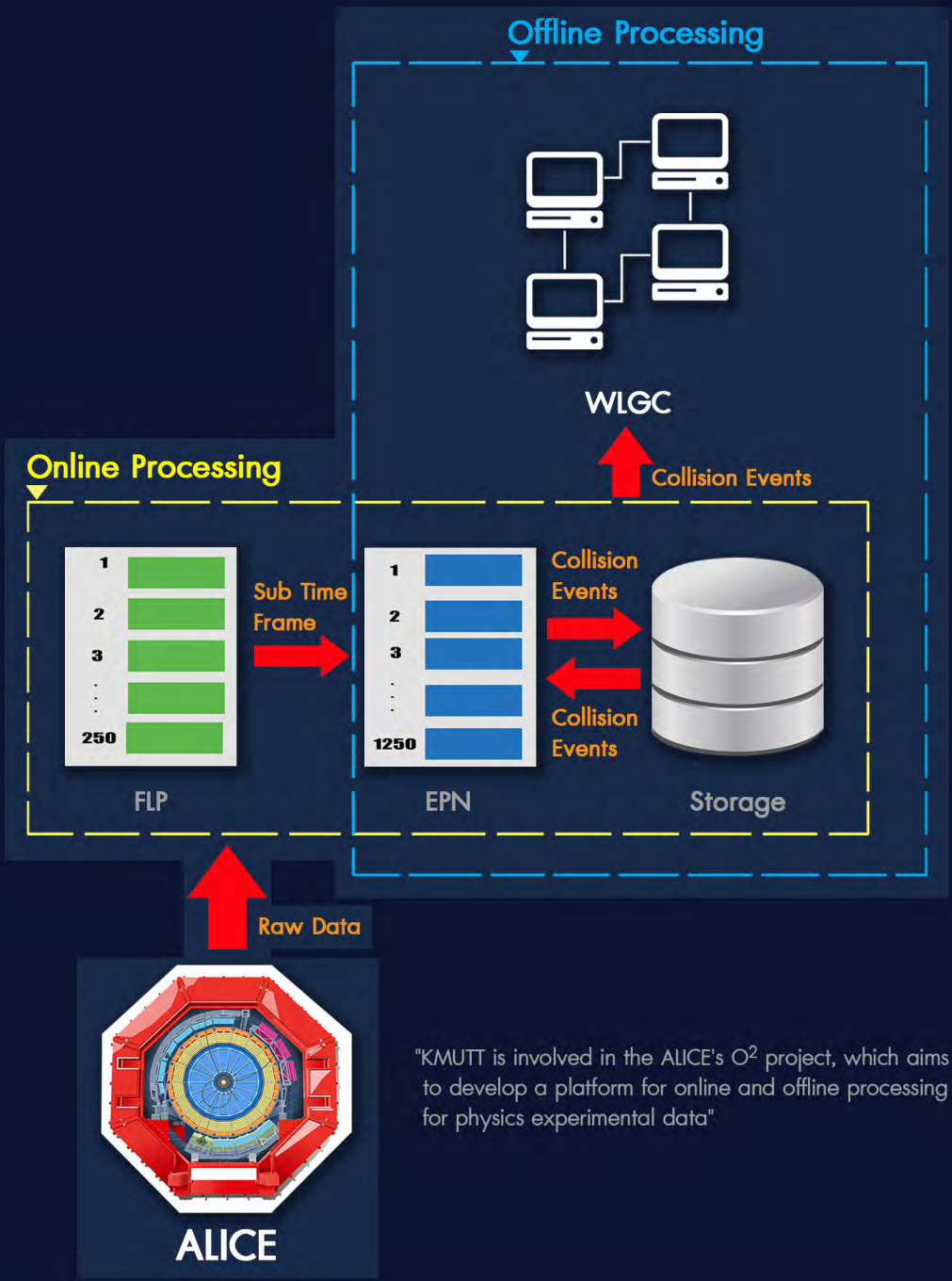
National e-Science Infrastructure Consortium

# e-Science 2015

www.e-science.in.th



" The image of NGC2207 and IC2163, two colliding spiral galaxies at 80 million light-year away from us, taken with the 2.4m Thai National Telescope, Chiang Mai. "




"KMUTT is involved in the ALICE's $O^2$ project, which aims to develop a platform for online and offline processing for physics experimental data"



# e-Science 2015

This booklet gives an overview information of National e-Science Infrastructure Consortium including the motivations, the current status and the achievements of the consortium. Short introduction to each member institutes, the research groups, and, the available computing resources are included.

Readers who are interested in participating in the consortium either as a member to contribute computing resources or as a researcher to utilize the computing resource for research should kindly contact the consortium office.



## Message from Prof. Pairash Thajchayapong
### Advisor of Steering Committee
### National e-Science Infrastructure Consortium

H.R.H. Princess Maha Chakri Sirindhorn has graciously initiated the collaboration between Thai scientists and the European Organization for Nuclear Research (CERN) on High Energy Physics. The significance of this collaboration is that it shows the capability of Thai scientists to participate in the world class scientific research and it raises Thai public awareness of the importance of basic scientific research. This cooperation opens up many opportunities for example for students, high school and university levels, to visit CERN laboratories, training for physics teachers, and, organizations of summer schools in Thailand. This also inspires domestic scientific research and educational collaborations including the foundation of National e-Science Infrastructure Consortium. Since its establishment in 2011, the consortium has played a significant role to support the collaboration with CERN. The consortium has formally entered the Worldwide LHC Computing Grid (WLCG) Collaboration led by CERN in 2013, and, has been operating three WLCG Tier 2 sites, which provide computing resources for data storage and analysis. More than 13 High Energy Physics research projects have been conducted under the collaboration with the Compact Muon Solenoid (CMS) experiment and the A Large Ion Collider Experiment (ALICE) of CERN.

Through our engagement with international and domestic collaborations, I hope we develop technical capabilities as well as leadership and skills for teamwork. The success of the consortium has been achieved through the open mindedness and hard working of its members. And, I would like to encourage all members to keep this spirit of sharing continue for our mutual long term benefit.

P. Thajchayapong

Pairash Thajchayapong, Ph.D.



## Message from Dr. Thaweesak Koanantakool
### Chair of Steering Committee
### National e-Science Infrastructure Consortium

The National e-Science Infrastructure Consortium aims to develop a sustainable research infrastructure relating high performance computers, storage systems and fundamental datasets for Thailand. The members collaboratively contribute to this infrastructure by investing in their resources and sharing them. This approach is believed to be sustainable, efficient and most suitable for shared resource development and open innovation is a developing country like Thailand.

Since its establishment in 2011, the consortium has provided computing services to 105 science research projects, producing 250 publications and 26 graduate students. To support this objective, our members continuously invested in the computing resources. In 2014, the total number of CPU cores has increased to more than 2,500 cores and the storage capacity reached 600 Terabytes. The number of projects utilizing our resource in each year has grown from 34 to 49 projects, and the number of publications per year has also grown from 40 to 86.

In 2014, the consortium has welcome a new regular member: the National Astronomical Research Institute of Thailand (Public Organization), and two associate members: The Center of Excellence for Ecoinformatics of Walailak University, and Faculty of Science of Kasetsart University.

Looking forward, I expect that this national computing resource pool will continue to grow in size and activities to produce more output and impact. An exciting new area is Big Data and Analytics. Our consortium will try to facilitate data sharing and encourage researchers to investigate and develop new algorithms for analyzing the data. Finally, I wish to thank all members for actively working together over the past years and look forward to more successful collaborations.



Hugh T. Koanantakool, Ph.D.













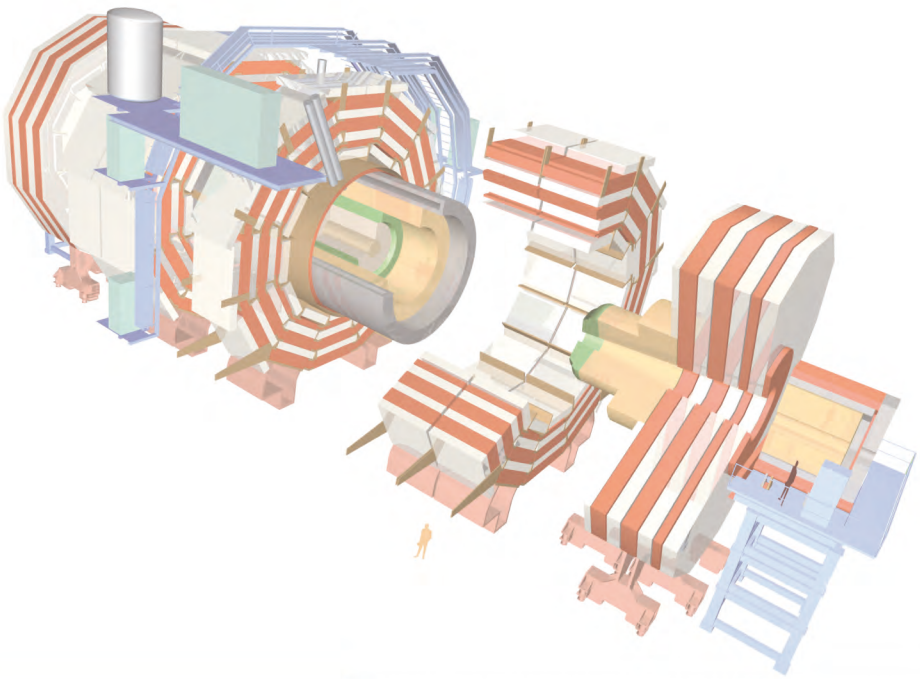
**WLCG MOU signing** between CERN and Chulalongkorn University, Suranaree University of Technology, and National Science and Technology Development Agency, October 2013

# Contents

**Message from Prof. Pairash Thajchayapong (Advisor of Steering Committee)**
**Message from Dr. Thaweesak Koanantakool (Chair of Steering Committee)**

Overview 8
e-Science Members 10
Resources 16
Virtual Organizations 20
- High Energy Particle Physic 21
- Computational Science and Engineering 24
- Computer Science and Engineering 28

Achievements 32
Committee and Working Groups 34
Contact Details 36



# Overview

High performance computing infrastructure in Thailand has been continuously developed by different groups of researchers and research institutes. National Electronics and Computer Technology Center (NECTEC) provided high performance computing service since 1995 to support computational science and engineering research. The objective is to stimulate the use of computational methods to complement theoretical and experimental approaches. Since then, research communities have developed around the development and application of high performance computing such as Thai Grid community and Computational Science and Engineering Association. In 2004, many organizations participated in Thai National Grid project, and, in 2008, NECTEC and HAII joined the EUAsiaGrid project which was partially supported by the European Commission. These efforts provided a good foundation for the development of National e-Science Infrastructure Consortium.

Following the leadership of Prof. Dr. Pairash Thajchayapong, the founding members agreed to form the National e-Science Infrastructure Consortium to collaboratively develop computing, data storage and fundamental datasets as a sustainable infrastructure to support research in Thailand. The computing resources are used to support research projects in the areas of Computational Science and Engineering, Computer Science and Engineering and High Energy Particle Physics.

The consortium has two types of membership, the Regular member and the Associated member. Regular members have committed to provide computing resources to the consortium and the institutional head of each Regular member is a member of Steering Committee. Associated members do not have to provide computing resources to the consortium but they have other contributions of collaboration with the consortium. They are not in the consortium Steering Committee.

The consortium founding members are Chulalongkorn University (CU), Suranaree University of Technology (SUT), King Mongkut's University of Technology Thonburi (KMUTT), Hydro and Agro Informatics Institute (HAII), and, National Science and Technology Development Agency (NSTDA). In addition to the founding members, the consortium has welcomed the National Astronomical Research Institute of Thailand (Public Organization) or NARIT as a regular member; and; the Center of Excellence for Ecoinformatics of Walailuk University, and, Faculty of Science of Kasetsart University as associated members.

## Objective

To collaboratively develop sustainable e-Science infrastructure for supporting research in Thailand while ensuring the quality of service and maximizing resource utilization efficiency




















## Chulalongkorn University

Chulalongkorn University is Thailand's first institution of higher education producing the finest quality graduates with a high level of knowledge and skills in the arts and sciences. The Particle Physics Research Laboratory at Chulalongkorn University is dedicated to experimental and theoretical high energy particle physics researches. It focuses on Super Symmetric extension of the Standard Model (SUSY), the search for Large Extra Dimensions of space (LED), Superstring theory and Supergravity.

Our group participates in large international collaborations that revolve around the CMS, particularly at the Large Hadron Collider (LHC) situated at CERN. We are involved in the CMS experiment as a part of SUSY, Higgs and Exotica Physics Analysis Groups. We are the first CMS Center in ASEAN for CMS operations, sub-detector data quality monitoring (DQM), and data analysis. We also offer visibility and awareness to the general public about the ongoing research at the LHC through an online event display of the activity of the CMS detector in real time.

The laboratory collaborates with NECTEC for the development of the CMS Tier 2 node of Thailand under e-Science Infrastructure Consortium.



# Hydro and Agro Informatics Institute

Hydro and Agro Informatics Institute (HAII), a public organization under the Ministry of Science and Technology, was originally established by the initiative of His Majesty the King Bhumibol Adulyadej, with support from MIT[1], RDPB[2] and TRF[3] aiming to develop a coherent plan to improve water resource management in Thailand. With agriculture as the backbone of Thailand's economy, HAII's researches on water resource management and agricultural practices have been increasingly notable.

Since 2010, HAII has maintained the High Performance Computing facilities that enable researches branching from intelligent monitoring systems, weather and flood modeling, simulation, information processing, and information dissemination that support the policy makers in coping with flood and drought management.

Active research areas include:

- Short-term precipitation prediction using the Weather Research and Forecasting Model (WRF) and Coupled Modeling Systems
- Wind-Wave prediction using Simulating WAve Near-shore (SWAN)
- Seasonal precipitation prediction using a hybrid between dynamical and statistical models.
- Hydrological and flood modeling.

[1] MIT - the Massachusetts Institute of Technology
[2] RDPB - the Office of the Royal Development Projects Board
[3] TRF - Thailand Research Fund



## King Mongkut's University of Technology Thonburi

King Mongkut's University of Technology Thonburi (KMUTT) is a technological university with a mission on education and research excellence. KMUTT aims to produce quality graduates who serve our community and contribute to the sustainability of Thailand economics and society. As one of the designated national research universities in Thailand, KMUTT is striving in commercializing products from campus in order to bring our research and development to the new height.

The research cluster and its researcher teams have participated in the National e-Science Infrastructure Consortium project under the Computer Science and Engineering Virtual Organization. Works on high performance computing and mobile sourcing platforms are performed in collaboration with the European Organization for Nuclear Research or CERN, Switzerland. The data and opinion mining and the 3D medical imaging engines are example research frameworks that results in publications, award winning software applications, and startup companies. Both engines are readily available commercially. Currently, the research cluster is expanding to include multidisciplinary research in the fields of bio-engineering and bioinformatics, Computation Fluid Dynamics, and particle physics simulation, just to name a few.

It has always been a belief of KMUTT that National e-Science Infrastructure Consortium will be an important platform that contributes to Thailand's competitiveness in the global economy. KMUTT computational Science and engineering research cluster will continue its mission in research and its support for Thailand's e-Science platform into the future.



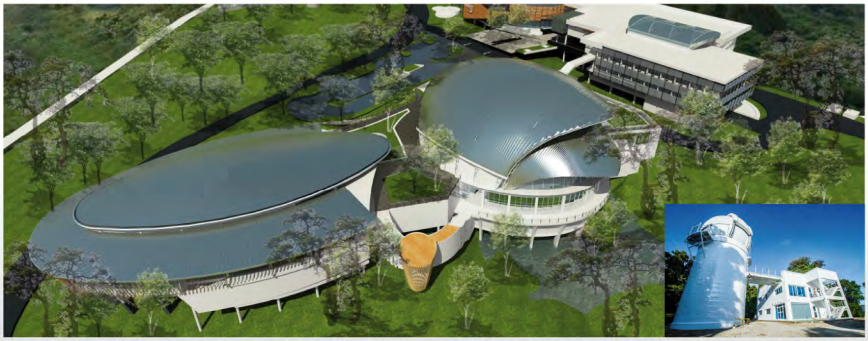
NARIT

## National Astronomical Research Institute of Thailand

National Astronomical Research Institute of Thailand (NARIT) is a public organization under the Ministry of Science and Technology. Our main missions are astronomical research, infrastructure development, public awareness and astronomy education. The organization has set its goal to increase the national astronomical research capability to that of the international community and to become the leader in the South East Asia region. We are also a key and a founding member of the South East Asian Astronomy Network or SEAAN.

NARIT owns and operates the 2.4-metre (currently the largest in South East Asia) Thai National Telescope (TNT) located on Doi Inthanon, Chiang Mai, Thailand. We also operate the remotely controlled 0.6-metre "PROMPT-8" telescope installed at Cerro Tololo Inter-American Observatory (CTIO), Chile, in collaboration with the University of North Carolina at Chapel Hill. The data obtained from these facilities are of great importance for astronomy that require properly managed and reliable database. Furthermore, the on-going researches at NARIT involve handling and analysis of big dataset as well as complicated modeling of astrophysical processes and simulations that require High Performance Computer (HPC) cluster. The computational astronomy at NARIT covers a wide range of subjects from stellar, extra-galactic astrophysics, astroclimate to cosmology. Many of these works are carried out in collaboration with our partner institutes both national and international.

Currently, NARIT HPC cluster is relatively small compared to other members of the consortium but we committed to increase the size of our e-Science infrastructure in the next few years, to ensure that the needs of national computational astronomical community are met.



NSTDA

## National Science and Technology Development Agency

NSTDA, under the administration of Ministry of Science and Technology, plans and executes four mandated missions: research and development, technology transfer, human resources development, and, infrastructure development. NSTDA is comprised of four national R&D centers: the National Center for Genetic Engineering and Biotechnology (BIOTEC), the National Metal and Materials Technology Center (MTEC), the National Electronics and Computer Technology Center (NECTEC) and the National Nanotechnology Center (NANOTEC). In addition, NSTDA reaches out to other research organizations and universities through joint collaboration, contracted research, and, other mechanisms to ensures the best resources are being captured for the country's innovation needs. To tie all these organizations together, the Technology Management Center (TMC) serves as a linkage between scientists and end users, and it provides applicable technology services.

NSTDA has played an important role in developing and applying high performance technology in Thailand. Its laboratories have been using computational approaches in research areas such as nanoscience, molecular biology, bio-informatics, engineering designs, and, environmental sciences. It is also very active in the areas of networking infrastructure, technology and application development. NSTDA also maintains a number of national scientific databases such as Genome Databases, Life Cycle Inventory Database, and, Annotated and Multimedia Corpus.



## Suranaree University of Technology

Suranaree University of Technology (SUT) was established as a state autonomous university, outside the civil service system, under the supervision of the Royal Thai Government, promoting administrative proficiency and efficiency in its operations; a scholarly community consisting of the knowers and the learners, as well as all knowledge in the arts, sciences and technology, beneficial to the individual and society. This university firmly pledges to maintain excellence in all commitments; to advance the quality of life; to seek applications in the collection and creation of knowledge, moral ethos and wisdom, for the eternal growth of humankind.

SUT was selected by the Office of the Commission on Higher Education (OCHE) to be one of the nine "national research universities," and has operated continually in accordance with three research strategic dimensions: building a world-class quality knowledge base, efficient research management with good governance, and tackling national issues and problems. SUT is determined to create even more strength in its research by increasing resources in many forms. For examples, SUT has up-to-date scientific equipment laboratories for instruction in engineering, agricultural technology, science, health and social technology, as well as academic services to the public. Moreover, the backbone for the computer network of SUT (SUTnet), a 10 Gigabit type network linking together primary buildings with single mode and multimode fiber optic cables, thus connecting computing resources and communication equipment.



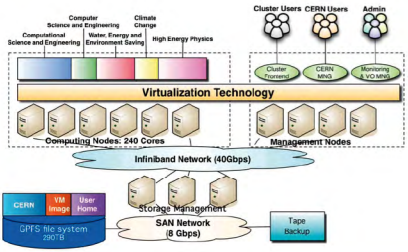
Each consortium member contributes computing resources to the consortium. The resource development plan and coordinations are taken care by the Resource Working Group. While the consortium do not interfere with the procurement process of its members, it provides standard hardware and software configurations to ensure the interoperability among the share computing resources. It also put the best effort in matching the resource requirement set by research projects and the existing infrastructure.

At the moment, the consortium has the following computing resources

| Site | CPU (Cores) | Storage (TB) |
|---|---|---|
| HAII | 896 Cores | 112 TB |
| NSTDA | 688 Cores | 290 TB |
| SUT | 656 Cores | 150 TB |
| CU | 208 Cores | 10 TB |
| KMUTT | 224 Cores | 25 TB |
| Total | 2,672 Cores | 597 TB |

The available software packages are

- ABINIT 7
- ANSYS R12
- AMBER 9
- AUTODOC 4.2
- AUTODOC_VINA 1.1
- BLENDER
- GAUSSION 09
- GROMACS 4.6
- SYBYL X 2.0
- Total View Debugger
- QUANTUM ESPRESSO 5
- User Licenses Software
- Other Open sources Software

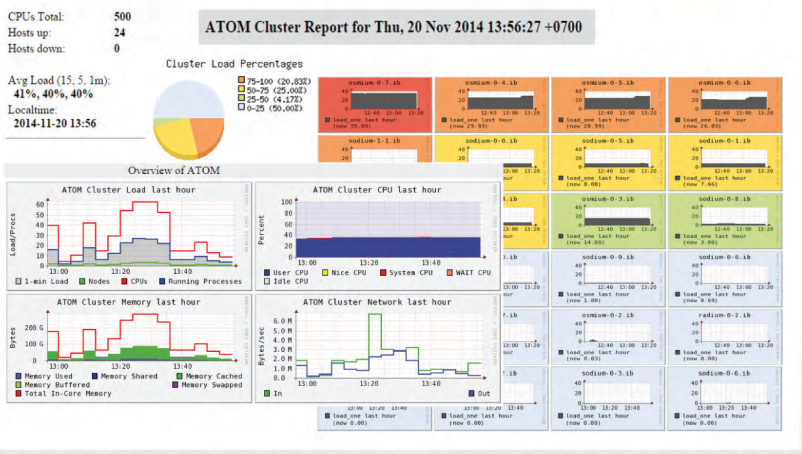





Currently, the consortium have a total of 2,672 CPU-cores and 597 TB of storage. The resources are located at CU, HAII, KMUTT, NSTDA and SUT.

By the end of 2015, NARIT will provide computing resources to the consortium, and NSTDA also plans to increase the storage to 700 TB.





## Connection with CERN

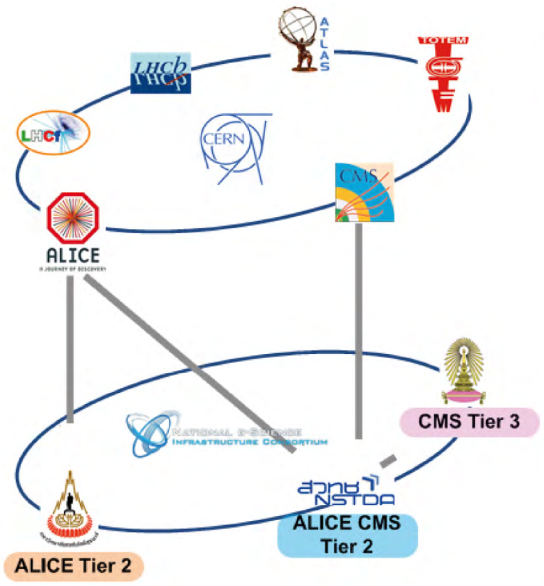
High Energy Particle Physics is an important research area that the consortium aims to support, particularly the research collaborations with CERN.

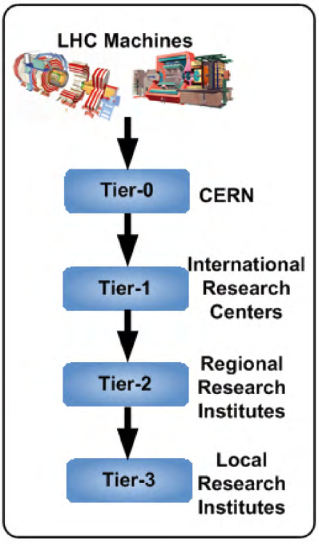
At CERN, the seven experiments have been setup around the world largest and most powerful particle accelerator, the CERN's Large Hadron Collider (LHC). These experiments use different designs of particle detector to detect the myriad of particles produced by collisions in the accelerator. The seven experiments include (i) ATLAS (A Toroidal LHC Apparatus) and (ii) CMS (Compact Muon Solenoid), the two general purpose detectors to investigate various physics phenomena where the highly massive particles are produced from the proton-proton collisions. These particles are important keys, especially for physics beyond the Standard Model, i.e. the explanation of the dark matter, or additional space dimensions. (iii) ALICE (A Large Ion Collider Experiment) is designed to be the heavy-ion detector used to study the quark-gluon plasma state, a state of matter thought to have formed just after the Big Bang. (iv) LHCb (Large Hadron Collider beauty) is a special designed detector, to focus on b-physics, i.e. to measure parameters of the CP violation which could explain the dominance of the matter over the antimatter in our universe. (v) LHCf (Large Hadron Collider forward) is a particle detector specially designed to study the origin of ultra-high -energy cosmic rays. (vi) TOTEM (TOTal cross section, Elastic scattering and diffraction dissociation Measurement at the LHC) is a unique experiment designed to measure the proton-proton interaction cross section, and also to study the proton structure which is still poorly understood. The last but not the least, (vii) MoEDAL (Monopole and Exotics Detector At the LHC), the experiment which is designed to detect the Highly Ionized Particles (HIPs), i.e. the magnetic monopole.

Currently, three Thai universities have joined two experiments at CERN. Physicists at the Chulalongkorn University (CU) join the CMS experiments, while those at Suranaree University of Technology (SUT) and King Mongkut's University of Technology Thonburi (KMUTT) join the ALICE experiment. To support the physics studies, the consortium currently operates three Tier-2 sites used for physics studies. Two sites for the ALICE experiment located at NSTDA and SUT. Another one for the CMS experiment located at NSTDA, using computing resources from CU and NSTDA. These sites are under the Memorandum of Understanding (MoU) of the Worldwide LHC Computing Grid (WLCG). This MoU has been signed on Oct 10th, 2013. The last updated MoU can be found at http://wlcg.web.cern.ch/collaboration/mou.

## Computing resources contributed to WLCG, CERN

| Site | CPU (Cores) | Storage (TB) |
|---|---|---|
| T2-TH-ALICE-NSTDA | 60 Cores | 30 TB |
| T2-TH-CUNSTDA | 260 Cores | 100 TB |
| T2-TH-SUT | 128 Cores | 100 TB |



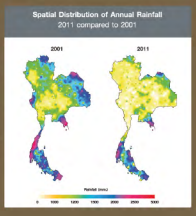
# Virtual Organizations (VO)

The consortium uses the concept of Virtual Organization to allocate computing resources. A Virtual Organization or VO is a group of researchers who share a common research goal. The members of a VO may, and usually do, belong to different real organizations, but, due to their common research interest, decide to work together planning their research projects, sharing a pool of computing resources and exchanging knowledge and experience. Taking advantage of this concept, the consortium will be able to more efficiently manage the infrastructure, and, the Steering Committee can execute their policies through the resource allocations.

The consortium realizes that achieving the profound collaboration within a VO is extremely challenging. Each VO requires a good leading researcher to be the Head, and, a group of researchers who have a certain level of existing collaborations. Therefore, the consortium chooses to start from a small number of VOs, and, hopes to have more VOs to cover other research areas in the future. To assist the management tasks of VO Head, we develop a VO management tool to register the member names, projects, resource utilization and research outputs.



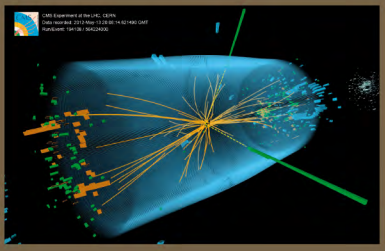


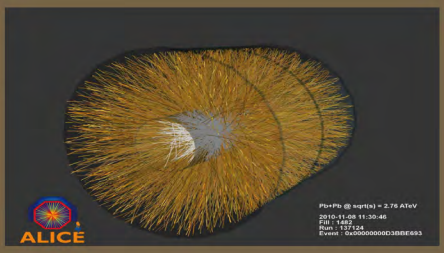



Currently, the Steering Committee has approved three VOs, namely, High Energy Particle Physics VO, Computer Science and Engineering VO, and, Computational Science and Engineering VO. More details of each VO can be found in the following sections.

## High Energy Particle Physics Virtual Organization

**VO's Head :** **Dr. Burin Asavapibhop**
**Chulalongkorn University**






One of the main tasks of the National e-Science Infrastructure Consortium of Thailand is to build Tier-2 nodes of Thailand to serve for ALICE and CMS experiments. The computing facilities provided by Chulalongkorn University, Suranaree University of Technology and the National Electronics and Computing Technology Center (NECTEC) are integrated into the Worldwide LHC Computing Grid (WLCG). This will allow physicists from both universities to simulate the Monte Carlo events, or to analyze the experimental data using personal computers at their institutes. This infrastructure will be beneficial not only to the physics community, but also to other scientific collaborations which need computing power, i.e. Biology, Computational chemistry, Climate study, Engineering, Mathematics, and Medicine.



## CU Research with CMS, CERN

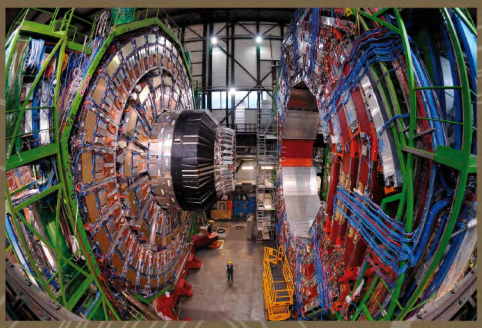
*Burin Asavapibhop, Kittikul Kovitanggoon, Gurpreet Singh, Norraphat Srimanobhas,* and *Narumon Suwonjandee*

The Particle Physics Research Laboratory (PPRL) at Department of Physics, Faculty of Science, Chulalongkorn University has joined the international collaboration working on the Compact Muon Solenoid (CMS) experiment at the Large Hadron Collider (LHC) at CERN since 2012. In 2015, the LHC machine will provide the proton-proton collision at the highest energy level, 13 TeV. With the colossal amounts of collected data in the next few years, this may help physicists to explain more about the early universe and some unsolved problems.

We, physicist at CU, are currently interested in the standard model and beyond the standard model physics. The topics on interest include

1. Example research projects carried out under the HEP-VO:
   + Analysis of the Standard Model Higgs boson produced in association with a W or a Z boson and decaying to bottom quarks
   + Invisible Higgs study using the Vector Boson Fusion (VBF) channel

2. Beyond standard model physics
   + Search for the new physics using the monojet and missing transverse energy topology
   + Search for supersymmetric partners of the third generation quarks
   + Search for highly ionized particles





# SUT Research with ALICE, CERN: Detector simulation

*Chinorat Kobdaj, Mario Sitta* and *Parinya Namwongsa*

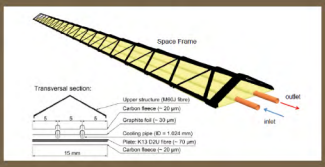
One key point of the new ITS upgrade design is the requirement of rapid accessibility for maintenance and inspection. To achieve this goal, the mechanical removable structures or barrels have been introduced for both ITS inner and outer layers. Each barrel is composed of a detector section and a service section. The detector barrel is the host for sensor modules or staves which are connected via electrical signal connections (e-links) and power cables to patch panels. While the service barrel integrates the cable trays that support the e-links and power cables through their routes from the detector staves to the patch panels. However, to minimize the material used in the detection area, the details geometry of these barrels are created and, later, will be used in the material budget calculation of the ITS detector.

**Objective of the simulations :** To investigate the mean material budget of the inner barrels and to answer the question "Is it possible to reduce material budget: X/X0 /layer of the inner barrels to approximately 0.3% ? "

**The structure of inner barrels**

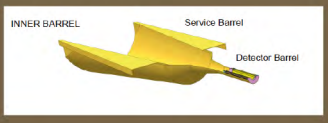
- Detector stave

Each detector stave composes of the supporting structure, pixel chips and flexible printed circuit strip. The pixel chips are glued to the space frame on one side and soldered to the flexible printed circuit on the other side.




- Detector barrel and service barrel

The service barrel is connected to the detector barrel while the staves are mounted on the detector barrel with the holders and pins.




**Current results (work in progress)**

Geometry shapes written in c++ class of AliITSUv1Layer. {cxx, h } and AliITSUv1. {cxx, h }



Updated direction is using different private methods, removing hardcoded numbers, transforming composite shapes into real volumes and solving for overlap problems. All of which need to comply with the Coding Conventions of Aliroot.

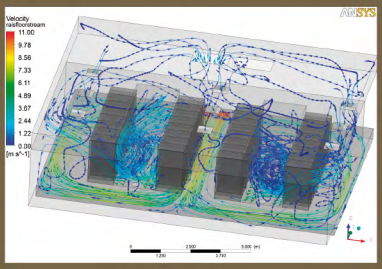
**Outlook and future work**

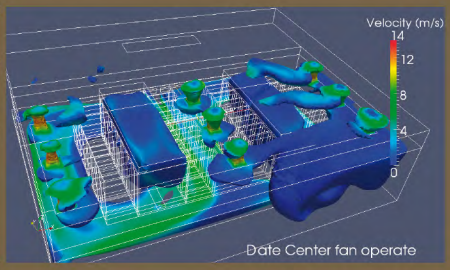
Once the geometry files are completed we will calculate the mean material budget used in the sensitive area of the detector barrels and compare it with our goal at 0.3%.

## Computational Science and Engineering Virtual Organization

**VO's Head :** **Dr. Sornthep Vannarat**
**National Science and Technology Development Agency**

Computational Science and Engineering (CSE) is a discipline where computer simulation is used as a main tool to pursue scientific research and technology development. This approach has been used extensively to complement experimental and theoretical approaches especially to study complex systems. There are plenty examples in various fields such as the simulation of early universe; atmospheric and oceanic circulations; mechanical stress and fluid flows in vehicles, engines, and, circulatory systems in organisms; electronic band structure of materials, etc. CSE covers vast research fields and is significantly important for advancing science and technology.



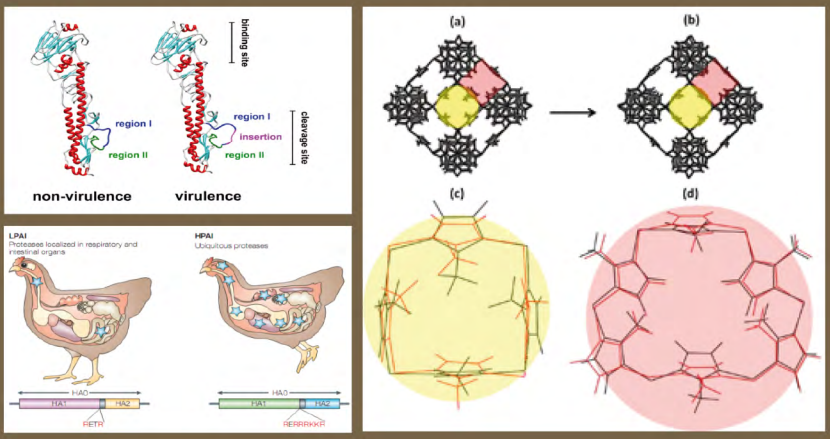




Even though CSE covers wide application areas, CSE researchers face similar challenges. They need to have a model that accurately captures the essential physical phenomena, but, is not too computationally complicated to be handle by available computing resources. The researchers also need to optimize the model in order to consider more realistic systems and study cases. The computational experiments must be carefully designed to yield key information to the research questions. The CSE VO will encourage the interaction among the researchers within and across scientific disciplines so that lessons and experiences can be shared. This VO will also try to accommodate as many research projects as permitted by the computing resources we received.

## Research at Computational Chemistry Unit Cell (CCUC),

*Department of Chemistry, Faculty of Science, Chulalongkorn University*
*Associated Professor Dr. Vudhichai PARASUK*

Research carried out currently at CCUC ranges from physics to pharmacology, with special emphasis on molecular interactions, molecular structures and species distribution of solutions, as well as development of new methodological approaches. Scopes of our research could be summarized into 2 main areas, Material and Bio-science. The research in Material area is composed of the study on novel materials such as carbon nanotubes and graphene, porous materials such as Metal Organic Frameworks (MOF) and Zeolititc Imidazolate Frameworks (ZIF), and catalysts such as Ziegler-Natta and metallocene. For the research in Bioscience, we focus on modeling of proteins which relate to human pathogens such as humanflu and birdflu, hepatitis C, cancer, and neuro-diseases. In addition, we also study on fundamentals such as ion transportation through membranes and drug-delivery systems. All studies were carried out using computational methodologies such as quantum calculations (QM), Molecular Dynamics (MD)/Monte-Carlo (MC) simulations.



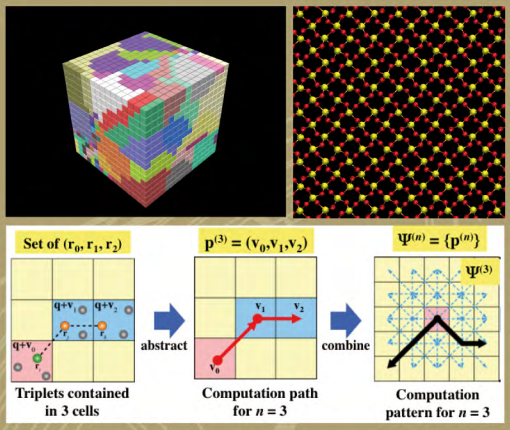

Left : The cause of high pathogenicity of avian flu
Right : Transform of the linkers in the ZIF-8 framework from low density to high density by guest molecules.

## Fast and Scalable Reactive Molecular Dynamics Simulation Program for Large-Scale Parallel Computing Platforms

*National Science and Technology Development Agency*
*Manaschai KUNASETH, Ph.D*

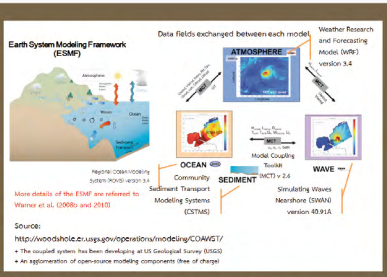
Molecular dynamics (MD) simulation has become a vital tool to solve a broad range of scientific and engineering problems. However, larger and longer simulations, along with sophisticated modeling of real-world problems, are required in order to characterize realistic systems. In the scope of chemically reactive MD simulation, reactive force-fields is one of the most common methods. Despite the well-developed computational methods for non-chemical reactive MD, limited studies were achieved on improving performance of reactive MD for a large-size and long-time simulation.

In order to fully utilize immense computation power of emerging large-scale parallel computing platforms such as GPGPU and MIC, a novel Shift/Collapse (SC) algorithm has been developed for fast and highly scalable reactive MD simulations. The Unified Computational Framework (UCF) has also been developed allowing range-limited MD computation based on cell method to be analyzed for correctness and optimality in a mathematically rigorous fashion. Under UCF analysis, SC outperforms the conventional short-range many-body calculation in terms of communication and computation costs. SC algorithm has been included Shift/Collapse Reactive Molecular Dynamics Simulation Program (SCoReMD). SCoReMD benchmark shows significant improvement in terms of wall-clock time and scalability on large-scale supercomputers and MIC computing platforms.

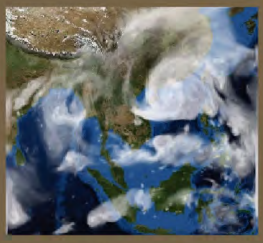


## Challenges of Climate Change and Current Research Cutting Edge

*Hydro and Agro Informatics Institute*

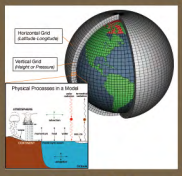



Coupled Modeling Systems Atmosphere-ocean coupling helps in understanding multi-components of climate system and interactions between them. It allows the surface fluxes to influence the stability of the atmospheric boundary layer, the momentum, heat and moisture.



As Thailand is located between the Indian Ocean and the South China Sea which is a portion of the Pacific Ocean, its weather prediction system could benefit from the coupled atmosphere-ocean model. The Hydro and Agro Informatics Institute (HAII) has been developing a coupled atmosphere-ocean model to predict the precipitation in Thailand. The model employs the Coupled-Ocean-Atmosphere-Wave-Sediment Transport (COAWST) Modeling System obtained from U.S. Geological Survey (USGS).

### GCM Bias Correction for Thailand




The global circulation model (GCM) is the model for predicting the future climate and it is also used in the study of climate change. Generally its resolution is too coarse to allow an assessment of the impact in the local hydrological scale. For this reason, we developed the Gamma-Gamma (GG) bias correction approach to improve the statistical inference between the GCM and observed climate data. We applied this technique to correct the bias from the 11 GCMs data under the Coupled Model Intercomparison Project Phase 5 (CMIP5) such as BCC-CSM1.1, BNU-ESM, CanESM2, CNRM-CM5, CSIRO-Mk3.6, EC-Earth, FGOALS, GFDL-CM3, HadGEM2-AO, MIROC5 and NorESM1-M. The numbers of rainfall and meteorological stations used for bias correction are 1183 stations and 101 stations, respectively.

## Computational Science and Engineering Virtual Organization

**VO's Head :** **Assoc. Prof. Dr. Tiranee Achalakul**
**King Mongkut's University of Technology Thonburi**

The Computer Science and Engineering Virtual Organization (CSE-VO) is set up with the mission to support the research works in the area of high performance computing (HPC) and its applications in Thailand. The VO also aims to promote the importance of HPC in enhancing the scientific advancement and technological innovation in the country.

Currently, the VO has recruited members from multiple agencies in Thailand including King Mongkut's University of Technology Thonburi, Kasetsart University, and the National Electronics and Computer Technology Center. In addition, the research works carried out under the VO has resulted in international collaborations with the European Organization for Nuclear Research (CERN), The Institute of High Performance Computing (Singapore), Shibaura Institute of Technology (Japan), and Virginia Tech (USA).

Research projects of CSE-VO are mostly multi-disciplinary works that emphasize computational modeling, simulation, and visualization methodologies. A few examples of the research works carried out under this VO will be presented next.

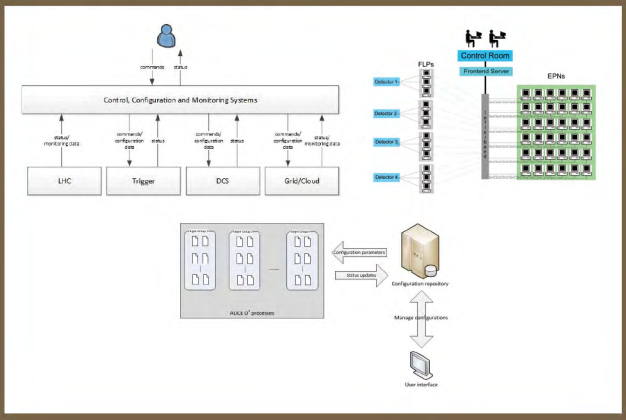


## Control, Configuration, and Monitoring: a Computing System Design for CERN's ALICE $O^2$ Processing

*Department of Computer Engineering*
*King Mongkut's University of Technology Thonburi*

The most recent particle accelerator at CERN is the Large Hadron Collider (LHC). Inside the LHC, two proton beams travel in the opposite direction in the separated pipes until they are allowed to collide at one of the detectors. An enormous number of collision events are detected and recorded by the detectors located along the LHC's ring. ALICE is one of four main detectors of the LHC. In 2018, the ALICE detectors will be upgraded and the amount of data produced will be much higher than the current system. For this reason, a new computing system has to be designed and developed entirely. KMUTT is the team assigned with a task to design and develop control, configuration, and monitoring (CCM) modules of the new computing system.

The CCM components will act as tightly-coupled entities that support users in a day-to-day operation. The Control system will be responsible for orchestrating all the components of the ALICE O2 system, based on state information as well as monitoring data. The Configuration system will ensure that both the application and the environment parameters are properly set up and can be re-configured dynamically during simulation runs. Finally, the Monitoring system will receive the status of different subsystems with the aim of determining unusual patterns and raising alarms. Currently, the design of a new state machine has been drafted by the KMUTT team. Later in 2015, the team will develop a prototype system, which will then be evaluated by the ALICE Experiment's engineers.



## SkyPACS: a High Performance, Mobile Medical Imaging Solution

*Department of Computer Engineering*
*King Mongkut's University of Technology Thonburi*



Lack of radiologists is a problem that arises in many parts of the world. Radiologists need to work long hours for multiple hospitals. In order to improve the quality of healthcare, SkyPACS is designed. It is a mobile solution that allows radiologists to work more conveniently. SkyPACS is a customizable medical imaging tool that can be used for prognosis. The solution is designed to be an assistive technology with the focus on simplicity, flexibility, and user experiences. The architecture of SkyPACS is designed based on service oriented Model-View-Controller. The customers can freely choose the backend services: cloud computing and storage on public cloud, private server, or hybrid system. The compute-intensive modules are deployed on a GPU-server taking advantage of data parallel with CUDA library. The main features include all standard tools for viewing and diagnosis in 2D and 3D, convenient tools for collaborations, and case management. In addition, advanced functions such as automatic blood vessel detection and reconstruction, and bone/skin/muscle segmentation are provided.

SkyPACS started as a series of research projects for graduate students at KMUTT. The study and experiments have been performed on storage virtualization technology, 3D reconstruction of blood vessel on GPUGPU, image data analytics, performance tuning for black-box scientific applications, and mobile cloud computing. Towards the end of the research stage, the results have been utilized and adapted to the SkyPACS software framework. The software has now been commercialized under a newly formed startup company and has been implemented at a few hospitals and radiology centers. We are looking to add more advanced features into the software as soon as new research results become available. We believe that SkyPACS will soon be able to reduce the cost of the healthcare platform in the near future.

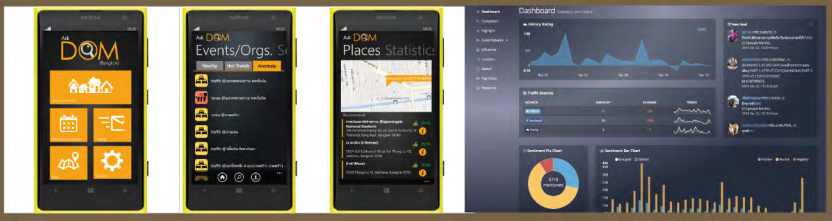
## DOM: A Data and Opinion Mining Framework

*Department of Computer Engineering*
*King Mongkut's University of Technology Thonburi*

In the past few years, social networks have been exponentially growing and connect our lives together in various dimensions. In every second, hundred thousands of messages are shared through social media such as Facebook, Twitter, and Foursquare. The information is about our life, feeling, experiences and opinions. This huge volume of data has been utilized across business domains. However, as much as 90% of the data stored is "unstructured," meaning that it is spontaneously generated and not easily captured and classified. To make user of such data, DOM was developed.

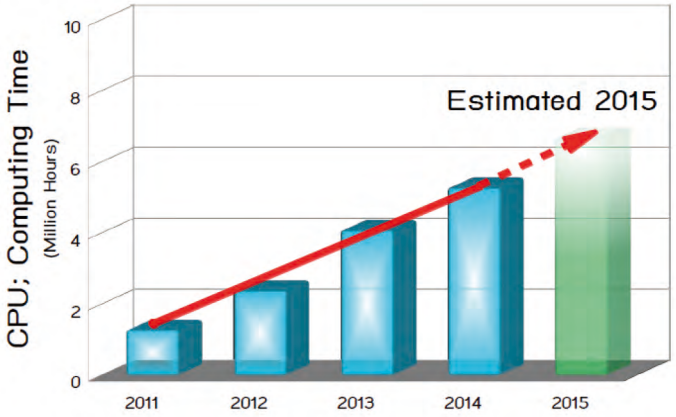
DOM is a big data processing engine designed to capture data from multiple well-known social network sources, and then processes them using MapReduce, a keyword-based sentiment analysis technique, and an influencer analysis algorithm to determine public opinions and sentiments of certain topics. The engine was evaluated its sentiment prediction accuracy by matching the predicted result with the human sentiment and tested on various case studies. The effectiveness of the approach demonstrates the practical applications of the engine.

DOM is developed as a part of a research theme in big data analytics at the department of computer engineering, KMUTT. The methods, algorithms, and techniques designed during the research stage have been implemented into a commercial framework. Currently, the DOM engine is incubated with one of the biggest IT companies in Thailand. The engine is being marketed and soon will be commercialized under the new startup venture making DOM another success story of the “KMUTT’s research to product” program.



# Achievements

- **Computing resource usages.**




- **Publications**

Between fiscal year 2012 and 2014, they are 105 research projects from 34 institutions using computing resources. The researchers have produced 210 publications as show in the table below

| | International Journal | National Journal | International Conference | National Conference | Others | Total |
|---|---|---|---|---|---|---|
| 2011 | | | | | | 40 |
| 2012 | 17 | 1 | 12 | 15 | 7 | 52 |
| 2013 | 17 | - | 28 | 6 | 21 | 72 |
| 2014 | 47 | 1 | 18 | 5 | 15 | 86 |

- **Graduated students**

| Institution | CU | KMUTT | SUT | Total |
|---|---|---|---|---|
| Bachelor degree | - | 9 | - | 9 |
| Master degree | 2 | 15 | 13 | 30 |
| Doctoral degree | 1 | 1 | - | 2 |

**Exhibition** on NSTDA Annual Conference (NAC); An International Annual Symposium on Computational Scientist and Engineering (ANSCSE)






**Seminar** on Future Research on Internet Development Initiative by Thailand Research Alliance at Conference on INET Bangkok

**Visit Universities** at University of Phayao, Chulalongkorn University and Walailak University





**Workshop** on Computer-aided Molecular Design at Chulalongkorn University and Standards-based Hydrologic Data Management and Visualization at NECTEC

# Committee and Working Groups

## Board of Steering Committees

| | |
|---|---|
| Prof. Dr. Pairash Thajchayapong | Advisory |
| Dr. Kopr Kritayakirana | Advisory |
| President of National Science and Technology Development Agency | Chair person |
| President of Chulalongkorn University | Committee |
| Director of Hydro and Agro Informatics Institute | Committee |
| President of King Mongkut's University of Technology Thonburi | Committee |
| Rector of Suranaree University of Technology | Committee |
| President of Electronic Government Agency (Public Organization) | Committee |
| Director of UniNet, Office of Higher Education Commission | Committee |
| Asst. Prof. Putchong Uthayopas | Committee |
| Mr. Chaicharearn Atibaedya | Committee |
| Chair Person of Usage Management Working Group | Secretary |
| Chair Person of Resources Working Group | Assistance Secretary |
| Chair Person of Tools Working Group | Assistance Secretary |
| Chair Person of Network Working Group | Assistance Secretary |

## Usage Management Working Group

| | |
|---|---|
| Dr. Sornthep Vannarat | Chair Person |
| Prof. Dr. Kritsana Sagarik | Committee |
| Assoc. Prof. Dr. Tiranee Achalakul | Committee |
| Dr. Burin Asavapibhop | Committee |
| Miss Jarumon Limtipdara | Committee |

## Resources Working Group

| | |
|---|---|
| Mr. Suriya U-ruekolan | Chair Person |
| Dr. Norraphat Srimanobhas | Committee |
| Dr. Supakit Prueksaaroon | Committee |
| Dr. Thara Angskun | Committee |
| Mr. Atip Peethong | Committee |
| Mr. Rajchawit Sarochawikasit | Committee |

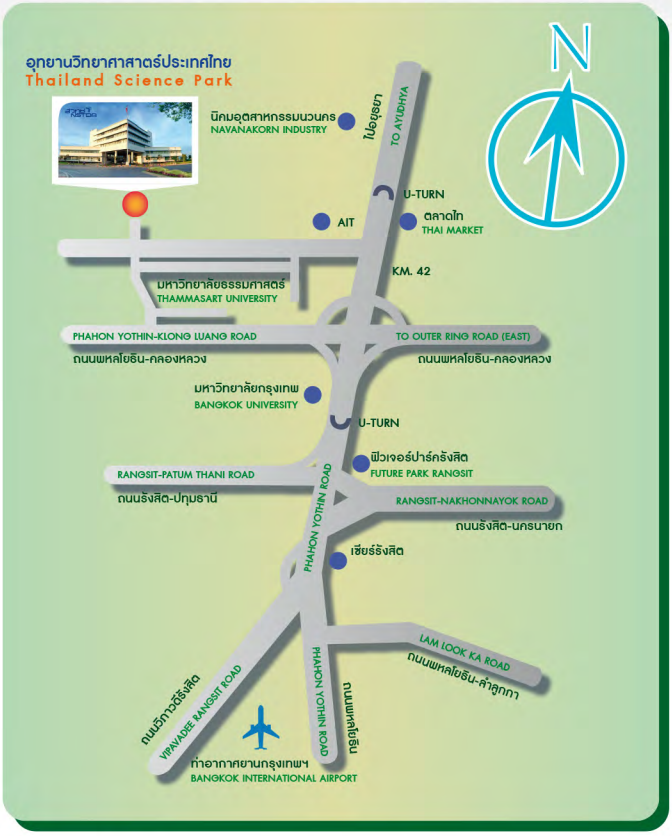
## Tools Working Group

| | |
|---|---|
| Assoc. Prof. Dr. Vudhichai Parasuk | Chair Person |
| Assoc. Prof. Dr. Tiranee Achalakul | Committee |
| Dr. Ayut Limphirat | Committee |
| Dr. Ekasit Kijsipongse | Committee |
| Dr. Surajate B.Aroonnet | Committee |

## Network Working Group

| | |
|---|---|
| Deputy Director of UniNet | Chair Person |
| Office of Higher Education Commission | Committee |
| President of Electronic Government Agency (Public Organization) | |
| Director of Computer Center | Committee |
| King Mongkut's University of Technology Thonburi | |
| Head of Network Technology Laboratory | Committee |
| National Electronic and Computer Technology Center | |
| National Science and Technology Development Agency | |
| Director of University Office of Information Technology | Committee |
| Chulalongkorn University | |
| Director of the Center for Computer Service | Committee |
| Suranaree University of Technology | |

# Contact Details




## Consortium Office

### Location

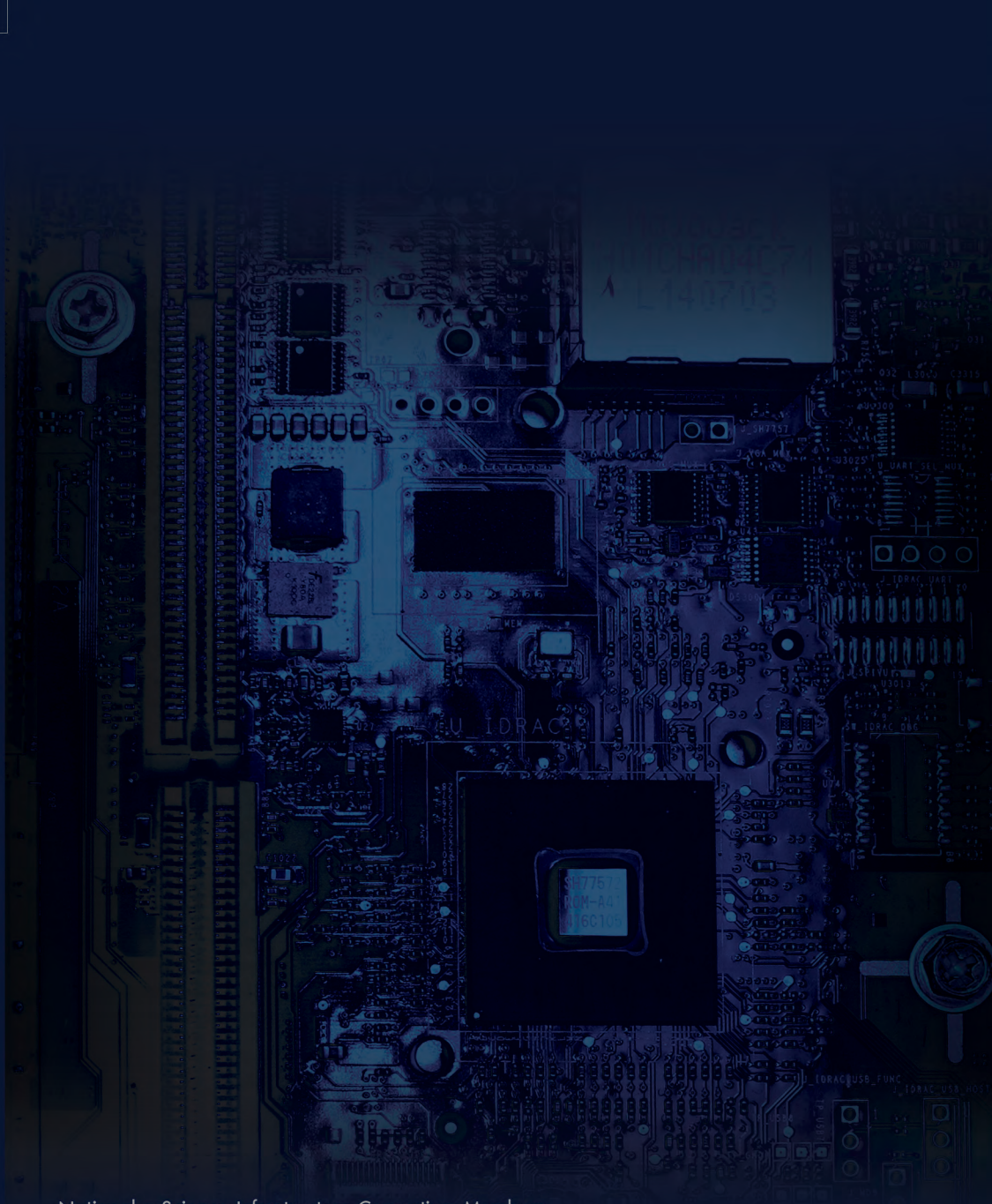
Large Scale Laboratory Research
National Electronic and Computer
Technology Center (NECTEC)
112 Thailand Science Park,
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Klong 1, Klong Luang, Pathumthani,
12120, Thailand

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National e-Science Infrastructure Consortium Members