

eHPC2017

Workshop on e-Science and High Performance Computing

About eHPC

eHPC is a one day workshop aiming to bring together a community of researchers, developers, practitioners, and user involved with e-Science and high performance computing technology from both academic institutions and industries to discuss and exchange ideas. The objectives of the workshop are to build collaborations for interdisciplinary research, and to increase the awareness on technological advancement in e-science and HPC fields. The event will offer technical paper presentations, invited talks, discussions, and technology demonstrations by the e-Science and HPC communities.

Areas of interest include but not limited to e-Science applications, infrastructure and services; cloud computing; data analytic; scientific computing applications and tools. eHPC2017 is organized in conjunction with JCSSE 2017.

Who can attend

Anyone who are interested in e-Science and High Performance Computing are welcome to join this seminar

Date and Venue

July 13, 2017 (11:00-17:00 hrs.) at Oraphin room, Twin Lotus Hotel, Nakhon Si Thammarat

Program for eHPC2017

*eHPC seminar will be started after JCSSE's keynote speakers (09:00-11:00hrs)

Time	Session
08:30-09:00	Registration
09:00-10:40	JCSSE's keynote I / JCSSE's keynote II
10:40-11:00	Break
eHPC2017 : Room Oraphin 2	
11:00-11:15	<ul style="list-style-type: none">• Welcome Message <i>by Asst. Prof. Dr.Putchong Uthayopas</i>• Opening Remark <i>by Dr. Sarun Sumriddetchkajorn</i>
11:15-12:30	Panel discussion: Integrating HPC, Cloud, Data Analytic and Scientific Computing <u>Invited Moderator:</u> <i>Dr.Piyawut Srichaikul (NECTEC)</i> <u>Invited Panelists:</u> 1. <i>Asst.Prof.Dr.Putchong Uthayopas</i> <i>(Kasetsart University)</i> 2. <i>Dr. Adisak Srinakaran</i> <i>(Executive Vice President, EGA)</i> 3. <i>Asst.Prof.Dr.Natawut Nupairoj</i> <i>(Chulalongkorn University)</i>
12:30-13:30	Lunch (1 hr)

Time	Session
13:30-14:00	Invited Speaker 1: Energy Function for Grain Boundary in Body-Centered Cubic Metals by Mr. Rajchawit Sarochowikarit (King Mongkut's University of Technology)
14:00-14:30	Invited Speaker 2: Cloud Caching by Dr. Thepparit Banditwattanawong (Kasetsart University)
14:30-14:45	Technology Update by Acer, Thailand
14:45-15:00	Break (15 mins)
15:00-15:30	Invited Speaker 3: Shift/Collapse on Neighbor List: An Algorithm for Fast and Scalable Dynamic Many-Body Potential Molecular Dynamics Simulation by Dr. Manaschai Kunaseth (NANOTEC)
15:30-16:00	Invited Speaker 4: Astronomical Big Data with Gravitational-wave Optical Transient Observer (GOTO) By Dr. Utane Sawangwit (National Astronomical Research Institute of Thailand)
16:00-16:30	Invited Speaker 5: Ecoinformatics Applications in the IoT and Cloud Era by Assoc.Prof.Krisanadej Jaroensutasinee (Walailak University)
16:30-16:45	Closing Ceremony by e-Science Project manager

About each session

Panel discussion: Integrating HPC, Cloud, Data Analytic and Scientific Computing

How is this?

"High Performance Computing", "Cloud Computing", "Scientific Computing" and "Data Analytics": these 4 terms were born in separate timeframe and yet they co-exist today. How are they different or how are they alike? What will be the future of them?

The seminar should touch on

- historical background on each of them
- their transformation, then and now
- their characters and suitability
- their ecosystems
- their roles in the big picture, enterprises, society, social and economics impact
- and their future

Invited Talks: Abstracts

Energy Function for Grain Boundary in Body-Centered Cubic Metals

Mr. Rajchawit Sarochowikarit

King Mongkut's University of Technology

This research presents a large-scale calculations of grain boundary energies in body-centered cubic (bcc) metals, Fe, Ta, Mo, and W, are calculated based on the atomistic simulation. We construct 408 distinct grain boundaries for each metal. The characteristics of a large set of grain boundaries are composed of 127 tilt, 24 twist, and 257 mixed boundaries. This indicates that the energies of these grain boundaries in the bcc metals are strongly correlated,

although the microscopic configurations are not essentially the same. We conclude that the grain boundary energies in the bcc metals might have a universal characteristic, which is scaled to fit between coherent twin energy and cohesive energy.

Cloud caching

Dr. Thepparit Banditwattanawong,
Kasetsart University

Big data has been increasingly hosted in off-premise clouds, for example, high-definition multimedia, electronic documents, social media contents, opensource packages, and cloud-hosted web contents. This is because cloud enables not only fast and economical big data analytics but also highly-scalable and distributed sharing of the data. This is the evolution of data volume, data placement and data consumption behavior that altogether has led to several cloud-computing problems including the downstream bandwidth saturation, increase in external cloud data-out charge imposed by public cloud providers, and delayed cloud service responsiveness.

To address these problems, we would present the consumer-initiated partial replication of cloud-hosted data to consumer locus. We refer to this solution as client-side cloud caching.

Shift/Collapse on Neighbor List: An Algorithm for Fast and Scalable Dynamic Many-Body Potential Molecular Dynamics Simulation

Dr. Manaschai Kunaseth,
National Nanotechnology Center (NANOTEC)
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Reactive Molecular dynamics (ReMD) allowing dynamic many-body bond formation and breakage requires significantly more computation power compared to the conventional static bond method. Recently, we developed a shift/collapse (SC) algorithm, a novel MD computation algorithm that utilizes optimal communication scheme for n -tuple interaction, which significantly improves computation performance of ReMD [1]. Nevertheless, the original SC algorithm is incompatible with force computation based on neighbor list, which is a commonly used method for reactive potentials such as embedded-atom method (EAM), bond-order potentials (BOD), and reactive force fields (ReaxFF).

In this work, we have presented a new neighbor list-based force computation scheme for SC algorithm (NBL-SC), which enable both fast computation based on the commonly used neighbor-list method and the optimal communication scheme of SC algorithm. Implementation of the new method has been verified and the simulation results have been validated using a force fields with 2- and 3-body bond-breakable interactions. Here, performance benchmark showed significant simulation performance improvement of NBL-SC over the original SC algorithm with 1.33x and 3.29x speedups on small and large granularities (24 and 24,000 atoms per compute core), respectively. Large-scale benchmark also indicated simulation performance of up to 267 ns/day for grain size of 24 atoms/core on 1,296 cores of Intel Xeon processors. This ongoing work highlighted an important step towards highly efficient parallel MD algorithm for reactive MD simulation.

[1] Kunaseth *et al.*, A Scalable Parallel Algorithm for Dynamic Range-Limited n -Tuple Computation in Many-Body Molecular Dynamics Simulation, *Supercomputing SC13*, ACM, New York, NY (2013)

Astronomical Big Data with Gravitational-wave Optical Transient Observer (GOTO)

Dr. Utane Sawangwit

National Astronomical Research Institute of Thailand

To be update

Ecoinformatics Applications in the IoT and Cloud Era

Assoc.Prof.Dr. Krisanadej Jaroensutasinee

Center of Excellence for Ecoinformatics, Walailak University - NECTEC

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Ecoinformatics are applications of informatics to the field of Ecology to understand, monitor and manage efficiently. We have been working in this area ranging from underwater to cloud forest ecosystems with various types of sensor and various type of networking architectures. A number of Ecoinformatics applications such as coral sensor network, sound scape, tourism portal, smart farming and cloud-based smart city portal, in the recent developments of Cloud and IoT, will be discussed.

Registration

Advanced registration is not required, but due to the limited capacity, please reserve your seats by email to contact@e-Science.in.th

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