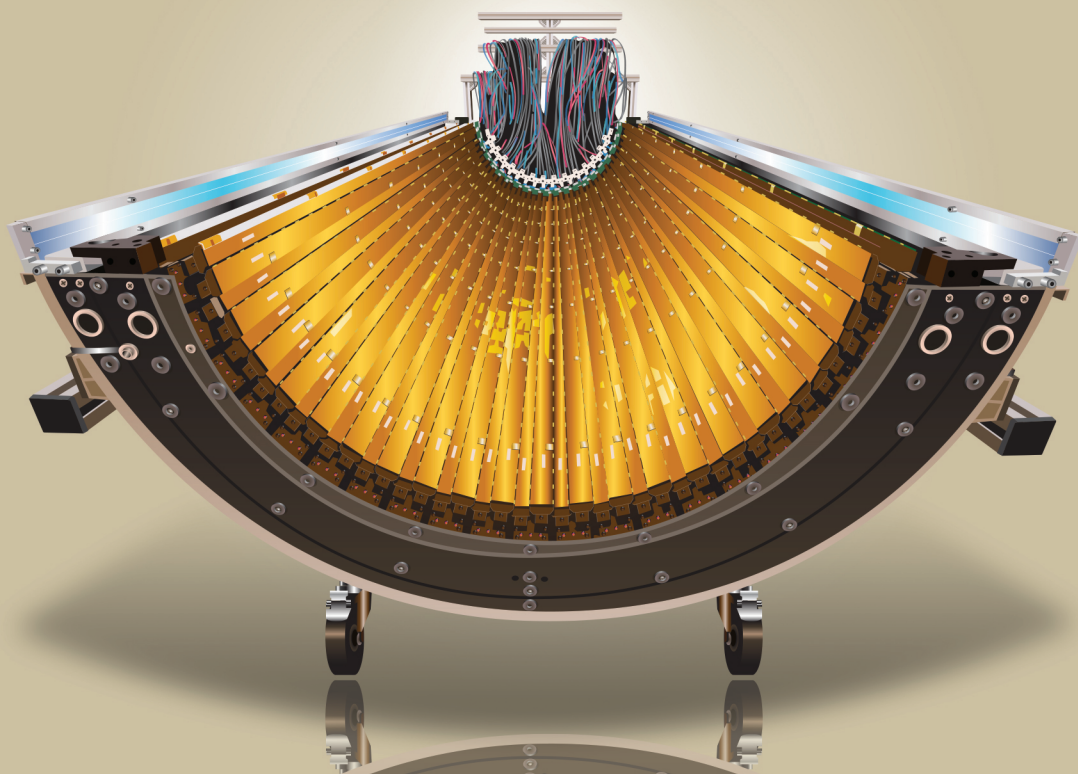


# e-Science 2020

[www.e-science.in.th](http://www.e-science.in.th)



## “World Class Innovation Project from Thailand”

This figure shows the bottom section of the outer barrel, which is a part of the Inner Tracking System (ITS) of the ALICE experiment. Researchers from Suranaree University of Technology, Thai Micro Electronics Center (TMEC), and Synchrotron Light Research Institute (SLRI) have participated in this intense global R&D program since the year 2012.

# e-Science 2020

This booklet gives an overview of the information on the National e-Science Infrastructure Consortium including motivations, current status and achievements of the consortium. Short introduction to each member institute, 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 computing resources for research can contact the consortium office or email: [contact@e-Science.in.th](mailto:contact@e-Science.in.th)



The Inner Tracking System (ITS) of the ALICE experiment is a detector located next to the beam pipe in which particles generated by a Large Hadron Collider (LHC) collide. Its function is to record trajectories of charged particles scattering out of the collision point. The new ITS consists of seven cylindrical layers of high-speed CMOS sensors. By collaboration with this research project, Thailand has obtained advanced knowledge of CMOS technology from ALICE, CERN, and their potential applications in making the proton Computed Tomography (pCT) prototype for medical usages.





Her Royal Highness Princess Maha Chakri Sirindhorn's first visit to CERN on May 18, 2000.  
Photo from CERN

*"I hope that this collaboration can lead to better and conflict-free international corporation based on the scientific principle. For the Thai scientists, researchers and students involved, to be accepted for participation in a scientific endeavor like this is a very positive sign on our standard of education and quality of the people"*

Remarks of Her Royal Highness Princess Maha Chakri Sirindhorn on the occasion of the presentation of an Honorary Doctorate in Physics from Suranaree University of Technology to Professor Rolf-Dieter Heuer, the director of CERN at Sra Pathum Palace in Bangkok on October 10, 2013



## The 20<sup>th</sup> year Anniversary of the Thai-CERN Collaboration

Over 20 years, several collaborations between Thailand and CERN (The European Organization of Nuclear Research) has been established by the initiative of Her Royal Highness Princess Maha Chakri Sirindhorn. In 2000, Her Royal Highness paid the first visit to CERN and since then, she has paid . another five visits. Her Royal Highness wishes to see Thai scientists have the opportunity to collaborate with CERN in high-energy physics and relate technologies. On her third visit in March 2019, Her Royal Highness presided as a chairperson in the signing of “The Expression of Interest in Participation from Thailand in the CMS Experiment at the CERN LHC Accelerator”. Such collaboration has opened an opportunity for Thai physics students and teachers to participate in a CERN summer program and join in experiments in high-power particle physics. After this, there are several Memorandum of Understandings between Thai institutes and experiment at CERN on various areas.

The National e-Science Infrastructure Consortium, a program initiated by Her Royal Highness after she visited CERN for the third time, was established with the purpose to develop the High Performance Computing (HPC) resources. These HPC resources facilitate Thai Scientists to compute and store the LHC data from CERN. Besides the collaboration with CERN, Her Royal Highness wanted Thai scientists to get the most beneficial from this national infrastructure. This leads to the expansion of services and applications to other scientific areas such as Computational Science and Engineering.

This booklet was published on occasion of the 20th year anniversary of the Thai-CERN collaboration. The purpose is to provide a summary of the collaboration on High Energy Particle Physics between Chulalongkorn University and Suranaree University of Technology. The details are presented in High Energy Particle Physics Virtual Organization, page 26 – 29.

## Collaborative Activities of Thai Institutes and CERN



Students (high school) visit at CERN, 2019

Scholarships for students and Physics teachers to join CERN Summer student Program and CERN Physics High School Teacher Program.



Activities of CERN Summer School, 2019

Programs for distribution of knowledge of Particle Physics, operated through various programs, such as CERN School Thailand (Master and Doctor), and Thailand Experimental Particles Physics Novice Workshop (Graduate level).



MOU Signing of CU, SUT, NSTDA and WLCG, 2013

A joint research between Thai researchers working with CERN and CERN scientists.



MOU Signing of e-Science Consortium, 2011

The National e-Science Infrastructure Consortium collaboration to develop computing infrastructure and networking support to CERN and other research areas.



## Message from Advisor of the Steering Committee National e-Science Infrastructure Consortium

The year 2020 is the 20th anniversary of Thailand and CERN (The European Organization for Nuclear Research) collaboration which is one of the science and technology initiatives of H.R.H. Princess Maha Chakri Sirindhorn. The collaboration not only provides benefits on expanding knowledge and expertise in high-energy physics and related technologies but also on establishing the foundation of The National e-Science Infrastructure Consortium in 2011 which aims to develop computational instrument, data storage and fundamental datasets as a sustainable infrastructure to support research in Thailand.

At present the consortium has nine regular members that are from universities and research institutes. Furthermore, we are pleased to announce the launch of NSTDA Supercomputer Center or ThaiSC which is one of our consortium's supporting centers located in Thailand Science Park. Its mission is providing cutting-edge high performance computing research and service for the national R&D community.

Although our consortium has predominantly focused on several areas of research interest relevant to computational science and engineering, computer science and engineering, water resource, energy and environment management, climate change, and high energy particle physics, we have provided some computational resources and services for other research projects. In addition, we also currently provide our resources and services to projects working on the 2019 Coronavirus disease (COVID-19) pandemic and related topics in order to assist scientists to speed up science, technology and innovation discovery to fight against the pandemic.

The mission of the consortium has been successful because of the great dedication of all members for years. I, therefore, would like to thank to all members for strengthening the consortium and fondly anticipate seeing the consortium's next successful years filled with great accomplishments and with great collaboration.

**Prof. Dr. Pairash Thajchayapong**

Secretary General, Information Technology Foundation under the Initiative of H.R.H. Princess Maha Chakri Sirindhorn  
Senior Advisor to the President, National Science and Technology Development Agency



## Message from Chairperson of the Steering Committee National e-Science Infrastructure Consortium



The National e-Science Infrastructure Consortium is one of the projects under Her Royal Highness Princess Maha Chakri Sirindhorn initiatives. With a launch of the NSTDA Supercomputer center (ThaiSC) last year, 2019, as one of the National Science and Technology Infrastructure (NSTI), we have a plan to promote our activities together with ThaiSC for wider research communities in Thailand, including industries.

However, due to the Covid-19 outbreak worldwide, working from home is going to be a new normal even for the research communities in Thailand. In this crisis, we would like to explore if it is possible for our users, whose homes are scattered throughout the country, to access our resources located at various places in Thailand.

The stability and security of network infrastructures within our country are among the topmost key factors since they guarantee the accessibility, availability, and reliability of all resources associated with the consortium. Besides, the user-friendly interface and web portal are the essential parts to interact with our users. It is interesting to see whether the consortium could facilitate in developing a common framework or a service portal to serve our Thai researchers by exchanging ideas with our international collaborators and partners.

During pandemic and economic recession, I would like to urge all members of the consortium to work more closely together and coordinate our activities remotely so that mutual benefits can be fully achieved and realized by our society.

Assoc. Prof. Dr. Weerapong Pairsuwan  
Rector of Suranaree University of Technology

# ANNOUNCEMENT

## "New and most advanced resource"

**NSTDA Supercomputer Center (ThaiSC)**, founded in 2019, is one of the national science and technology infrastructure (NSTI) located in Thailand Science Park. As a leadership center, ThaiSC aims to provide cutting-edge high performance computing research and service for national R&D community.

### Vision

Leading HPC facility and computational science R&D center in ASEAN

### Mission

1. Provide HPC computing service for Thailand R&D
2. Perform frontier computational science R&D
3. Promote development of HPC workforce
4. Develop HPC roadmap for Thailand
5. Establish HPC partnership and visibility

### ThaiSC Resource in 2020

- 4,320 compute cores
- 28 NVIDIA V100 GPU
- 0.8 PB Storage
- 42.2 TB overall memory

### Planned ThaiSC Resource in 2022

- > 28,000 compute cores
- > 200 NVIDIA A100 GPU
- > 5 PB storage
- > 100 TB memory

### Who are ThaiSC Users

Scientist and Engineer with HPC demands to rapidly boost research and innovation development

- Basic research
- Frontier & Big Science
- Industrial problem
- Translational R&D
- Multi-disciplinary R&D

**Contact Detail**

[www.thaisc.io](http://www.thaisc.io)

E-mail: [thaisc@nstda.or.th](mailto:thaisc@nstda.or.th)

## Contents

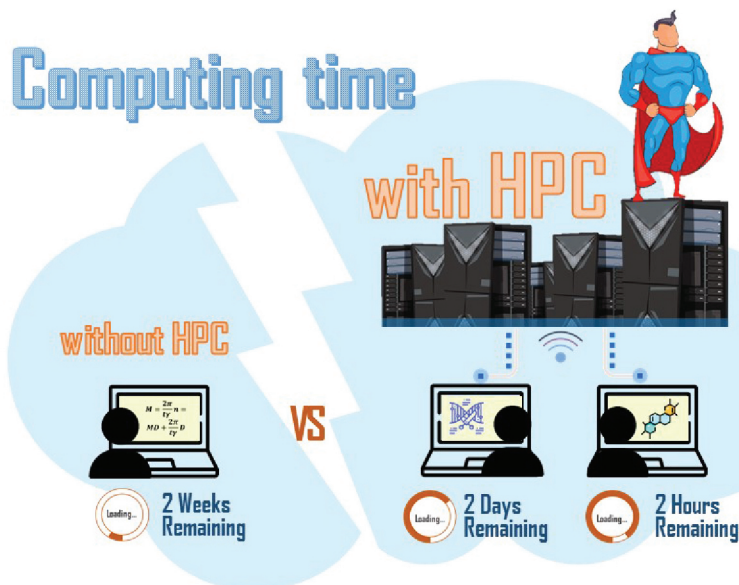
○ The 20th year Anniversary of the Thai-CERN Collaboration	2
○ Message from Advisor of the Steering Committee	4
○ Message from Chairperson of the Steering Committee	5
○ What is HPC?	8
○ What is National e-Science Infrastructure Consortium?	10
○ e-Science Members	12
○ Chulalongkorn University	12
○ Digital Government Development Agency	13
○ Hydro Informatics Institute	14
○ King Mongkut's University of Technology Thonburi	15
○ National Astronomical Research Institute of Thailand	16
○ National Science and Technology Development Agency	17
○ Synchrotron Light Research Institute	18
○ Suranaree University of Technology	19
○ Thailand Institute of Nuclear Technology	20
○ HPC Resources 2020	21
○ HPC Resources 2020	21
○ Connection with CERN	22
○ Virtual Organizations	24
○ High Energy Particle Physics Virtual Organization	26
○ Computational Science and Engineering Virtual Organization	30
○ Computer Science and Engineering Virtual Organization	33
○ Business and Industrial Communities Supported by ThaiSC	36
○ Achievements	37
○ Committee and Working Group	39
○ Contact detail	41

## What is HPC?

High-Performance Computing: A set of computers built to handle advanced computational and engineering problems. HPC consists of several computing-intensive nodes, GPU node, large memory per node, and vast storage capacity. It is an essential tool in many innovative applications by increasing the ability to process massive amounts of data and carry out complex computations in industrial and scientific sectors. Altogether, HPC offers maximum efficiency and speedy results.

HPC is most used for 2 types of problems:

- Highly complex work that requires a large processor to solve problems, e.g., weather forecasts and climate change.
- High throughput for medium to large works, including many sub-works. Many processors are required for complex tasks, e.g., drug design and animation.

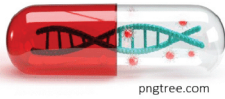


Wait times for complex calculations are drastically reduced by using the power of multiple processors!

Source: <https://www.pomona.edu/>

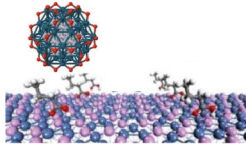


## HPC Use Cases



pngtree.com

**Genomics & Drug design –**  
Sequencing personalize  
medicine

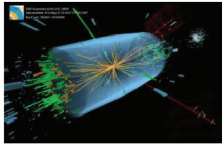


**Chemistry –** nanomaterial,  
efficient catalysts and new  
methods of energy storage



pngtree.com

**Physics –** Simulations of  
space affects Earth



**High energy particle physic –**  
study dark Matter



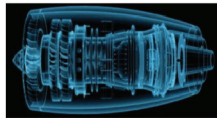
pngtree.com

**Environmental –** Climate  
simulation, weather  
forecasting, and early  
warning



pngtree.com

**Agriculture –** management of  
water and resources,  
numerical simulations of plant  
growth, estimate plant  
genetic

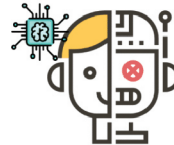


epsrc.ukri.org

**Energy Consumption,**  
Simulate industrial power  
generation



**Services –** optimizes supply  
chains, logistic management,  
risk analysis



flaticon.com

**AI – Machine learning**



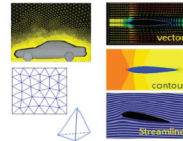
pngtree.com

**Financial Analysis, future  
trade, stock analysis**



blender.org/

**3D Animation - Rendering**



**Industrial –** Product  
prototyping in automotive,  
aerospace, and  
pharmaceutical industries

## What is National e-Science Infrastructure Consortium?

The National e-Science Infrastructure Consortium was 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. The objective of the collaboration is to help support computational science, Big Data and AI in Thailand. The consortium members provide computing systems which support High-Performance Computing (HPC) and Cloud Computing infrastructures.

The consortium maintains e-Science-related research projects in general, but with an emphasis on climate change, high-energy particle physics, drug design and material design. The number of research projects has increased rapidly in the past few years and scalability of computing resources is always needed. Four new organizations have joined the consortium to support this growth: National Astronomical Research Institute of Thailand, Electronic Government Agency, Synchrotron Light Research Institute, and Thailand Institute of Nuclear Technology.

Last year, the consortium supported computing resources for 112 research projects in both academic and industrial sectors. Our users consist of more than 102 researchers and students. In the coming year, we will increase the number of computing resources to support various applications, and promote the consortium in order to enhance the HPC community.

## Objective

Our objective is to collaboratively develop sustainable e-Science infrastructure that supports 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. High Performance Computing Cluster project at Chulalongkorn University had been set up 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. In 2012, we were the first ASEAN university to officially join the Compact Muon Solenoid (CMS) Collaboration at the European Organization for Nuclear Research (CERN).

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 2<sup>nd</sup> Century Project Advancement Project. CUniverse research is dedicated to theoretical, experimental and astrophysics. Topics of interest include physics beyond Standard Model, including supersymmetric particles, Large Extra Dimensions (LED) of spaces, dark matter, superstring theory and supergravity. In 2019, CUniverse-Phase 2 has started. The additional effort is to combine several academic disciplines or professional specializations between faculties in Chulalongkorn University, for example, an effort between Physics and Computer engineering to develop the new e-Science computing cluster and CMS Tier-2 on private cloud technology, or between Physics and Electrical engineering to develop the magnet coil model for Jiangmen Underground Neutrino Observatory (JUNO).





## Digital Government Development Agency

Digital Government Development Agency (Public Organization) (DGA) is under supervision of the Prime Minister, the Office of Prime Minister. The Prime Minister has assigned Deputy Prime Minister [Mr.Somkid Jatusripitak] to supervise the DGA on his behalf. The DGA's duty is to provide services and supports to all government agencies with regard to digital government transformation. At present, the DGA's core mission is to Promote and endorse the integration and exchange information among government agencies, and Implement standards, and approaches in the form of digital technology as well as the transaction process in order to bridge information and work systems among government agencies legitimately and concordantly.

DGA also provides Government Cloud, also known as G-Cloud, is an infrastructure component with shared resource for several government agencies, where sources of information will be stored on the Internet. G-Cloud offers a broad range of benefits to various IT-based services, where government personnel can generate greater working performance to ensure the highest quality of public services for everyone.



## Hydro Informatics Institute

Hydro Informatics Institute (HII), a public organization under the Ministry of Higher Education, Science, Research and Innovation, 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, because water and agriculture is the backbone of Thailand's economy, HII's researcher on water resource management. Since 2010, HII has maintained High Performance Computing facilities that enable researches branching from intelligent monitoring systems, weather and flood monitoring, simulation, information processing, and information dissemination to support policy makers in coping with flood and drought management in Thailand.

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 the 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 research and development to the new height.

KMUTT research teams work on high performance computing and mobile sourcing platforms are performed in collaboration with the European Organization for Nuclear Research or CERN, Switzerland. Frontier research teams work on Quantum information, computing, and programming, collaborate with many universities in Thailand and Japan. In addition, new trend on big data, the analytical modeling is researched for consulting and training with the organizations in Thailand. Moreover, the research teams also work on scientific and mathematic research based on computational platform, such as bio-engineering and bioinformatics, computation fluid dynamics, and material science and engineering.

KMUTT education teams build the manpower to serve our country with new learning tools and techniques. Including new curriculums that have a direct answer to Thailand and International market, such as Health Data Science and Computational Science program that results in publics, award winning, and start-up companies.

KMUTT believes that National e-Science Infrastructure Consortium will be an important platform that contributes to Thailand's competitiveness in the global economy and KMUTT will support for 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. NARIT 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 meters (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-meter "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 partner institutes both national and international.





## National Science and Technology Development Agency

NSTDA, under the administration of Ministry of Higher Education, Science, Research and Innovation. NSTDA plans and executes four mandated missions of research and development, technology transfer, human resources development, and, infrastructure development. NSTDA is comprised of four national R&D centers: BIOTEC, MTEC, NECTEC, and NANOTEC. As part of NSTDA's strategic plan, the Focus Centers, the National Quality Infrastructure Centers, and the National Science and Technology Infrastructure (NSTI) have launched. One of the NSTI facilities is the NSTDA Supercomputer Center (ThaiSC). ThaiSC aims to perform frontier research in computational science, data analytics and AI as well as provides high performance computing service to researchers in Thailand.

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 Technologies in Thailand. Its laboratories have been using computational approaches in research areas such as nanoscience, molecular biology, bio-informatics, engineering designs, environmental sciences, big data and AI. Furthermore, the areas of networking infrastructure, technology and application development are also very active.



### **Synchrotron Light Research Institute**

Synchrotron Light Research Institute (SLRI) is a public organization under supervision of the Ministry of Science and Technology, Thailand. The institute operates “Siam Photon Laboratory” (SPL) which is the first synchrotron facility of Thailand, providing synchrotron radiation and total solutions for users from academic and industrial sectors. The wide spectral range of synchrotron light, with photon energies spanning from infrared to x-rays make it an indispensable investigating tool for a variety of applications. Currently, SPL utilizes 7 techniques with 11 experimental stations and 2 stand-alone industrial research labs ready to welcome both domestic and international users.



## Suranaree University of Technology

Suranaree University of Technology (SUT) is Thailand's first autonomous university and was founded on 27 July 1990. It is located in the north-eastern part of Thailand, approximately 250 kilometers or a three-hour drive by car from Bangkok. SUT was chosen to be "one of nine national research universities," in 2010, a university providing excellence in research and teaching in Thailand. SUT is the first state university to become a "University of Technology," with emphasis on training and research in science and technology, with Baccalaureate, Masters, and Ph.D. programs. Every year, around 2,500 students graduate after studying in one of the seven institutes, for Science, Engineering, Agricultural Technology, Social Technology, Nursing, Medicine, and Dentistry. From SUT's graduates, 96% obtain jobs, with initial salaries among the highest in Thailand. From the assessment of the research of the individual schools conducted by the Thailand Research Fund (TRF), the School of Physics has received 1<sup>st</sup> excellence for Thailand for 10 consecutive years, 2008-2017.





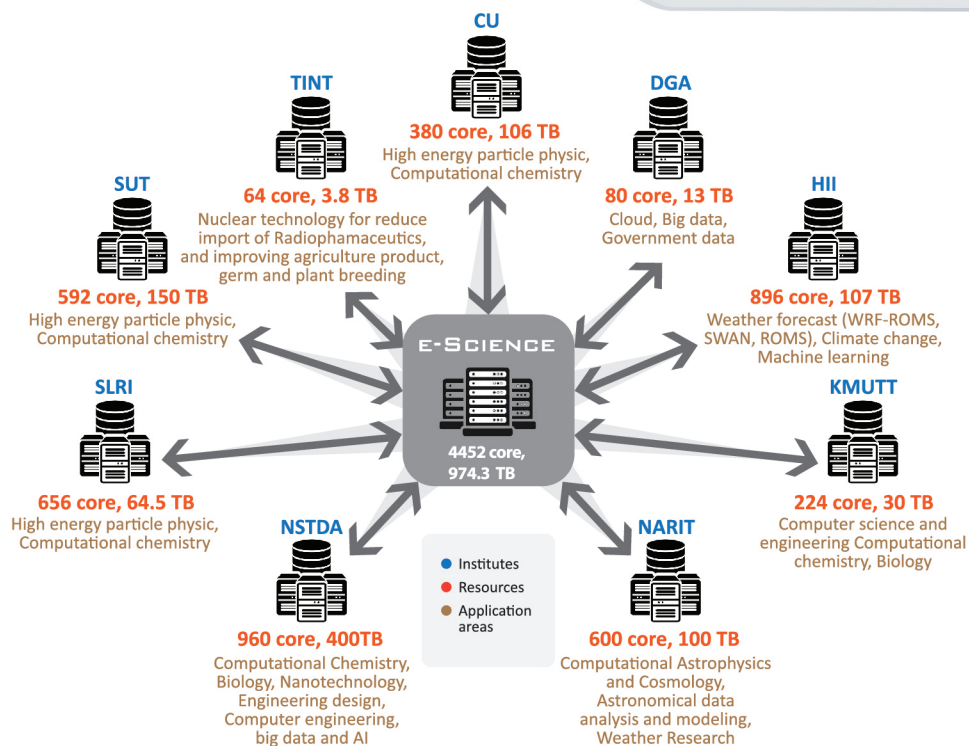
### **Thailand Institute of Nuclear Technology**

Thailand Institute of Nuclear Technology (TINT) is a public organization under the Ministry of Science and Technology. On 21st April 2006, TINT was separated from the Office of Atoms for Peace and then the organization was reformed to focus on nuclear technology research and application. TINT provides facilities such as nuclear reactor, electron accelerator, gamma irradiation, radiopharmaceutical production laboratory, and isotope hydrology laboratory. These facilities increase the capability and competitiveness of Thai research and industry. In the future, TINT will be able to install new facilities include cyclotron for radiopharmaceutical production, TT-1 Tokamak for plasma and fusion research, and next-generation of Thailand nuclear reactor.



## HPC Resources in 2020

The resources of National e-Science Infrastructure Consortium are provided by each member. These include computing time and scientific applications. The resources of each member may have different architectures and application bases according to the individual objectives and missions. However, the consortium strives to customize contributions to each research project and the existing infrastructure.



HPC resources of e-Science members in 2020

Available software packages depend on which cluster users are using. Each member has specific commercial licenses and various open-source software to serve users. Users are also welcome to install their own licensed software packages.

## Connection with CERN

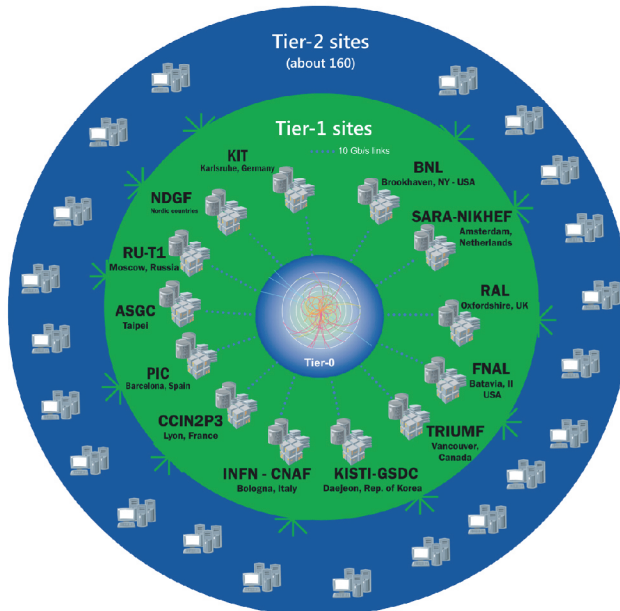
High energy particle physics is a research area that the consortium supports, particularly through research collaborations with CERN. We anticipate supporting the JUNO experiment in China when it starts operation.

At CERN, seven experiments have been set up around the world's largest and most powerful particle accelerator, the Large Hadron Collider (LHC). These experiments use different designs and techniques of particle detection to detect the myriad particles produced by collisions in the accelerator. They are run by collaborations of scientists from institutes all over the world. Chulalongkorn University (CU) contributes to the CMS experiment by investigating a wide range of physics phenomena where highly massive particles can be produced from the proton-proton collisions. Suranaree University of Technology (SUT) and King Mongkut's University of Technology Thonburi (KMUTT) joined the ALICE experiments, which use a heavy-ion detector to study the quark-gluon plasma state, a state of matter thought to have formed just after the Big Bang.

To join the CERN collaborations, Thailand became a member of the Worldwide LHC Computing Grid (WLCG). The MOU was 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 centers in 42 countries, linking national and international grid infrastructures. Currently, Thailand has two Tier-2 sites: the ALICE Tier-2 experiment located at SUT, Nakhon Ratchasima; and the CMS Tier-2 located at CU.

## Tier Centers

WLCG is made up of four layers, or "tiers"; 0, 1, 2 and 3. Each tier provides a specific set of services



**Tier 0:** safe-keeping of the raw data (first copy), first pass reconstruction, distribution of raw data and reconstruction output to the Tier 1s, and reprocessing of data during LHC down-times.

**Tier 1:** safe-keeping of a proportional share of raw and reconstructed data, and safe-keeping of corresponding output, distribution of data to Tier 2s and safe-keeping of a share of simulated data produced at these Tier 2s.

**Tier 2:** store sufficient data and provide adequate computing power for specific analysis tasks. They handle analysis requirements and proportional share of simulated event production and reconstruction.

**Tier 3:** Individual scientists will access these facilities through computing resources, which can consist of local clusters in a University Department or even just an individual PC. There is no formal engagement between WLCG and Tier 3 resources.

# Virtual Organizations

The consortium uses concept of Virtual Organization or VO which is 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 computing resources and exchanging knowledge and experience.

The consortium realizes that achieving the profound collaboration within a VO is extremely challenging. Each Head of VO have a certain level of existing collaborations. Therefore, the consortium starts with a small number of VOs, for instance, High Energy Particle Physics VO, Computer Science and Engineering VO, and Computational Science and Engineering VO. In the future, we hope to have more VOs to cover other research areas.





**HEP****High Energy Particle Physics****Head: Asst. Prof. Dr. Burin Asavapibhop, CU**

The HEP VO emphasis is on building Tier-2 nodes namely, T2-TH-CUNSTDA and T2-TH-SUT to serve ALICE and CMS collaborations. These allow physicists from Thailand to simulate Monte Carlo events, or analyze the experimental data using personal computers at their institutes.

**CSE****Computational Science and Engineering****Head: Dr. Chalee Vorakulpipat, NSTDA**

The CSE is a discipline where computer simulation is used as a main tool to pursue scientific research and technology development. CSE researchers need to have a model that accurately captures essential physical phenomena yet is not too computationally complicated to be handled by available computing resources. They also optimize the model to consider more realistic systems and case studies.

**COM****Computer Science and Engineering****Head: Assoc. Prof. Dr. Tiranee Achalakul, KMUTT**

CSE VO is set up with the mission to support research works in the area of HPC and its applications, and to promote the importance of HPC in enhancing scientific advancement and technological innovation in the country. Our research projects are mostly multi-disciplinary works that emphasize computational modeling, simulation, and visualization methodologies.

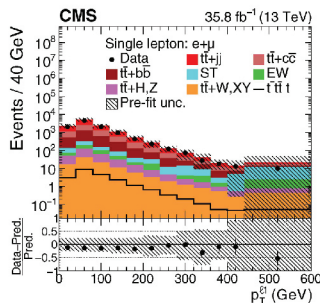


## High Energy Particle Physics Virtual Organization

### High Energy Physics at CU

Chulalongkorn University is the first university in Thailand and in ASEAN that has collaborated unofficially with CERN through the "Compact Muon Solenoid (CMS)" experiment since 2002. CMS experiment is a collaboration with approximately 4000 between physicists, engineers, computer scientists, technicians and students from around 200 institutes and universities from more than 40 countries. On July 14, 2012, Chulalongkorn University officially became a member of the CMS Collaboration. Her Royal Highness has granted the privilege to preside over the MOU signing ceremony between CMS and Chulalongkorn University held in Sra Pathum Palace, Her Royal Highness residence. Since then, Thai researchers have taken part in one of the world's leading experiments in the Higgs discovery, dark matter search and searches for physics beyond the standard model.

Currently, our topics of interest include Higgs, top quark, and beyond standard models physics. Research topics are varied from searching for new particles, measuring of the standard model in more precision, and improving analysis techniques, for example, applying modern machine learning techniques.



**Picture: A**

Combined lepton transverse momentum distribution in the search for the production of four top quarks in the single-lepton channel.

In addition to physics research, Chulalongkorn University also contributes to CMS in several ways. We contribute to the coordination area call "Physics Performance and Dataset (PPD)". PPD is responsible for the processing of the collision data recorded ( $\sim 10\text{B}$  events per year) with the detector, and for the production of simulated events ( $\sim 15\text{B}$  events per year). On the engineering side, we start participation in the new CMS endcap calorimeter project, target to operate in 2026. We also participate in the "Offline and Computing (O&C)" coordination area, to study the probability to improve CMS software using computer engineering techniques and to set up the high performance computing cluster project at Chulalongkorn University to support CMS and the National e-Science Infrastructure Consortium. The cluster has been operated since 2010. Currently, there is an effort between Physics and Computer engineering departments to build the new computing cluster and CMS Tier-2 on private cloud technology and to support GPU processing.

Furthermore, we are expanding our international research network internationally. Several engineering, physics student projects have been done with international collaborations such as the Jiangmen Underground Neutrino Observatory (JUNO) experiment, the Belle experiment, and the Karlsruhe TRitium Neutrino (KATRIN) experiment.

### CMS Activity in Thailand



#### CMS Remote Week 2019.

16-20 December 2019, Bangkok, Thailand, hosted by Chulalongkorn University. The CMS Collaboration members are meeting at Chulalongkorn University, Bangkok to discuss plans for the rest of Long Shutdown 2 (LS2), the upcoming LHC Run 3 and beyond.



## High Energy Particle Physics Virtual Organization

### High Energy Physics at SUT and its Activities in Short

The Nuclear and Particle Physics Research group at SUT was founded in 2000 by Prof. Yupeng Yan. In the beginning, we focused on the theory of the strong nuclear interaction, in particular hadronic interactions, exotic atoms, and chiral quark models. Within these fields, we have established fruitful and ongoing collaborations with groups from the University of Tübingen and GSI in Germany and the Institute of High Energy Physics in China. Later, we expanded our scope by investigating collective effects of the strong interaction in heavy-ion collisions, mainly via transport model studies with QMD and UrQMD. Hereby, significant progress in the understanding of hypernuclei production as well as strangeness and fluctuation phenomena was achieved also through new scientific collaborations and regular exchange visits with partners from Goethe Universität, Germany and the Chinese Institute of Atomic Energy Beijing, China. Financially, this early stage of high energy physics was mainly sustained by SUT, TRF, and DAAD scholarships.

In 2007, our group joined the Research Center for Computational and Theoretical Physics supported by the Thailand Center of Excellence in Physics (ThEP Center). As the first funding agency in Thailand with the sole purpose to promote physics activities in Thailand. It aims to enhance the quality of teaching and research in physics at Thai universities and to support local industries with well-prepared graduates and innovative ideas.

In 2010, Prof. Prasart Suebka, the previous rector of SUT, encouraged us to follow the Her Royal Highness Princess Maha Chakri Sirindhorn initiative in the area of experimental particle physics. With the support from Prof. Pairash Thajchayapong, chairman of the Thai-CERN committee, we set up the experimental particle physics group at SUT to participate in two prestigious international collaborations, Anti-Proton Annihilation at Darmstadt (PANDA) in 2011 and ALICE in 2012. Our strategy of initially contributing with detector simulations for the upgrade of the ALICE Inner Tracking System (ITS) and the PANDA Electromagnetic Calorimeter paid off and helped establish us as a reliable partner in both collaborations. Both projects were supported by the Center of Excellent in High Energy and Astrophysics at SUT and the National Science and Technology Development Agency (NSTDA).





Recently, we were able to significantly expand our international research network, with new areas of interest comprising the development and testing of sensors together with the Thai Microelectronics Center and the SLRI. In 2016, we joined the Jiangmen Underground Neutrino Observatory (JUNO) where we successfully contributed to the design of the Earth Magnetic Field (EMF) Shielding. In the same year, SUT has also proposed to work on the R&D of field cage and field-shaping for the Particle AND Astrophysical Xenon Time projection chamber (PandaX III).

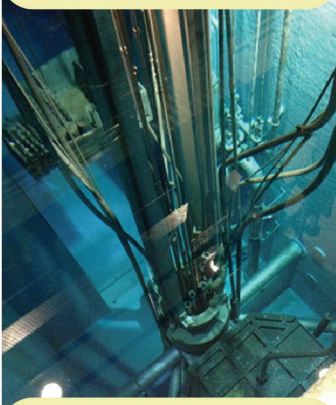
In 2019, SUT was accepted by the Beijing Spectrometer III (BESIII) at Beijing Electron-Positron Collider II (BEPCII) to participate in data analysis for the study of exotic particles. Furthermore, we have submitted a proposal to join the Karlsruhe TRItium Neutrino experiment (KATRIN). Our intended contribution hereby will be the development of the Magnetic Mobile Sensing unit together with teams from Chulalongkorn University and Chiang Mai University, which might ultimately allow for a measurement the mass of the neutrino.

Through all these invaluable experiences and exchanges with fellow researchers from throughout Europe and Asia, we have gained plenty of new strengths, skills, and knowledge, extending far beyond our efforts in fundamental research. We are going to use these for new and timely projects such the development of a proton Computed Tomography (pCT) prototype together with the University of Bergen, Norway. To improve the diagnosis and treatment of cancer, this system is going to be designed with the concept of an integrated scan/therapy approach. We are currently developing and implementing a realistic simulation for the description of particle beams, energy deposit, etc. in tissue and applying Machine Learning based algorithms to facilitate the diagnosis/treatment planning. All of this is possible thanks to the support of ThEP and International Research Network (IRN), Thailand Science Research and Innovation (TSRI).



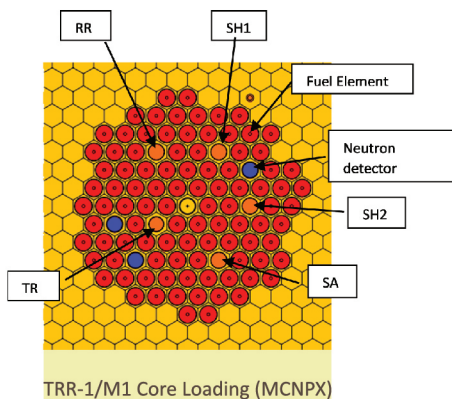
## Computational Science and Engineering Virtual Organization

### The HPC server utilization at TINT

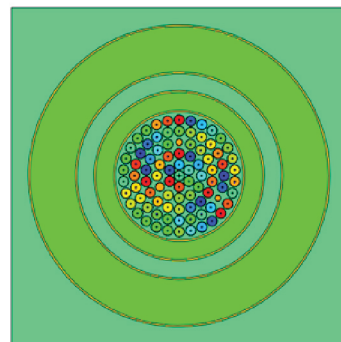


TRR-1/M1 Research Reactor

The HPC infrastructure at Thailand Institute of Nuclear Technology (TINT) is utilized by the Reactor Management Section particularly for neutronic calculation of the Thai Research Reactor (TRR-1/M1) core where extensive computing resources are required. The TRR-1/M1 core neutronic properties is currently calculated with Monte Carlo Methods using MCNPX and/or MVP programs. The core simulations are performed for TRR-1/M1 core management. The neutronic calculation results obtained from the simulations provide necessary information for subsequent safety analysis for the reactor such as the thermal-hydraulic analysis. Aside from the TRR-1/M1 core management calculation, TINT's HPC server is also used for the fuel burn-up calculation of TRR-1/M1 fuel elements and other research reactors under the International Atomic Energy Agency (IAEA) Coordinated Research Project "Benchmarks of Computational Tools against Experimental Data on Fuel Burnup and Material Activation for Utilization, Operation and Safety Analysis of Research Reactors".



TRR-1/M1 Core Loading (MCNPX)

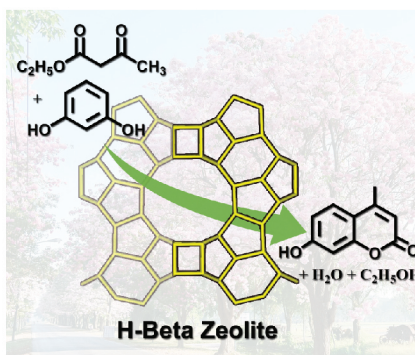


MCNPX model of ATI core

In our laboratory, we study the structure and reaction mechanism over heterogeneous catalysts with both experimental and theoretical studies. We would like to acknowledge National e-Science Infrastructure Consortium. With the high-end scientific computing resource, several projects can be completed including:

### i. Zeolite Catalysts

We study the adsorption and reaction mechanism of several compounds including biomass on Zeolite catalysts. Several computational techniques together with experimental investigation were developed to understand the reaction mechanism with the zeolite pore and their acid strength. For example, the Pechmann condensation reaction to synthesize coumarin which is the important substrate for drug synthesis were studied with conventional acid solution and several zeolites. The reaction mechanisms inside the zeolites were totally calculated with quantum calculation.



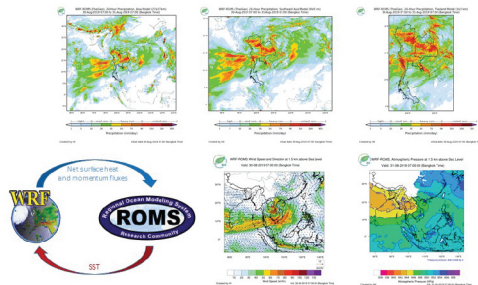
Picture from:  
ChemistrySelect, (2019) 4, 10660-10667

### ii. Metal-Organic Frameworks

In our work, the structure and acidity of the synthesized Zirconium-based Metal-Organic Frameworks, one of the most outstanding MOFs for heterogeneous catalysis owing to its high thermal and chemical stabilities, were characterized using experimental and theoretical techniques. The adsorption of base with several Density Functional Theory has been applied on the suitable calculation models. Then, the organic reactions in zirconium-based metal-organic framework functionalized has been theoretically investigated to guideline the development of the MOFs as catalysts.

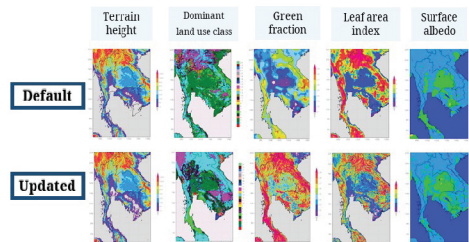
### ◦ Coupled Model (WRF-ROMS) for Weather Prediction

Short-term weather prediction using coupled atmosphere and ocean models (WRF-ROMS).



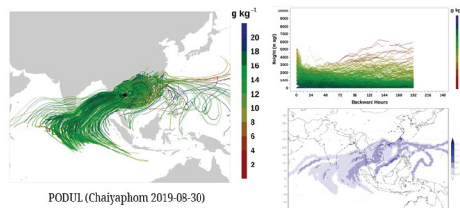
### ◦ Improving Input Spatial Information to Support Meteorological Modeling

Updating input surface data for WRF modeling to reduce uncertainty in the model due to unrealistic or unrepresentative surface data.



### ◦ Development of a Numerical Atmospheric Moisture Tracking System to Identify Potential Sources and Its Application to Enhance Rainfall Analysis for Thailand by LMTS

Lagrangian Moisture Tracking System (LMTS) can identify potential sources of moisture for a rainfall event of interest, which is useful to help enhance the weather forecast operation of Thailand.



PODUL (Chaiyaphom 2019-08-30)



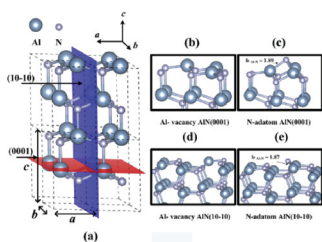
**Effects of  $N_2$ -Content on Formation Behavior in AlN Thin Films Studied by NEXAFS: Theory and Experiment**

Ratchadaporn Supruangnet, et al.

Synchrotron Light Research Institute (Public Organization)

anostructure of material has significant influence to the eletronics and mechanical properties of the film. For an example of a wide bandgap material, e.g. AlN film, researchers discover how to control its nano-architecture via only  $N_2$  gas flow. However, to clearly elucidate this phenomena, it require both synchrotron radiation experiment and power of high performed computer (HPC) for a computational materials calculation.

In this work, AlN thin films were deposited on glass slides by a reactive-radio frequency (RF) magnetron sputtering with various mixed ambient of  $N_2/(Ar + N_2)$  flow ratio at 20%, 40%, 60% and 80%. Later, X-ray diffraction (XRD) investigation showed (0002) plane of wurtzite-AlN for 60% and 80% of  $N_2/(Ar + N_2)$ . In contrast, samples with 20% and 40% of  $N_2/(Ar + N_2)$  could not exhibit the clear peak of the (0002) plane because of the low level of AlN crystal structure on glass slides. However, with the near edge X-ray absorption fine structure (NEXAFS) spectra using synchrotron radiation at nitrogen K-edge showed the evolution of thin film growth and local environment at the initial state of crystal's formation as such other experimental techniques cannot measure it yet. To reveal further understanding of this phenomena the density functional theory (DFT) was employed to calculate formation energy via SLRI-HPC system. An excellent agreement between the experiment and calculation on the formation mechanism was thus revealed.



Atomic structure of the wurtzite AlN. (a) Schematic of a 4-unit cell of AlN and red and blue plans represent (0001) and (10-10), respectively. Schematic representation of 2 x 2 unit mesh showing top two layers (b) Al- vacancy for the AlN (0001) model, (c) N adatom for the AlN (0001) model, (d) Al- vacancy for the AlN (10-10) model and N adatom for the AlN (10-10) model using in computational modeling.

**Keywords:** Aluminum nitride, Local structure, Density functional theory, X-ray absorption spectroscopy

<https://doi.org/10.1016/j.jallcom.2020.156128>

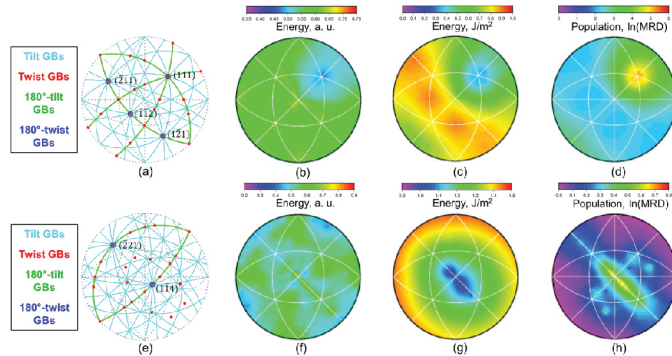
**References:**

- 1) R. Supruangnet, et al., J. Alloys Compd, 844 (2020), 156128.

**Study on Atomic Structure of Austenitic Steel with Atomistic Simulation**

**Asst. Prof. Dr. Sutatch Ratanaphan,**  
**Asst. Prof. Rajchawit Sarochawikarit, and Noppadol Kumanuvong**  
 King Mongkut's University of Technology Thonburi

This project studied on the energies of 388 grain boundaries with a range of misorientations and grain boundary plane orientations that have been calculated using the meta-atom embedded atom method (EAM) potential recently developed to simulate an austenitic twinning-induced plasticity (TWIP) steel. A comparison between the simulated grain boundary energies and the measured grain boundary population in an austenitic TWIP steel revealed that at fixed misorientations, there is a strong inverse correlation between the energy and the population. In addition, the Bulatov-Reed-Kumar (BRK) five-parameter grain boundary energy function for face-centered cubic (fcc) metals was used to produce a larger, more nearly continuous set of grain boundary energies. Interestingly, these interpolated grain boundary energies were consistent with the simulated energies and also inversely correlated with the measured grain boundary populations in an austenitic TWIP steel.

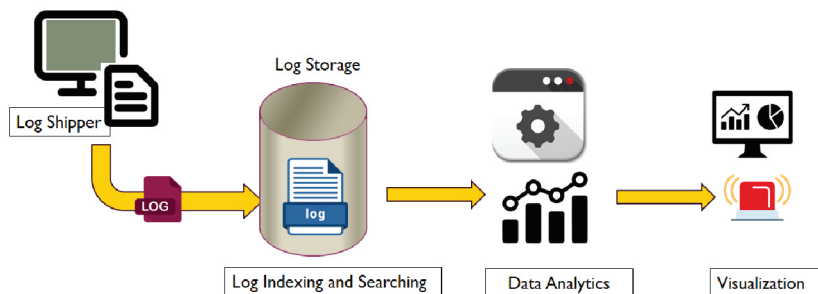


The figure shows schematic representation of grain boundaries at  $\Sigma 3$ ,  $60^\circ/[111]$  (a) and  $\Sigma 9$ ,  $39^\circ/[110]$  (e). The distributions of measured grain boundary energies, simulated grain boundary energies, and relative grain boundary areas for  $\Sigma 3$  (b, c, d) and  $\Sigma 9$  (f, g, h) misorientations. For the plots of simulated grain boundary energies, 41 and 23 distinct data points are used at the  $\Sigma 3$  and  $\Sigma 9$  misorientations, respectively. It should also be noted that the symmetry increases the numbers of data points. The distributions are plotted on a stereographic projection using the bicrystal reference frame with the  $[001]$  and  $[100]$  directions normal to the page and horizontal to the right within the page, respectively. The measured grain boundary population and energy were obtained from previous study. The relative grain boundary areas are plotted in units of multiples of a random distribution (MRD).

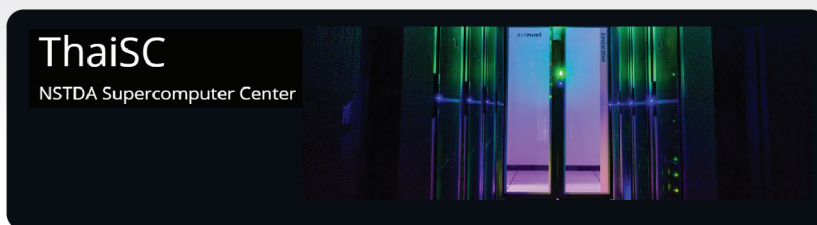
## AI-Based Logging System for ALICE O2 Facilities

Asst. Prof. Dr. Phond Phunchongharn and  
Assoc. Prof. Dr. Tiranee Achalakul  
King Mongkut's University of Technology Thonburi

CERN has four main particle detectors that will capture and record the effects of these collisions. ALICE (A Large Ion Collider Experiment) is a powerful particle detector on the Large Hadron Collider (LHC). It is designed to study the physics of interaction with high energy density substances, called plasma quark-gluon. O2 is the computing facility support team for ALICE experiments. O2 facilities have approximately 2000 nodes which is working all the time. Currently, there is no any logging system in ALICE O2. As a result, O2 operational team cannot provide preventive maintenance for the system effectively. We have, therefore, proposed an AI-based logging system for O2 facilities. Currently, the failure of computing nodes affects the loss of important data in experiments. Also, the total computation time of the cluster could be delayed. If the problem occur during the night time, it could delay time-to-recover due to the less manpower during the time. This proposed system could enhance the predictive maintenance and failure management for the support team. The proposed system must provide the following functions: 1. to collect, process, store and visualize the relevant information of the vast amounts of system logs that will be generated by the O2 hosts and services 2. to advance analyze the data to support preventive analytics. Advanced data analytics part contains 4 main components which are i) Anomaly Detection ii) Failure Detection iii) Survival Analysis and iv) Recommendation for Maintenance. Our team will take an ownership of the AI-based logging system in the full stack of software engineering activities from collecting the requirement from CERN, designing, implementing to maintaining the system for 3 years in the first phase.



## Business and Industrial Communities Supported by ThaiSC



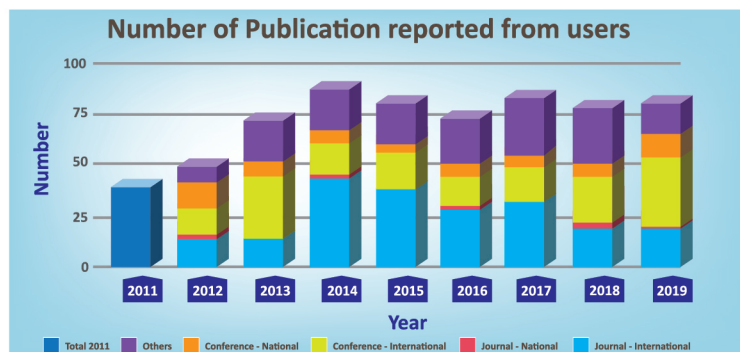
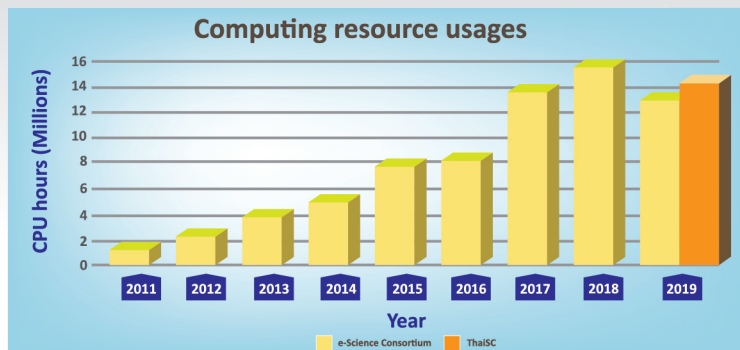
NSTDA Supercomputer Center's (ThaiSC) mission is to provide HPC infrastructure services for the R&D community in Thailand. We support the growing computing demand arising from advanced computational techniques such as machine learning, deep learning, computational engineering, and molecular and quantum mechanical simulations. Aside from academia and government, ThaiSC aims to boost Thailand's competitiveness through high-value industries.



In 2020, ThaiSC launched a pilot program to provide HPC services to private sectors by collaborating with The Siam Cement Group Public Company Ltd. (SCG) to conduct research on novel materials and chemicals using advanced computational techniques.



## Achievements



Active user 2019



- 156 total users
- 97 researchers
- 61 Students

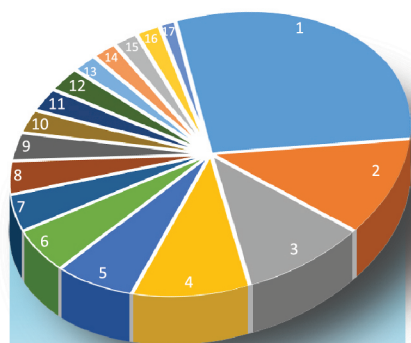


166 Projects



27 Institutes

## Projects Categorize



1. Computational Chemistry
2. Computational Physics
3. Biology Chemistry
4. Material Science
5. Mechanical Engineering
6. Atmospheric science
7. Cosmology
8. Nanomaterial
9. High Energy Particle Physics
10. Weather forecast
11. High Energy Astrophysics
12. Big Data & Machine Learning
13. Nuclear technology
14. Molecular Chemistry
15. Pharmaceutical Chemistry
16. Computer Science & Engineering
17. Bioinformatics

## Activities of Consortium and Members



Panel discussion on "National Computing Platform" at Chiang Mai University, 2019 Advisory



Conference on "CMS Week Bangkok 2019" Organize by CU, Bangkok



Workshop on "Exabyte scale Storage (EOS)" Organize by SUT, 2019



Attended "5th Asian Tier Center Forum and the 1st Asia HTCondor workshop" India, 2019



Exhibition at ANSCSE 23rd, Chiang Mai University, 2019



Introduction of "HPC in Thailand" at Supercomputer conference, USA, 2018



Workshop on "HPC and e-Science in Thailand" at The Sukosol Hotel, 2018



Workshop on "e-Science and High Performance Computing" at Mahidol University, 2018



## Committee and Working Group

### o Board of Steering Committees

Prof. Dr. Pairash Thajchayapong	Advisory
Dr. Kopr Kritayakirana	Advisory
Mr. Nart Liuchareon	Advisory
Dr. Thaweesak Koanantakool	Advisory
Rector of Suranaree University of Technology	Chairperson
President of Chulalongkorn University	Committee
President of Digital Government Development Agency	Committee
Director of Hydro Informatics Institute	Committee
President of King Mongkut's University of Technology Thonburi	Committee
Director of National Astronomical Research Institute of Thailand	Committee
President of National Science and Technology Development Agency	Committee
Director of Synchrotron Light Research Institute	Committee
Executive director of Thailand Institute of Nuclear Technology	Committee
Director of Office of Information Technology Administration for Educational Development (UniNET)	Committee
Asst. Prof. Dr. Putchong Uthayopas	Committee
Mr. Chaicharearn Atibaedya	Committee
Dr. Chalernpol Charnsripinyo	Committee
Chair Person of Usage Management Working Group	Secretary
Chair Person of Network Working Group	Assistance Secretary
Chair Person of Resources Working Group	Assistance Secretary
Chair Person of Tools Working Group	Assistance Secretary
Asst. Prof. Dr. Chinorat Kobdaj	Assistance Secretary

### o Usage Management Working Group

Dr. Sornthep Vanarat	Advisory
Dr. Chalee Vorakulpipat	Chairperson
Prof. Dr. Kritsana Sagarik	Committee
Assoc. Prof. Dr. Tiranee Achalakul	Committee
Asst. Prof. Dr. Burin Asavapibhop	Committee
Miss Jarumon Limtipdara	Committee



#### o Resources Working Group

Mr. Suriya U-ruekolan  
Dr. Noraphat Srimanobhas  
Dr. Supakit Prueksaaron  
Dr. Thara Angskun  
Mr. Atip Peethong  
Mr. Rajchawit Sarochawikarit

Chairperson  
Committee  
Committee  
Committee  
Committee  
Committee

#### o Tools Working Group

Assoc. Prof. Dr. Vudhichai Parasuk  
Assoc. Prof. Dr. Tiranee Achalakul  
Dr. Ayut Limphirat  
Dr. Ekasit Kijispongse  
Dr. Surajate B.Aroonnet

Chairperson  
Committee  
Committee  
Committee  
Committee

#### o Network Working Group

Deputy director of Office of Information Technology Administration  
for Educational Development (UniNET)  
President of Digital Government Development Agency  
Director of Computer Center,  
King Mongkut's University of Technology Thonburi  
Head of Network Technology Laboratory,  
National Electronic and Computer Technology Center  
Director of University Office of Information Technology,  
Chulalongkorn University  
Director of the Center for Computer Service,  
Suranaree University of Technology

Chairperson  
Committee  
  
Committee  
  
Committee  
  
Committee  
  
Committee



## Contact detail



### Consortium Office

#### Location

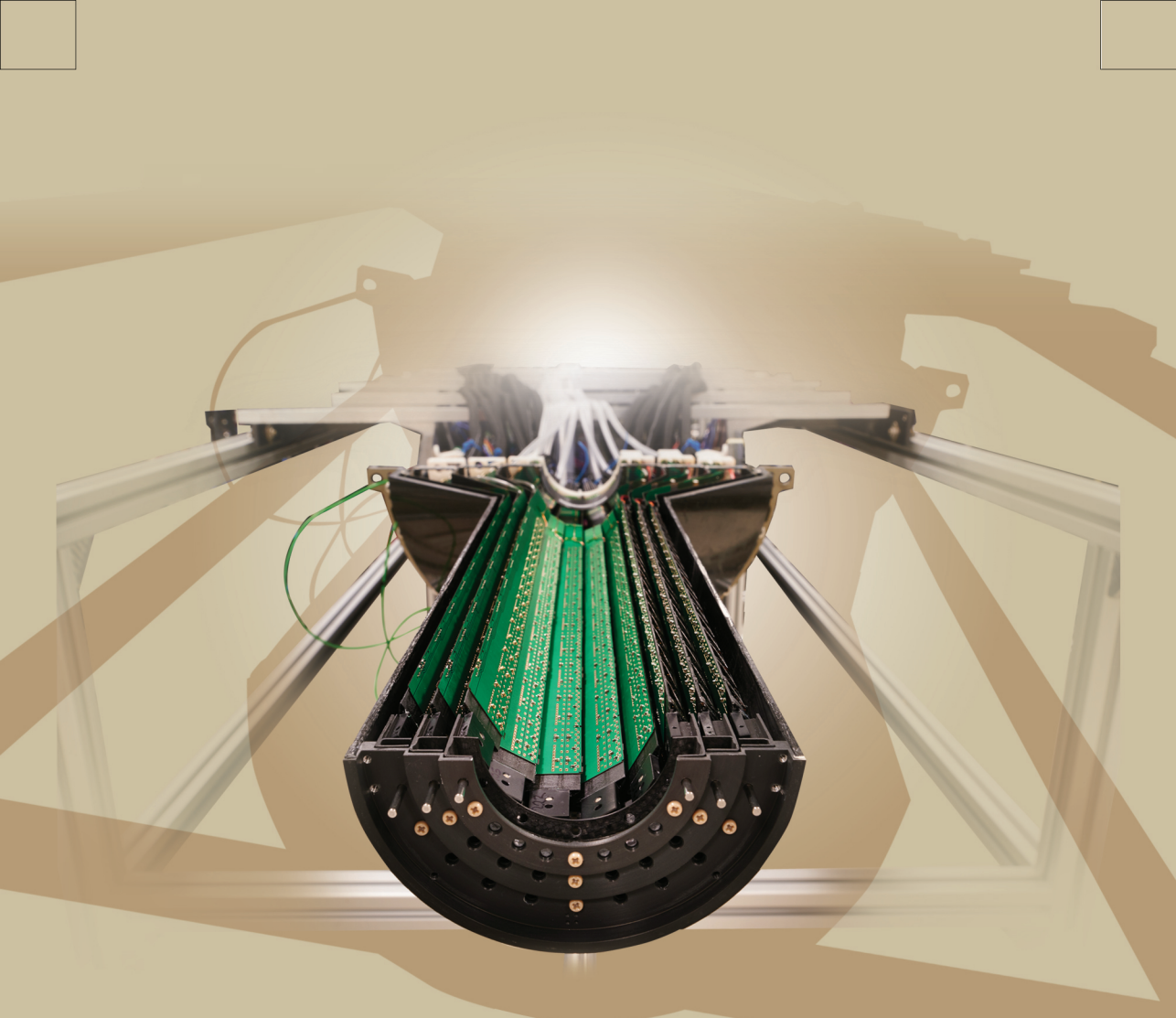
National Electronic and Computer  
Technology Center (NECTEC)  
112 Thailand Science Park,  
Pahonyothin Road,  
Klong 1, Klong Luang, Pathumthani,  
12120, Thailand

### Contact

**Dr. Chalee Vorakulpipat**  
**Miss Sunutha Phromma**  
**Miss Natsuda Kasisopha**  
**Miss Sineenat Tienkouw Watanavisit**  
Tel. +66 2564 6900 ext. 2551, 2443, 2517, 2066  
E-mail: [contact@e-science.in.th](mailto:contact@e-science.in.th)

#### Further Information

[www.e-science.in.th](http://www.e-science.in.th)  
[www.facebook.com/eScienceConsortium](https://www.facebook.com/eScienceConsortium)



This figure shows the bottom section of three inner barrels, which are now assembled and tested in Building 167 of CERN's Meyrin site, preparing for the final phase of installation and commissioning by the end of year 2020.

National e-Science Infrastructure Consortium Members

