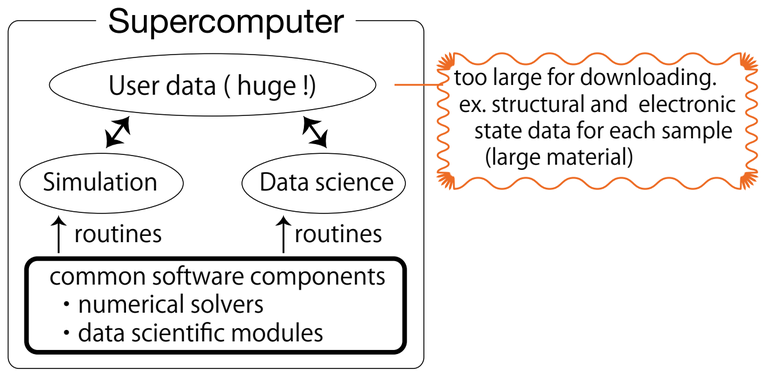
Concept

→The whole research activity, simulation and data science, are carried out on a supercomputer



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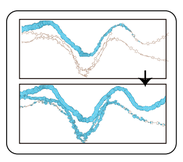
Basics of software components

Fortran (+MPI+OpenMP)
→ numerical linear algebraic solver
ex. our code: EigenKernel (https://github.com/eigenkernel/)
→ generalized real-symmetric eigenvalue problem
H. Imachi and T. Hoshi, J. Inf. Process. 24, 164 (2016)
H. Imachi D. Thesis, Tottori U, Mar. 2017.

Python (+mpi4py)
→ Pre/post simulation tools,
• data scientific analysis (module : sci-kit learn)
• 3D visualization (module : VTK)
ex. our code: VisBAR (https://github.com/visbar/)
→ batch visualization (off-screen rendering) for quantum wave dynamics →
• other data analysis
(module: numpy, scipy, matplotlib and so on ..)
Note: All the Python modules are preinstalled on Oakforest-PACS, except VTK



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Large-scale quantum material simulator (1) : ELSES

Paper and URL: T. Hoshi, H. Imachi, K. Kumahata, M. Terai, K. Miyamoto, K. Minami and F. Shoji, Proc. ScalA16 in SC16, pp.33-40 (2016); http://www.elses.jp/
Method: Order-*N* algorithm by the shifted Krylov-subspace theory, based on the Green function formalism in electronic states / *Ab initio* based modelled (transferable TB) theory

Fig. (a) Strong scaling bench mark of 10^8-atom condensed organic polymers on the K computer

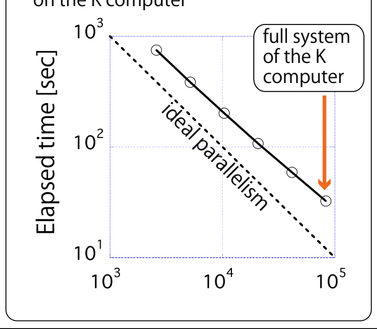
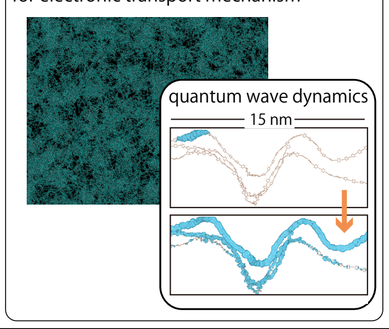


Fig. (b) Research example: 10^8-atom (100nm-scale) condensed organic polymers for electronic transport mechanism



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Large-scale quantum material simulator (2) : LDC-DFT

Recent paper: K. Shimamura, F. Shimojo, A. Nakano, and S. Tanaka, Scientific Reports 6, 38953 (2016).
Method: Order-*N* first-principle quantum material simulator (LDC-DFT=Lean Divide-and-Conquer Density Functional Theory)

Fig. (a) Strong scaling bench mark of 77,889-atom LiAl-water systems on Blue/Gene Q

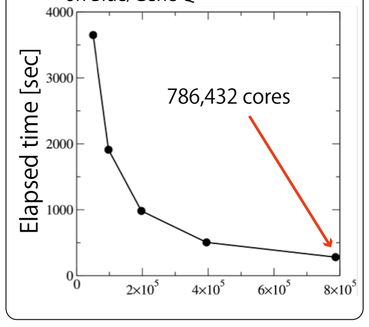
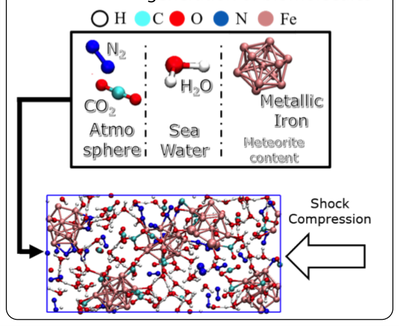


Fig. (b) Research example: 'Origin of life'; Simulation for meteorite shock-induced generation of biomolecules



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Organic polymer research as a combined research between large-scale simulaiton and data science (1)

Background : organic material
- The foundation of ultra-flexible device or the next-generation Internet of Things (IoT) products, like display, lightening device, sensor and battery
- The structural disorder in organic polymer is crucial for device performance or the mobility (Terao et al, Nat. Commun. 4, 1691(2013))

Fig. Examples of organic material devices:
(a) Sumitomo Chemical Co. (b) Sony (c) U. Tokyo. (d) Konika Minolta

(a) https://www.sumitomo-chem.co.jp/english/pled/about.html
(b) https://www.sony.net/SonyInfo/News/Press/201005/10-070E/
(c) Yokota, et al., Sci. Adv. 2, e1501856 (2016).
(d) Watanabe, et al., KONICA MINOLTA TEC. REP. 13, 16 (2016)

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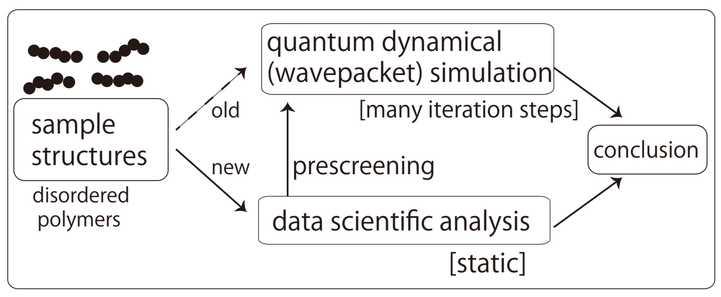
Organic polymer research as a combined research between large-scale simulation and data science (2)

Strategy for data science
- The device performance (mobility) can be estimated by the quantum wave dynamics simulation, like p.4 Fig(b), but the simulation requires many iteration steps for the real-time evolutions.
- The present research gives a data scientific analysis as a prescreening procedure, so as to choose 'hopeful' samples among disordered polymers



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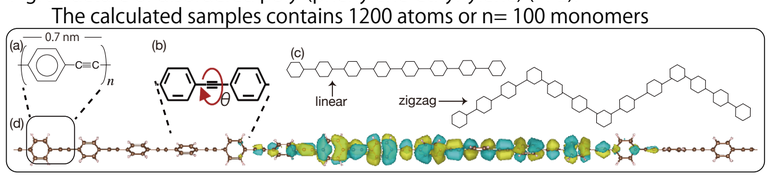
Organic polymer research as a combined research between large-scale simulation and data science (3)

Procedures of data scientific analsys
Step 1. Prepare 40,000 samples of disordered organic polymer with 1200 atoms for poly-(phenylene-ethynylene) (PPE) (See the below figure)
Step 2. Calculate the electronic states for each polymer by ELSES
Step 3. Calculate the participation ratio, a measure for the spatial extentaion, for each wavefunction.
→ descriptors in the data scientific analysis
Step 4. Solve the classification problem of the 40,000 samples by the k-means clustering method (not shown) or the principle component analysis (See the next page)

Fig. Structure of disordered poly-(phenylene-ethynylene) (PPE). The calculated samples contains 1200 atoms or n= 100 monomers



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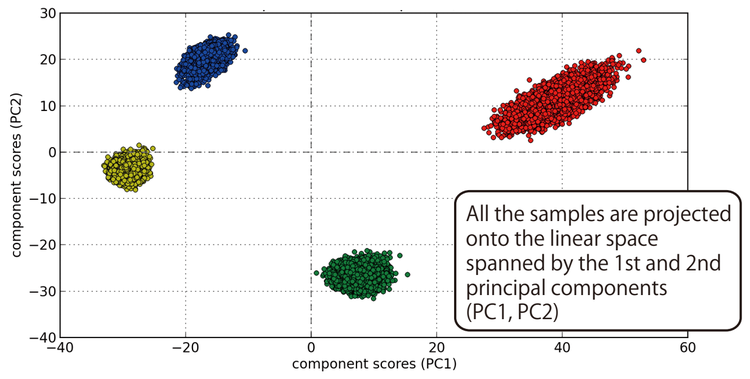
Organic polymer research as a combined research between large-scale simulation and data science (4)

As a result, the principal component analysis classify, successfully, the 40,000 samples into the four groups, as expected.



Note: The organic polymer research of pp.6-9 was carried out in the collaboration with Koji Hukusima (U. Tokyo) and Hiroto Imachi (Tottori U; The current affliation: Preferred Networks Inc.);
H. Imachi et al., ASIAN19, Taiwan, Oct. (2016); H. Imachi, D. Thesis, Tottori U, Mar. (2017);
T. Hoshi et al., JPS meeting, Mar. (2017) and Sep. (2017); Paper in preparation.