
National e-Science
Infrastructure Consortium
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2017
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เทิด ธ
เสด็จสรวง
น้อมส่ง
สถิตแล้ว
เสียงโศก
พระภูมินทร์
เสด็จสู่
ราษฎร์ร่ำไห้

พระพ่อหลวง
ล่วงลาแล้ว
องค์พ่อแก้ว
สุราลัย
ดั่งโลกสิ้น
ธ ดวงใจ
สวรรคาลัย
ไปทั่วแดน

ด้วยเกล้าด้วยกระหม่อม ขอเดชะ
ข้าพระพุทธเจ้า คณะผู้บริหาร พนักงาน สวทช.
และประชาคมอุทยานวิทยาศาสตร์ประเทศไทย

ผู้แต่ง ธนภัทร์ ศรีโมรา

The members of National e-Science Infrastructure Consortium had an audience with and presented a 2016 Annual Report of the National e-Science Infrastructure Consortium to HRH Princess Maha Chakri Sirindhorn in the meeting of the Executive Committee of the Information Technology Foundation under the Initiative of Her Royal Highness Princess Maha Chakri Sirindhorn, 1/2017

On January 12, 2017 at 09:00-12:00 Hrs. at Chaipattana building, Chitralada Palace, Bangkok

e-Science 2017

This booklet gives an overview information of National e-Science Infrastructure Consortium including motivations, current status and achievements of the consortium, short introduction to each member institutes, the research group, 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

PROFESSOR DR. 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 research scientists and the European Organization for Nuclear Research (CERN) on High Energy Physics. This collaboration led to the foundation of The National e-Science Infrastructure Consortium in 2011, aiming to develop computational instrument, data storage and fundamental datasets as a sustainable infrastructure to support research in Thailand. In 2013, the consortium joined the Worldwide LHC Computing Grid (WLCG), and has operates two tier-2 sites including T2-TH-CUNSTDA and T2-TH-SUT (formerly TH-SUT-NPP) until the present.

Today, the consortium consists of seven regular members from a number of universities and research institutes which work closely to accomplish the consortium goals. Originally, the consortium has focused on research areas such as computational science and engineering, computer science and engineering, water resource, energy and environment management, climate change, and high energy particle physics. However, due to an increasing interest in research on big data analytics on cloud today, the consortium considers an inclusion of research studies relevant to big data issues.

I expect that the success of the consortium will give Thai scientists inspiration to keep moving forward on research and development, and the infrastructure pool will allow them to create and share new knowledge among each others in a sustainable way. Finally, I would like to thank all members for hard working over six years and look forward to seeing the successful outcomes in the very near future.

MESSAGE FROM

PROFESSOR DR. PRASART SUEBKA
Chair of Steering Committee
National e-Science Infrastructure Consortium

It has been 6 years since the National e-Science Infrastructure Consortium was founded in 2011 as a research infrastructure related to high-performance computing in Thailand. An important factor to our success is the contribution from each member by investing and sharing their resources. As a result, the consortium has grown from five to seven members with three associate members. The total numbers of CPU cores now become more than 3,300 cores with the total storage capacity around 1,200 Terabytes. In year 2016, there are 99 research projects have been using our infrastructure and produced 79 research publications. All users can access and use the infrastructure via internet connectivity provided by the Inter-University Network (UniNet) and Thailand Research and Education Network (ThaiREN).

As a new chairman of the consortium, which is rotated every three years among members, I would like to thank all members for their long and fruitful collaboration over the first phase of the consortium. I am confident that the National e-Science Infrastructure Consortium is now ready to elevate itself as a national infrastructure to cooperate with the private sector and deliver a wide range of activities to support digital economy in the Thailand 4.0 model.

CONTENTS

OVERVIEW

The National e-Science Infrastructure Consortium was initially formed by a number of universities and research institutes including Chulalongkorn University, Suranaree University of Technology, King Mongkut's University of Technology Thonburi, Hydro and Agro Informatics Institute, and National Science and Technology Development Agency as founding members. The objective of the collaboration among the consortium members is to help support computational science and engineering research in Thailand. To accomplish the consortium goal, it is necessary to provide computing systems which support high performance computing (HPC) and cloud infrastructures. Today, the consortium focuses on an integration of HPC and big data driven services in a cloud computing system.

The consortium maintains e-Science-related research projects in general, but with an emphasis on water resource, energy and environment management, climate change, and high energy particle physics. The number of research projects has increased rapidly in the past few years and the scalability of the computing resources is always needed. To support this growth, two new organizations in addition to the founding members, National Astronomical Research Institute of Thailand and Electronic Government Agency participate in the consortium as a regular member. Electronic Government Agency offers the Government Cloud service (G-Cloud) which addresses big data storage issues.

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 may have other contributions or collaborations with the consortium. They are not in the consortium steering committee.

OBJECTIVE

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

Workshop on e-Science and High Performance Computing
Left: eHPC2015, Right: eHPC2016

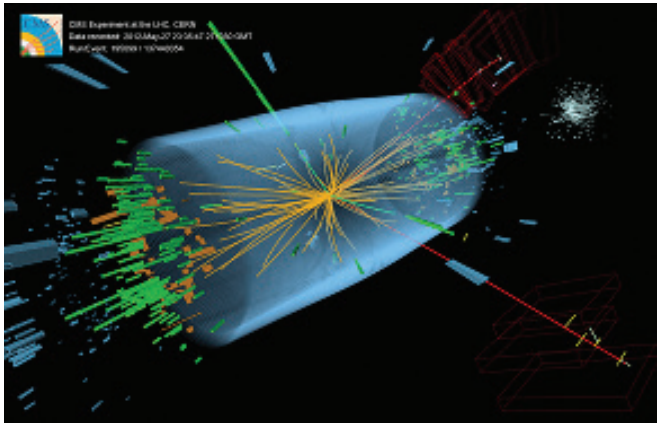
1

E-SCIENCE MEMBERS

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 high performance computing cluster project at Chulalongkorn University had been setup to support the National e-Science Infrastructure Consortium in 2010. Currently, our cluster is opened for researchers from both inside and outside the university. The current research projects include physics, chemistry, material science, and computer science.

Since 2015, the Particle Physics Research Laboratory at Chulalongkorn University together with theoretical physics group, and astrophysics group formed "Chulalongkorn University Next-Generation Initiatives for Experimental High Energy, Elementary Particle, and Extragalactic Astrophysics Research Excellence" (a.k.a. CUniverse) under the support of the Chulalongkorn Academic into Its 2nd Century Project Advancement Project. CUniverse research is dedicated to theoretical experimental high energy physics and astrophysics. It focuses on searches beyond Standard Model, including supersymmetric particles, Large Extra Dimensions (LED) of spaces, dark matter, neutrino physics, superstring theory and supergravity. Our university collaborates with Compact Muon Solenoid (CMS) collaboration and NECTEC for the development of the CMS Tier-2 node of Thailand under National e-Science Infrastructure Consortium in parallel with the high performance computing cluster.

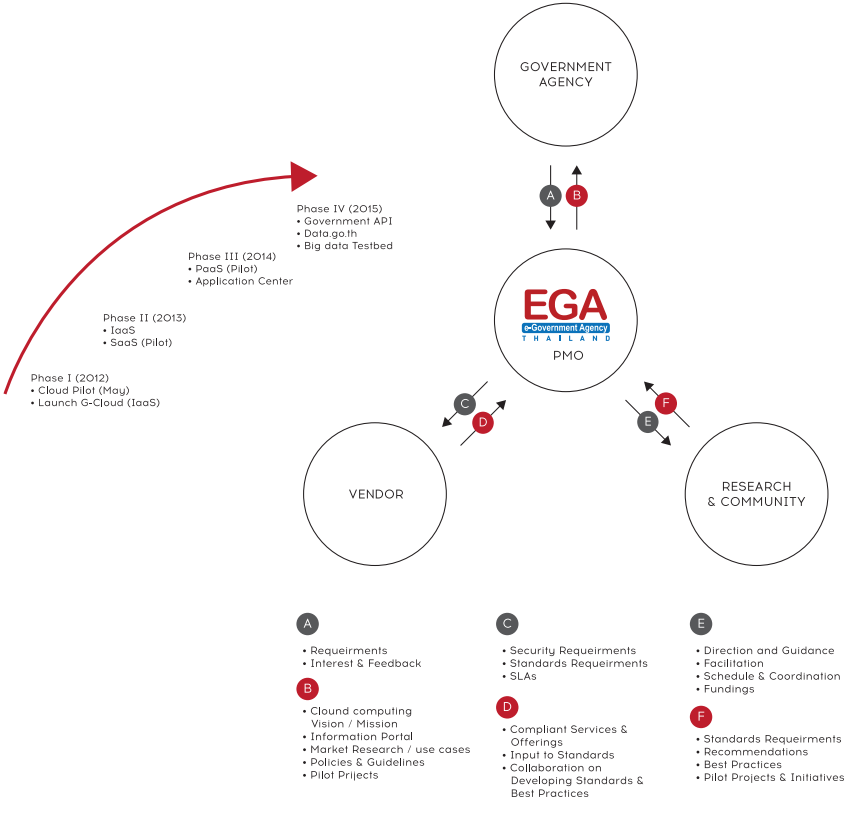


Electronic Government Agency

EGA is under supervision of the Ministry of Information and Communication Technology, EGA is the key organization with responsibilities of promoting and supporting the development of e-Government services. In the beginning, significant projects were transferred from the National Science and Technology Development Agency. In 2012, EGA continued to run those projects and initiated various projects to support e-Government development progress. EGA also provides consultancy, technical services and manages information and communication technology projects.

Government Cloud Model

EGA's responsibilities:
Project Management Office



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 researchers 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 monitoring, simulation, information processing, and information dissemination that support the policy makers in coping with flood and drought management.

Active research areas include:

- Short-term weather prediction using coupling atmosphere and ocean models (WRF-ROMS)
- Wind-Wave prediction using Simulating WAve Near-shore (SWAN) model and storm surge
- Seasonal precipitation prediction
- Flood forecasting system and DSS
- Hydroinformatics

[1] MIT – the Massachusetts Institute of Technology
[2] RDPB – the Office of the Royal Development Project 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 multi-disciplinary research in the fields of bio-engineering and bioinformatics, Computation Fluid Dynamics, and particle physics simulation, just to name a few.

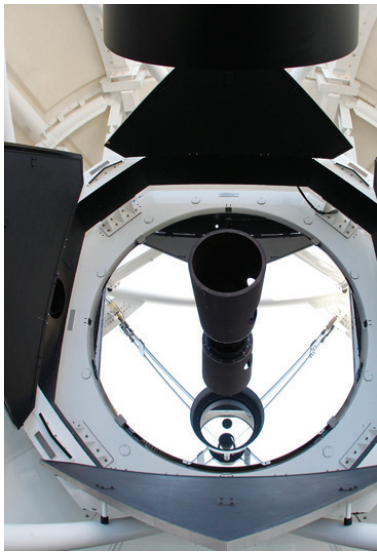
It has always been a belief of KMUTT that National e-Science Infrastructure Consortium will be an important platform that contributes to Thailand's competitiveness in the global economy. KMUTT computational Science and engineering research cluster will continue its mission in research and its support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

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.

From the beginning, NARIT HPC cluster was relatively small compared to other members of the consortium, but we currently have increased the size of our infrastructure which meets the needs of national computational astronomical community.



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 ensure 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) is Thailand's first autonomous university founded on 27 July 1990. It is located in the north-eastern part of Thailand approximately 250 kilometers from Bangkok. Flexible in administration, SUT speeded forward and in a few years, was chosen to be the "one in the nine of the national research universities," a university excellent in research and teaching in Thailand.

SUT is the first state university to become a "University of Technology," with emphasis on instruction and research in science and technology, with Baccalaureate, Masters and PhD programs. SUT has 7 Institutes: Science, Engineering, Agricultural Technology, Social Technology, Nursing, Medicine and Dentistry. SUT's annual output of 2,500 graduates has up to 96% rates of obtaining jobs, with initial salaries averaging the leading in Thailand.

SUT is the prototype and leader in Thailand's cooperative education. The first to adopt the work integrated education system to train graduates to respond to the needs of the labor market, today SUT is a "silver" member of the World's Association for Cooperative Education (WACE), as well as one in two institutions selected to be an WACE International Satellite Office (WACE ISO@SUT) for the Asia Pacific Region.

From the assessment of the research of the individual schools conducted by the Thailand Research Fund (TRF), the School of Physics has received 1st excellence for Thailand for 8 consecutive years, with the other 9 schools receiving distinguished marks being Mathematics, Chemistry, Biochemistry, Electrical Engineering, Telecommunications Engineering, Civil Engineering, Animal Husbandry Technology, Biotechnology and Food Technology.

Regarding research, Suranaree University of Technology has instituted 5 Centers of Excellence, i.e., Food Technology and Biotechnology Center, Nano-and Advanced Material Center, Nuclear Physics High Energy and Particle Physics Center, Advanced Construction Materials Center and Biomass Technology driving our National Research University to become a World Class University.

The university has taken into consideration its geographical location and is taking part in promoting the Nakhon Ratchasima Province as the center for 5 areas, including the Education Hub, Medical Hub, Transportation and Logistics Hub (land, car, rail and air transports), Food Hub or Food Valley and Tourism and Sports Hub.

2

RESOURCES

Each consortium member contributes computing resources to the consortium. The resource development plan and coordination are taken care by the Resource Working Group. The consortium provides standard hardware and software configurations to ensure the interoperability among the shared computing resources. It also put the best effort in matching the resource requirements set by research projects and the existing infrastructure.

Total resources

At the moment, the consortium has the following computing resources

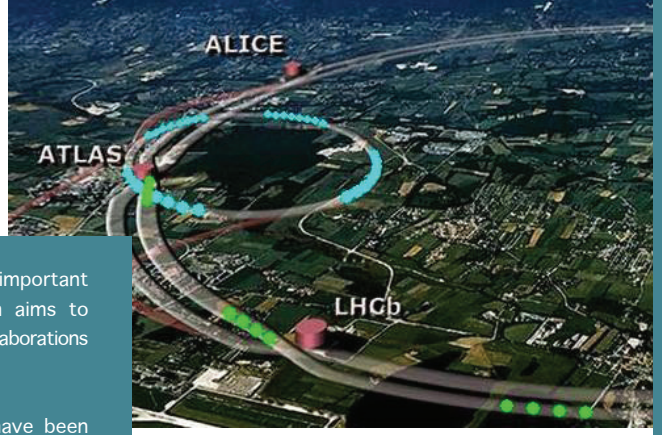
Site	CPU (Cores)		Storage (TB)	
HAII	896	Cores	112	TB
NSTDA	688	Cores	660	TB
SUT	656	Cores	150	TB
CU	340	Cores	106	TB
KMUTT	224	Cores	30	TB
NARIT	540	Cores	100	TB
EGA	80	Cores	13	TB
Total	3,424	Cores	1,171	TB

The available software packages:

- ABINIT
- AMBER 10
- AUTODOC
- AUTODOC_VINA
- GAUSSION 09
- GROMACS
- SYBYL X 2.0
- Total View Debugger
- QUANTUM ESPRESSO
- OpenMPI
- Mpich, Mpich2
- Omnet++
- Hummer
- Ncbi
- Clustal W
- User Licenses Software
- Other Open sources Software

Currently, the consortium has a total of 3,424 CPU-cores and 1,171 TB of storage which are located at site of each consortium members.

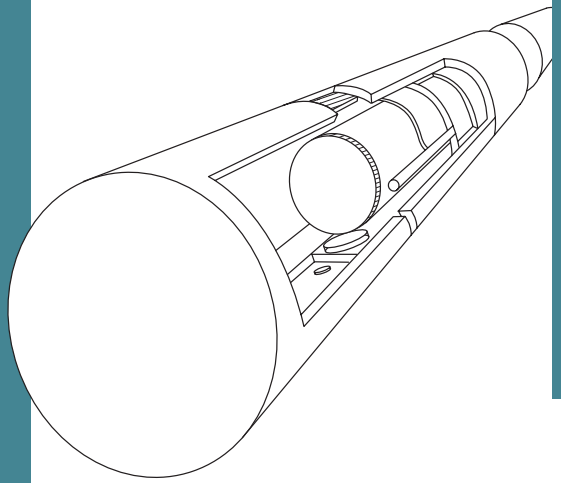
Connection with CERN

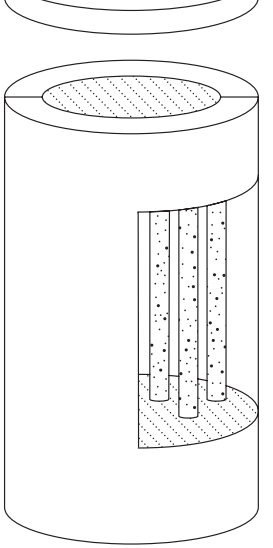


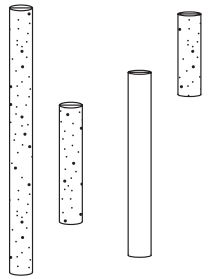
High energy particle physics is an important research area that the consortium aims to support, particularly the research collaborations with CERN.

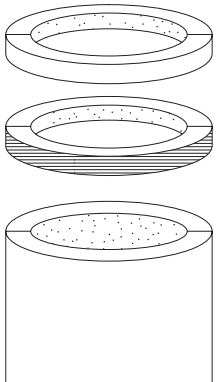
At CERN, the seven experiments have been setup around the world largest and most powerful particle accelerator, the CERN's Large Hadron Collider (LHC). These experiments use different designs of particle detector to detect the myriad of particles produced by collisions in the accelerator, and they run by collaborations of scientists from institutes all over the world. The seven experiments include (i) ATLAS (A Toroidal LHC Apparatus) and (ii) CMS (Compact Muon Solenoid), the two general propose detectors to investigate wide range of physics phenomena where the highly massive particles can be produced from the proton-proton collisions. Having two of them are important key to confirm new discoveries. (iii) ALICE (A Large Ion Collider Experiment), a detector which 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), a special design detector to focus on b-physics which could help to explain the dominance of the matter over the antimatter in our universe. (v) LHCf (Large Hadron Collider forward), a particle detecor specially designed to study the origin of untra-high-energy cosmic rays. (vi) TOTEM (TOTal cross section, Elastic scattering, and diffraction dissociation Measurement at the LHC), a unique experiment designed to measure the proton-proton cross-section, and also to study the proton structure which is not well understood. The last but not least, (vii) MoEDAL (Monopole and Exotics Detector At the LHC), the experiment which is designed to detect the highly ionized particles (aka HIPs), i.e. the magnetic monopole. Currently, there are three Thai universities which is officially joined CERN experiments. Chulalongkorn University joins the CMS experiment, Suranaree University of Technology (SUT) and King Monkut's University of Technology Thonburi (KMUTT) join the ALICE experiments.

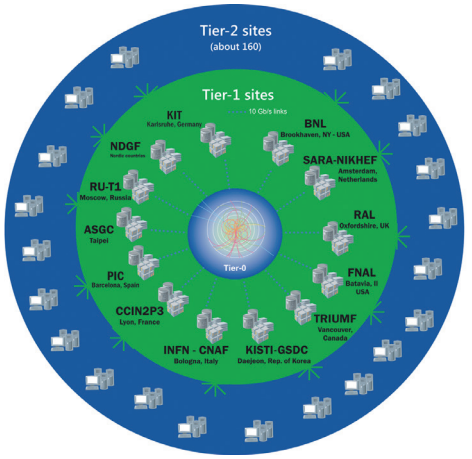
To join the computing resources with CERN and its collaborations, Thailand became the member of Worldwide LHC Computing Grid (WLCG). The MOU has been signed on Oct 10th, 2013. The last updated MoU can be found at http://wlcg.web.cern.ch/collaboration/mou. WLCG is a global collaboration of more than 170 computing centres in 42 countries, linking up national and international grid infrastructures. Currently, Thailand has two Tier-2 sites including the ALICE Tier-2 experiment locates at SUT, Nakhon Ratchasima, and the CMS Tier-2 locates at NSTDA using resources from CU and NSTDA.











3 VIRTUAL ORGANIZATIONS (VO)

The consortium uses a concept of Virtual Organization or VO to allocate computing resources. A VO is a group of researchers who share a common research goal. 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 starts from a small number of VOs, and, hopes to have more VOs to cover other research areas in the future.

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 VO

COMPUTATIONAL SCIENCE AND ENGINEERING VO

COMPUTER SCIENCE AND ENGINEERING VO

3 VO

VO 1

High Energy Particle Physics Virtual Organization

VO's Head: Asst. Prof. 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 collaborations. The computing facilities provided by Chulalongkorn University (CU), Suranaree University of Technology (SUT) and the National Electronics and Computing Technology Center (NECTEC) are integrated into the Worldwide LHC Computing Grid (WLCG). This allow physicists from both universities to simulate the Monte Carlo events, or to analyze the experimental data using personal computers at their institutes. In parallel with the Tier-2 nodes, the local high performance computing clusters are built to support both physics community, and other scientific collaborations which need computing power, i.e. biology, computational chemistry, climate study, engineering, mathematics, and medicine. Since 2015, the study of physics for the future experiment and colliders, i.e. Future Circular Collider (FCC), can also be done using the same infrastructure.

CU Particle Physics Researches with CMS, CERN and Future Machines.

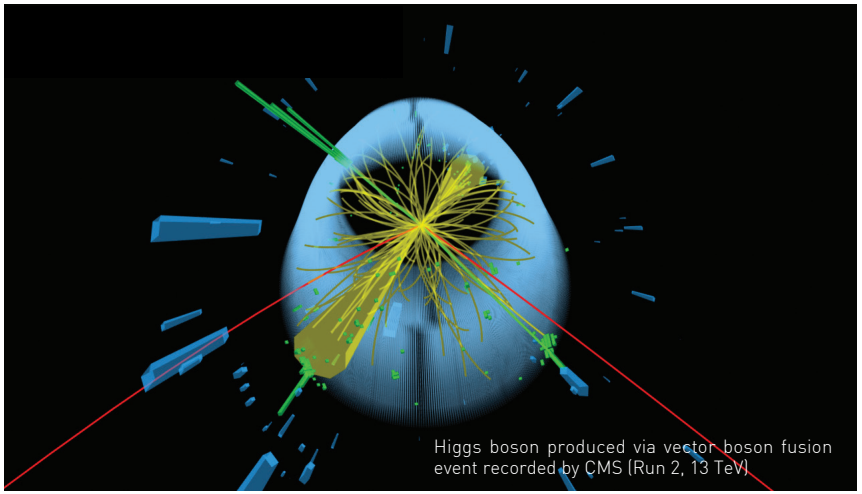
Dr. Norraphat Srimanobhas

The Particle Physics Research Laboratory (PPRL) at the 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 started to provide the proton-proton collision at the highest energy level, 13 TeV. With the colossal amounts of collected data in this several years, this may help physicists to explain more about the early universe and some unsolved problems.

We, physicists at CU, are currently interested in the standard model and beyond standard model physics. The current topics of interest include:

- Analysis of the Standard Model Higgs boson produced in association with a W or a Z boson and decaying to bottom quarks.
- Search for supersymmetric partners of the third generation quarks.
- Search for highly ionized particles.

In parallel with LHC physics, we also interest in neutrino physics at the Jiangmen Underground Neutrino Observatory (Juno) in China, and projection of Physics at 100 TeV for the future collider.



Higgs boson produced via vector boson fusion event recorded by CMS (Run 2, 13 TeV)

SUT Research

Asst. Prof. Dr. Chinorat Kobdej

Working under the center of excellence in Nuclear Physics High Energy and Particle Physics, the experimental particle physics group at SUT has just launched its activities and participated in international collaborations in the year 2011 with ALICE and PANDA. Having started in the simulation work for the upgrade of the ALICE Inner Tracking System (ITS) and PANDA Electromagnetic Calorimeter, later, the group has extended its research into the area of sensor development and testing by working together with Thai Microelectronics Center (TMEC) and Synchrotron Light Research Institute (SLRI). Recently, the group has also explored possibilities to work in neutrino physics with JUNO and dark matter search with PANDAX.

• PANDA (Anti-Proton Annihilation at Darmstadt)

SUT has joined PANDA in the year 2011 starting by setting up a GRID site for PANDA in Thailand and later working with researchers from Forschungszentrum Jülich in combining charged tracks with clusters in the Electromagnetic Calorimeter for PANDA.

• ALICE (A Large Ion Collider Experiment)

SUT is a full member of ALICE Collaboration since 2012 and participates in the Inner Tracking System(ITS) upgrade project. SUT has started by doing the detector simulations and the upgraded beam pipe studies. Now, the study has extended to cover material budget calculation for different stave models. Next, we plan to expand our studies to cover one or more physics channels related to the upgrade, especially in the sectors of charm baryons. Besides the current engagement in the detector and physics simulations, SUT has increased its activities into more hardware oriented areas such as sensor development/characterization and detector construction, assembly and test of detector modules. For sensor development, SUT works closely with Thai Microelectronics Center (TMEC) in the studies of resistivity profile of epitaxial layer of wafers, production of the dummy ships and fabrications of the silicon microchannel cooling unit. While in the sensor characterization, SUT has started a detector instrumentation group in Thailand by teaming up with the Synchrotron Light Research Institute (SLRI). SLRI is now developing 1.2 GeV electron beam test facility with the possibility to select the number of electron ranging from 100-1,000,000.

• JUNO (Jiangmen Underground Neutrino Observatory)

SUT joined JUNO as a full member in January 2016 and proposes to do phenomenological studies on two topics: i) Supernova neutrino and simulation and ii) Unitarity triangle and neutrino mixing parameters with matter effect. For hardware aspects, SUT will collaborate with CU to calculate and simulate the magnetic field produced by the shielding coils in veto region, then investigate the earth magnetic field (EMF) shielding test on the coil prototype, and finally install the EMF shielding coils around the JUNO center director.

• PandaX (Particle AND Astrophysical Xenon Time projection chamber)

SUT has joined PandaX in May 2016 and proposed to do the simulation of pulse shape to discriminate between the signals of Weakly Interacting Massive Particle (WIMP) and their background in Liquid Xenon Time Projection Chamber. SUT has also intended to do research and development for the acrylic panels inside the detector using the coating facility provided by SLRI and/or National Astronomical Research Institute of Thailand (NARIT).

The Activities

1. The 8th ALICE ITS upgrade, MFT, and O2 Asian Workshop at KMUTT Knowledge Exchange for Innovation Center (KX), Thailand, 5-6 Dec 2016

2. The 2nd ASIA TIER CENTER FORUM, Nakhon Ratchasima, Thailand, 30 Nov-2 Dec 2016

3. PANDA-Collaboration Meeting LVIII at Helmholtz-Institut Mainz, Germany, 12-16 Sep 2016

4. A group of 9 physicists from 3 Thai Institutes had participated in The 8th JUNO collaboration meeting in Beijing, China, 25-29 July 2016.

VO 2

Computational Science and Engineering Virtual Organization

VO's Head: Dr. Sornthep Vannarat

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.

CSE researchers 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. They 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.

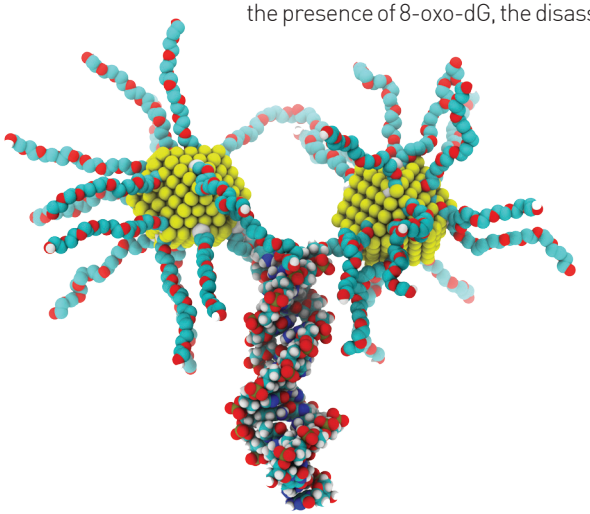
Designing Smart Nanoparticles for Nanomedicine

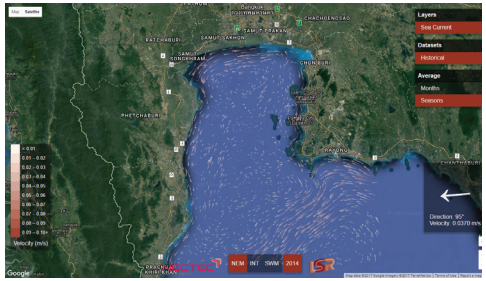
Asst. Prof. Dr.Theerapong Puangmali
Khon Kaen University

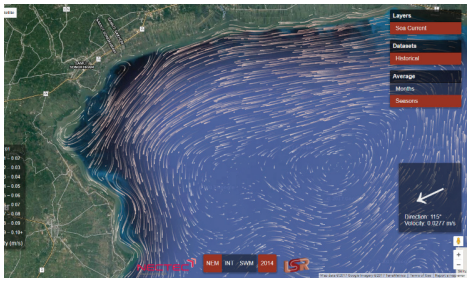
Computational simulation is therefore used to observe the interaction between the nanoparticles (NPs) and plasma membrane leading to the lucid understanding of how these nanoparticles travel through cell membrane. In addition to the study of the translocation through cell membrane, this opens the door for the realization of the toxicity of the nanoparticles and is also of great importance for the design of efficient drug delivery.

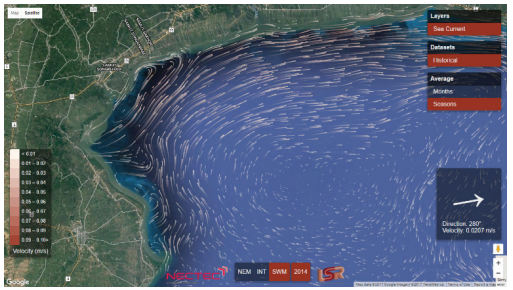
NPs can also be applied in biosensor. Herein, gold nanoparticles (AuNPs) are utilized as sensor probes for the detection of 8-oxo-dG which is a biomarker of cancer (cholangiocarcinoma). The working principle is based on the behavior of AuNPs in the solution. The solution is red provided that the NPs are uniformly distributed. Functionalized with single strand DNA, AuNPs can form dimer. In the presence of 8-oxo-dG, the disassembly of dimer is induced and the color of the solution is changed from blue to red. This can be observed by necked-eyes. To design smart biosensor, computer simulation is therefore used for the guideline of experimentalists.

The ultimate goal of our group is to design the functionalized nanoparticles that can be applied in drug delivery and biosensor. The study is beneficial for the design of the experiment as well-planed experiment can be designed by the computational simulation. Currently, our group is composed of PhD students, MSc students and undergraduate student. Recently, our undergraduate student was the winner from the research project competition in the Siam Physics Congress 2016 and was awarded the royal cup from Her Royal Highness Princess Galyani Vadhana, Princess of Naradhivas.









Coastal Ocean Circulation in the Gulf of Thailand

Sirod Sirisup, Saifhon Tomkratoke
National Science and Technology Development Agency

Reports from the many public organizations including DMR emphasize the severity of coastal erosion and accretion problems along Thai coastline nowadays. More than 800 kilometers along the coast have been facing such issue in various degree with the extreme rate of five meter per year. The problem greatly affects Thai coastal communities along the coastline hurting Thai's economy directly and indirectly intensifying Thai's social problems.

The project aims at developing mathematical model and generating knowledge on ocean circulation in the Gulf of Thailand. This circulation is resulted from the monsoon winds, tides and river discharges has the direct influence on sediment transport process. The mathematical model for wave and current interactions for a particular area is also developed as a tool to investigate the impact of the wave to shoreline in the area.

Coastal Ocean Circulation Visualization system is one of the project outputs. The system can be accessed through http://chaophraya.lsr.nectec.or.th/seacurrent. The system allow user to interactively visualize the monthly mean and seasonal mean velocity of the Gulf of Thailand in high resolution dynamically. The system can support and helps provide guidelines in deriving more overall, effective, efficient and sustainable erosion mitigation schemes.

VO 3

Computer 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.

KitWai:
Large-scale Data Analytics Cloud Platforms

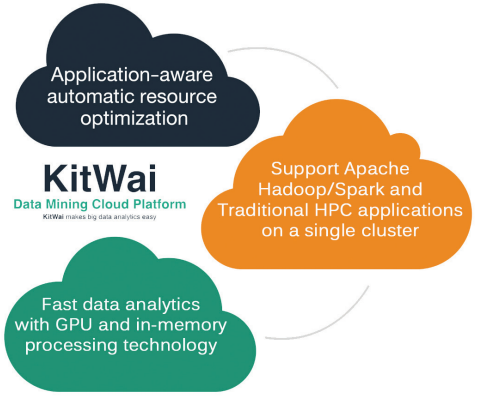
Dr. Ekasit Kijsipongse and Dr. Apivadee Piyatumrong
National Science and Technology Development Agency

In our data-driven world, scientists make use of data and insights derived from data to solve problems or discover the facts about nature. Modern data analytic techniques like data mining and machine learning are the top tools that have successfully been applied in various scientific disciplines to gain such insights. Applying these analytic techniques to process data having large volume, velocity and variety (the so-called big data) requires computing capabilities available from HPC systems in order to get the solution within a reasonable time. However, complexity arises from the heterogeneity of HPC architectures and tools comprising data analytics platforms, for example, lack of skills to configure the analytics tools or not being able to write programs to work efficiently on the HPC. This complication causes many hindrances for scientists to carry out their data analysis.

KitWai is a data analytics platform as a service (PaaS) on cloud computing. Users can provision an HPC cluster with the ability to scale up/down the cluster on-demand from the computing resource pool. The cluster comes with preconfigured and optimized data analytic tools such as the most well-known open source software, Apache Hadoop and Spark. As parts of the current research, KitWai focuses on using GPUs to speed up the performance of big data analytic tasks, as well as context-aware self-optimization platforms.

Contact us: kitwai@nectec.or.th

https://www.nectec.or.th/innovation/innovation-software/kitwai.html

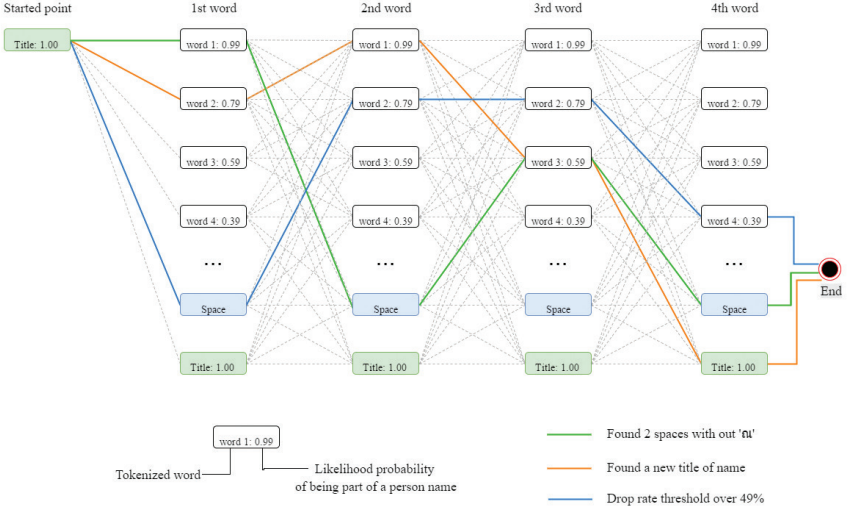


Natural Language Processing

Assoc. Prof. Dr. Tiranee Achalakul
King Mongkut's University of Technology Thonburi

Named Entity Recognition (NER) is very important in many natural language processing tasks, especially information extraction. The problem of NE extraction in Thai is much more complicated than English because Thai language lacks orthography and boundary indicator between words. In this project, we worked on NER with the emphasis on person name recognition (PNR) in Thai text. Our proposed method consists of 4 steps. First, text is tokenized into a set of words. Second, a part-of-name probability is computed for each word using Odds with Laplace smoothing and Logistic function. Third, name candidates are selected based on the likelihood probability. Finally, the end point of name is identified using a set of rules and a drop rate threshold. We then evaluated our method using 1,700 online news from the InterBEST 2009 corpus. The results show that the proposed method yields average precision, recall, F-measure and accuracy at 75.21%, 98.10%, 85.15%, and 81.05% respectively. This research was conducted as a part of the E-Science collaboration network.

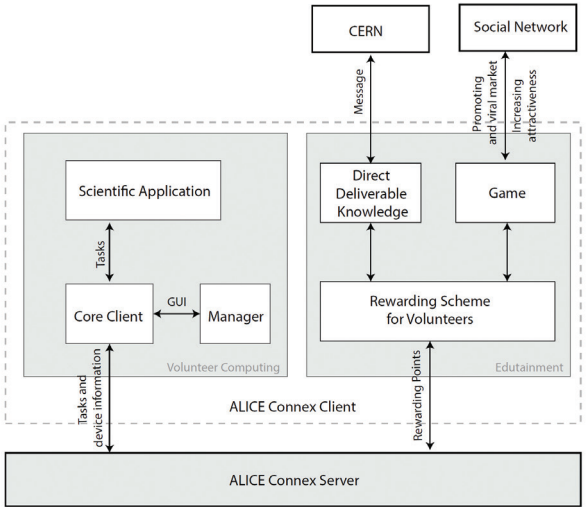
Identifying the End point of names



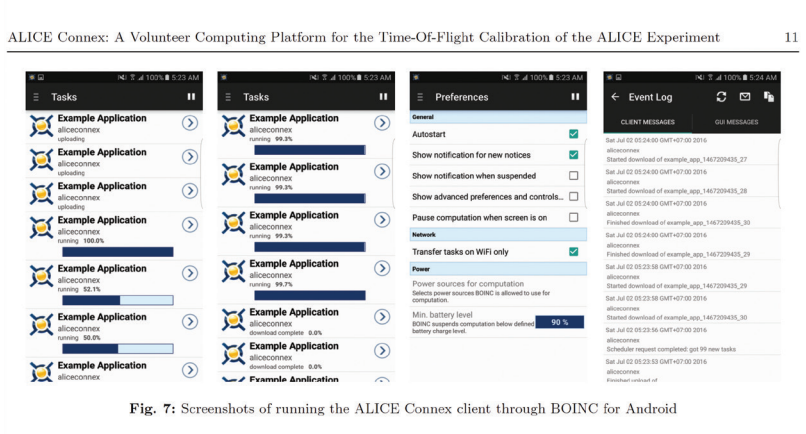
Thai-CERN Collaboration Project

Assoc. Prof. Dr. Tiranee Achalakul
King Mongkut's University of Technology Thonburi

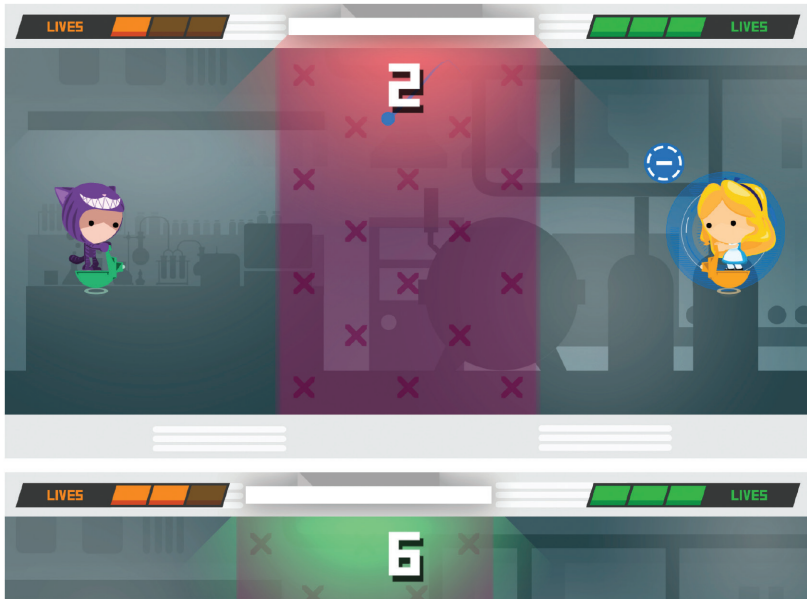
In this project, we propose the design and implementation of the ALICE Connex platform. ALICE Connex is a prototype of a volunteer mobile computing platform for the ALICE experiment at CERN. Untapped computing power of smartphones can be aggregated and exploited to help in the calibration of the ALICE's Time-of-Flight (TOF) particle detector. ALICE Connex is built based on the Berkeley Open Infrastructure for Network Computing or BOINC, which is a well-known volunteer computing middleware. In addition, ALICE Connex offers an outreach service to connect the ALICE experiment to the general public in Geneva and Bangkok by way of a game-based edutainment. Materials on basic physics can be delivered through our game. Students can get game coins for in-app purchases by donating computing time on their mobile devices to help the ALICE experiment. We believe that by offering a chance for students to be a part of the big experiments at CERN, they will be more excited about Science.



The connection between our volunteer computing front end and edutainment module



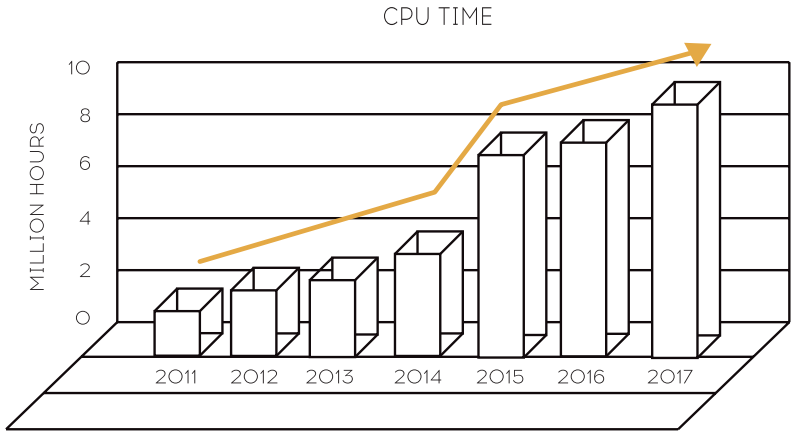
Screenshots: Running the ALICE Connex client app on Android



The ALICE Connex game

Achievements and Impacts

- Computing resource usages.



- Publications

Between the fiscal year 2011 and 2016, there are 167 research projects from 35 institutions using computing resources. The researchers have produced 417 publications as shown in the table below:

	International Journal	National Journal	International Conference Proceedings	National Conference Proceedings	Other	Total
2011						40
2012	17	1	12	15	7	52
2013	17	-	28	6	21	72
2014	47	1	18	5	15	86
2015	40	17	21	3	17	81
2016	37	1	18	5	26	86


1.


4.


2.

5.

3.

1. Workshop on Introduction to Smart Data at Kasatsart University
2. Workshop on Practical VASP for Materials Design at Chiang Mai University
3. Support computing resources for computational chemistry challenge
4. Panel Discussion on Big Data for National Productivity and Safety
5. Conference Exhibition at ANSCSE 20th, Kasatsart University

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Mr. Nart Liuchareon	Advisory
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President of King Mongkul's University of Technology Thonburi	Committee
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Director of National Astronomical Research Institute of Thailand (Public Organization)	Committee
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Head of Network Technology Laboratory, National Electronic and Computer Technology Center	Committee
Director of University Office of Information Technology, Chulalongkorn University	Committee
Director of the Center for Computer Service, Suranaree University of Technology	Committee

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