NSTDA HPC & DA
Research, Development, and Engineering

Manaschai Kunaseth

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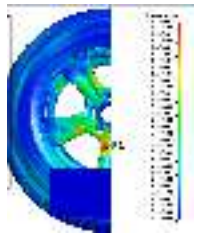
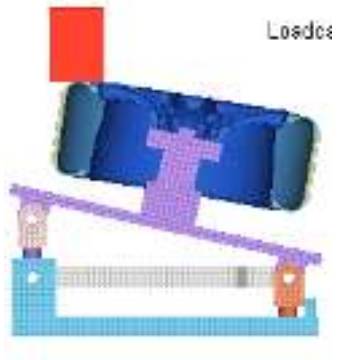




- Precision medicine
- Biobank
- Bioinformatics
- Plant genome

BIOTEC

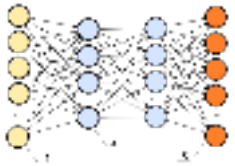
NECTEC

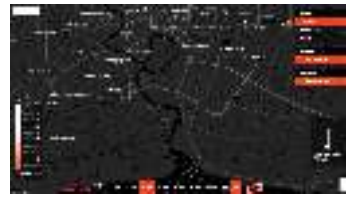
NSTDA

MTEC

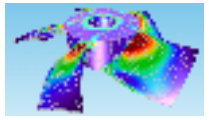
NANOTEC

- Salinity intrusion management
- Computer vision
- Deep learning for FR & NLP

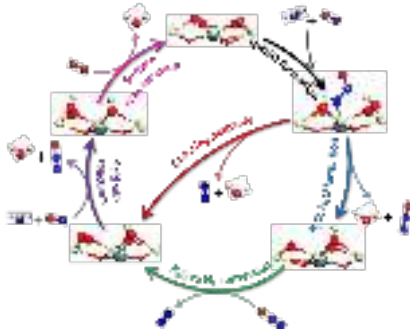


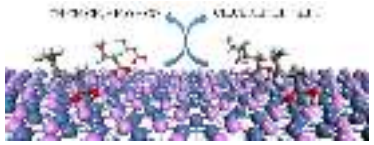


- Engineering testing
- Industrial design
- Computer-aided engineering



- Nanomaterials
- Catalysis and adsorbent
- Biofuel from biomass
- Carbon-based materials

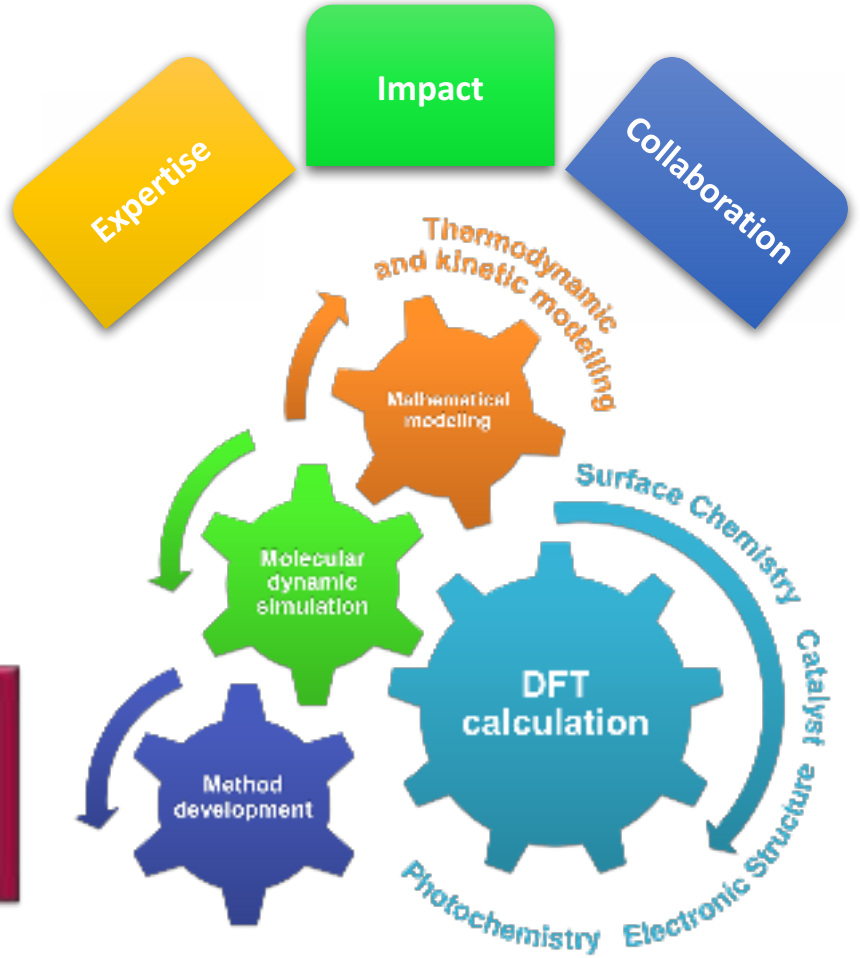




Nanomaterials Design and Simulations

Nanoscale Simulation Laboratory (NANOTEC) aims to design and predict the properties of functional nanomaterials, and to create a unique understanding of the physicochemical processes at nanoscale regime by using:

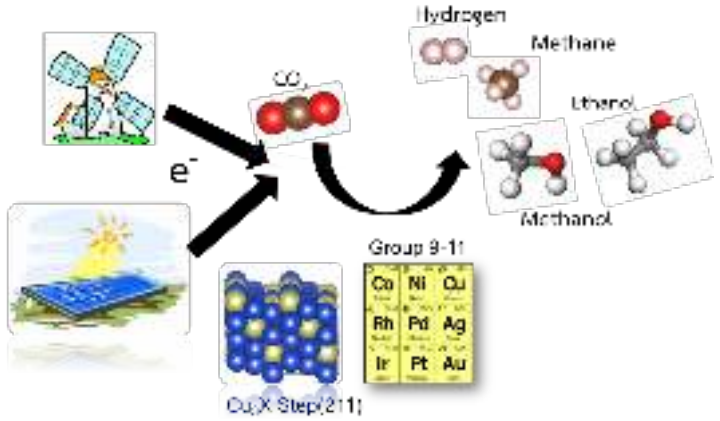
- ❑ first principle computational chemistry
- ❑ molecular dynamics simulations
- ❑ computational method development
- ❑ mathematical modeling based on continuum approach



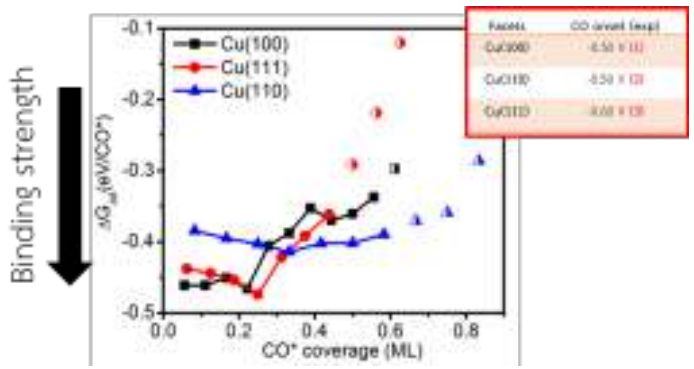
Catalysis for Green Energy Production

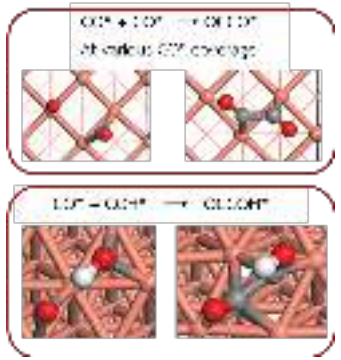
CO_2 Electrochemical Reduction to Methanol and Methane on Stepped Cu-based Alloys (211) Surfaces

P. Hirunsit *et al. J. Phys. Chem. C* 2013, *117* (16), 8262-8268.
P. Hirunsit *et al. J. Phys. Chem. C* 2015, *119* (15), 8238-8249.



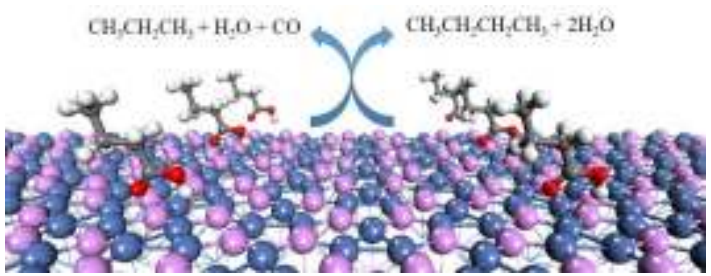
CO_2 Electrochemical Reduction to Ethylene on Cu(100), Cu(110) and Cu(111) Surfaces (Collaboration with Jason Yeo at NUS)



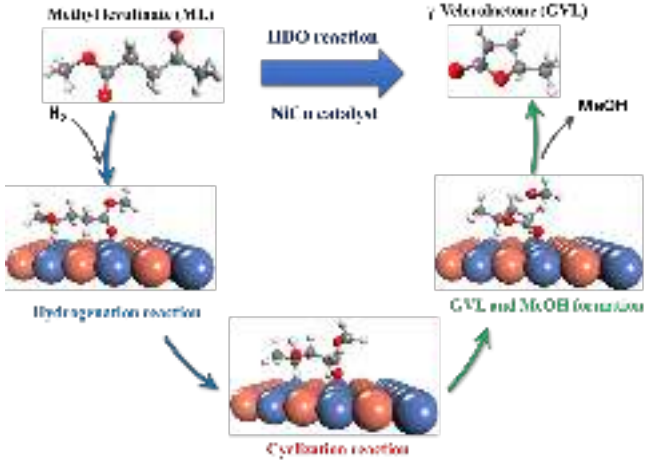


Y. Huang *et. al.*, *ACS Catal.* 2017, 7, 1749−1756.

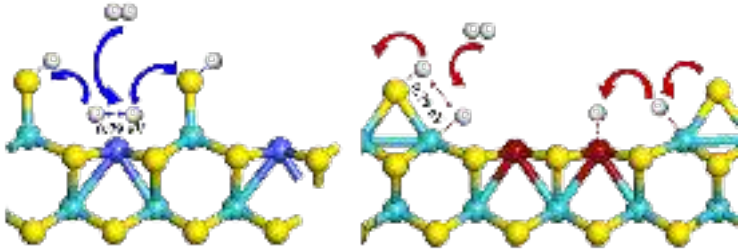
Palm Oil Conversion to Biofuel using Ni_2P Catalyst



Catalytic Transfer Hydrogenation for γ-Valerolactone (GVL) using NiCu Alloy



H_2 Activation on Partially Promoted Metal Edge of CoMoS and NiMoS



C. Sattayanon, *et al., Fuel Process. Technol.* 2017, 166, 217.

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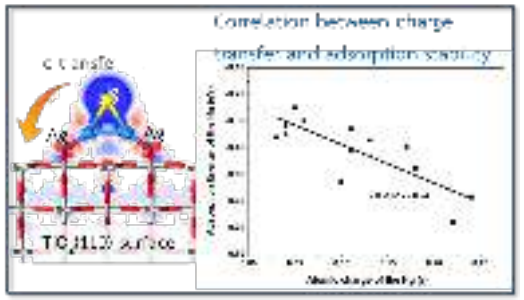
Catalysts and Adsorbents for Pollutant Removal

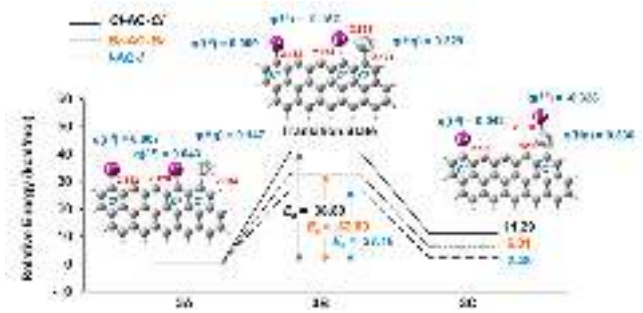
Development of Nanomaterials for Heavy Metal Removal

TiO_2-supported metal nanoparticles for Hg^0 removal



C. Rungnim, *et al., Chem. Eng. J.* 2015, 274, 132-142.

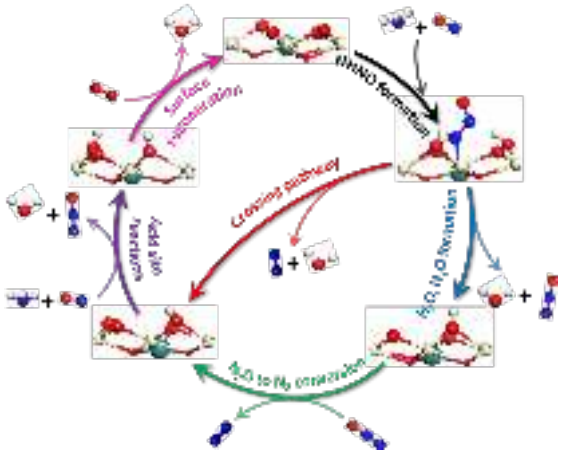
Activated carbon for Hg^0 removal



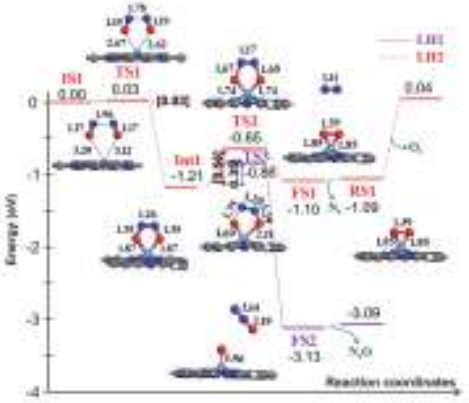
C. Rungnim *et al., J. Hazard. Mater.* 2016, 310, 253-260.

Nanomaterials for NO_x Removal

SCR-NH_3 of NO in metal oxide-based catalysts

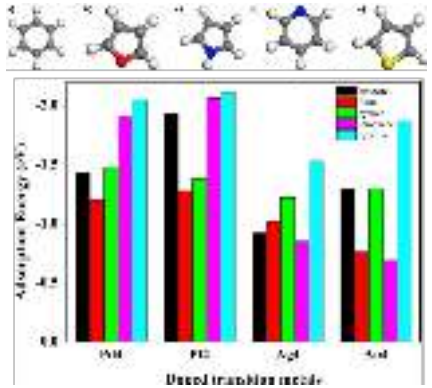


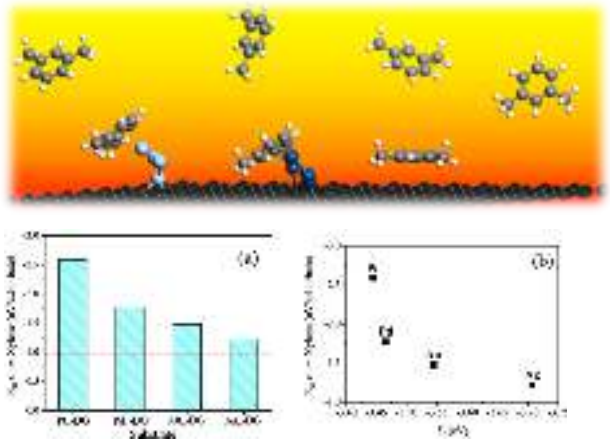
NO reactions in Metal complex and carbon-based catalysts



J. Meeprasert *et al., RSC Adv.* 2016, *6*, 20500-20506.
A. Junkaew *et al., RSC Adv.* 2017, *7*, 8858-8865.

Metal Deposited Defective Graphene for Volatile Organic Compound Removal

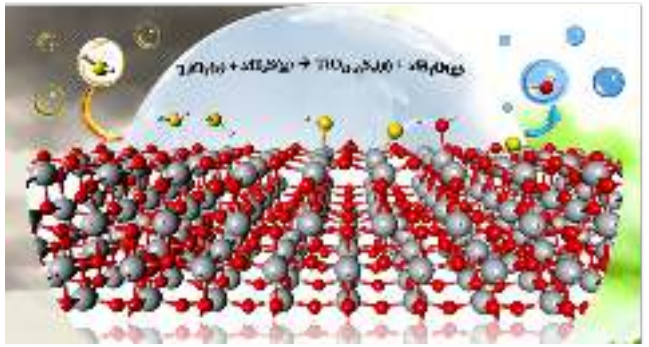




M. Kunaseth *et al. Appl. Surf. Sci.* 2017, 396, 1712-1718.

A. Junkaew *et al., New J. Chem.* 2015, 39, 9650-9658.

Nanomaterials for H_2S Desulfurization



$$TiO_2 + xH_2S(g) \rightarrow TiO_{(2-x)}\text{-}S_x^{*} + xH_2O(g)$$

$$TiO_2 + xH_2S(g) \rightarrow TiO_2\text{-}S_x^{*} + xH_2(g)$$

A. Junkaew *et al.*, *Catal. Sci. Technol.* 2017, 7, 356-365.

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NSTDA

Salinity Intrusion for Lower Chao Phraya Basin

River simulation includes a prediction model for **(1) water current (2) water level (3) salinity**. Information from these simulations helps water management from upper river's dams, water gates, and reservoirs.

- ❑ 7-day prediction with daily automatic update
- ❑ Perform "what-if scenario" for water management
- ❑ Data assimilation for accurate prediction
- ❑ Based on deterministic, and potentially, on ensemble models

Water Current Prediction

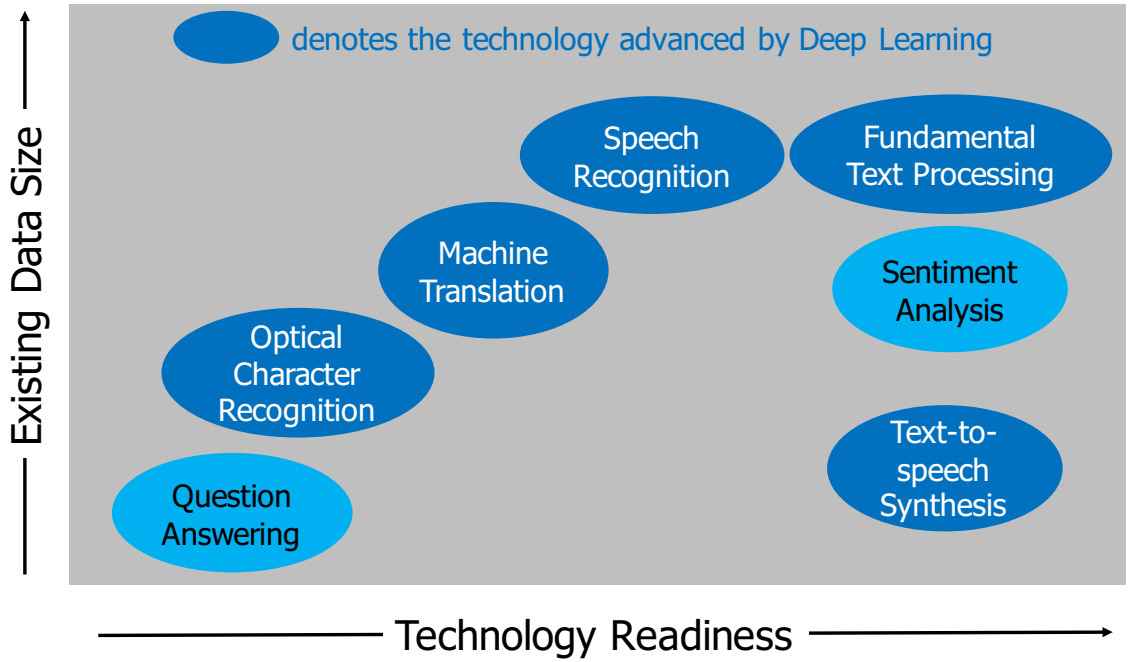
Water Salinity Prediction

Contact: Dr. Sirod Sirisup, NECTEC

NECTEC a member of NSTDA สวทช NSTDA

Artificial Intelligence & Big Data Technologies

NECTEC State-of-the-Art NLP



Computer Vision

Particle analysis

- Rice breed classification
- Car park monitoring
- Silk egg monitoring
- Plant-hopper detection

Computer Vision

CCTV image analytics

- Vehicle classification
- Vehicle tracking
- Surveillance

Contact: Dr. Chai Wutiwiwatchai, NECTEC

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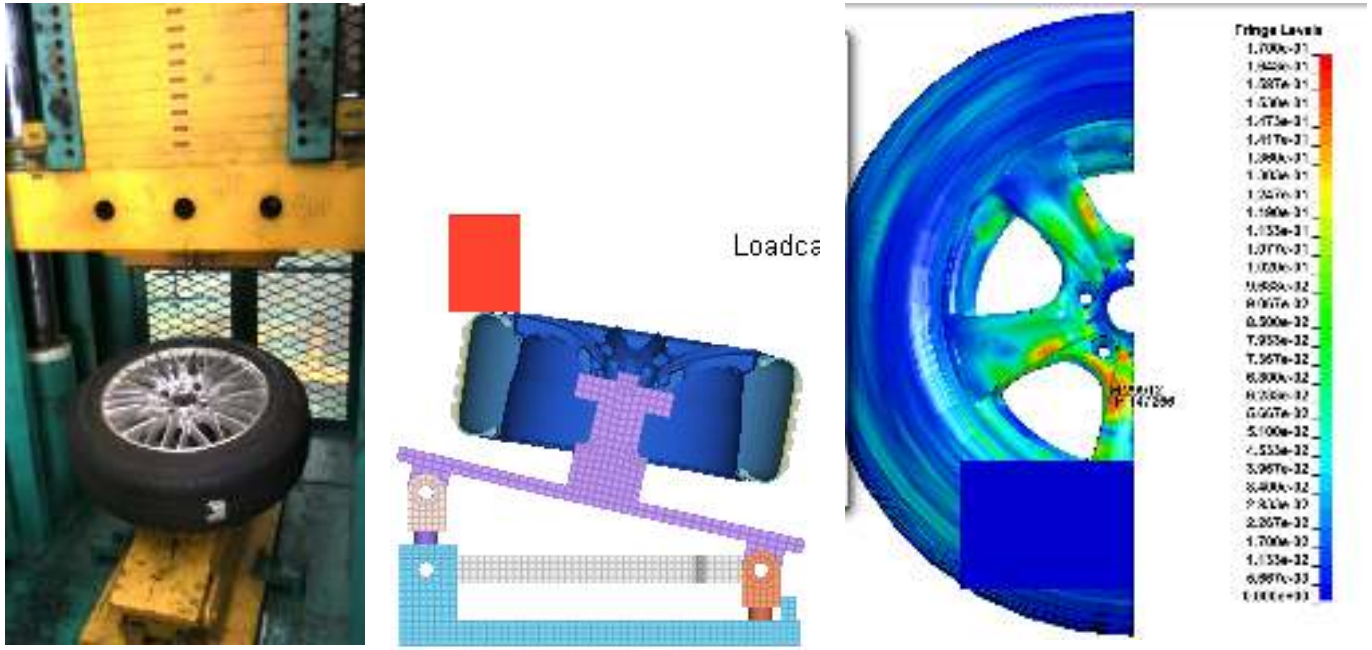
สวทช NSTDA

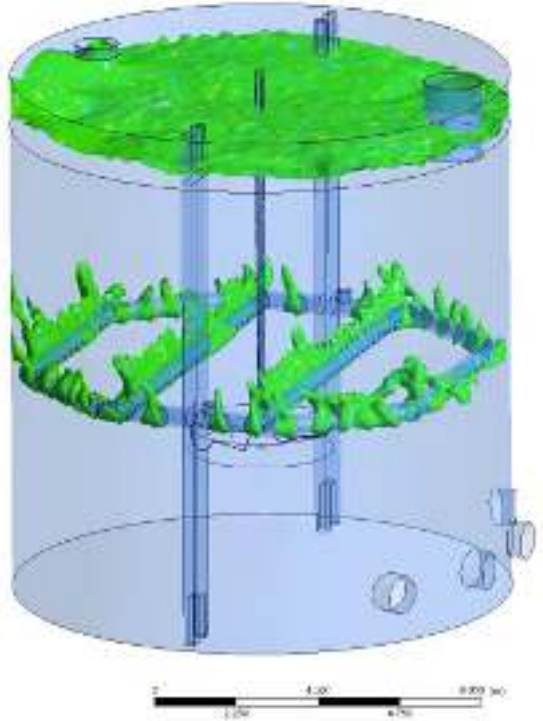
HPC for Computer-Aided Engineering (CAE)

- Finite element analysis (FEA) of dynamic structural problems
- Computational fluid dynamics (CFD) of fluid flow problems

ANSYS
MSC Software Simulating Reality. Delivering Certainty
COMSOL
XFlow
SolidWorks
Altair HyperWorks



The Wheel Impact Test



O_2 Gas Distribution in A Chemical Reaction Tank

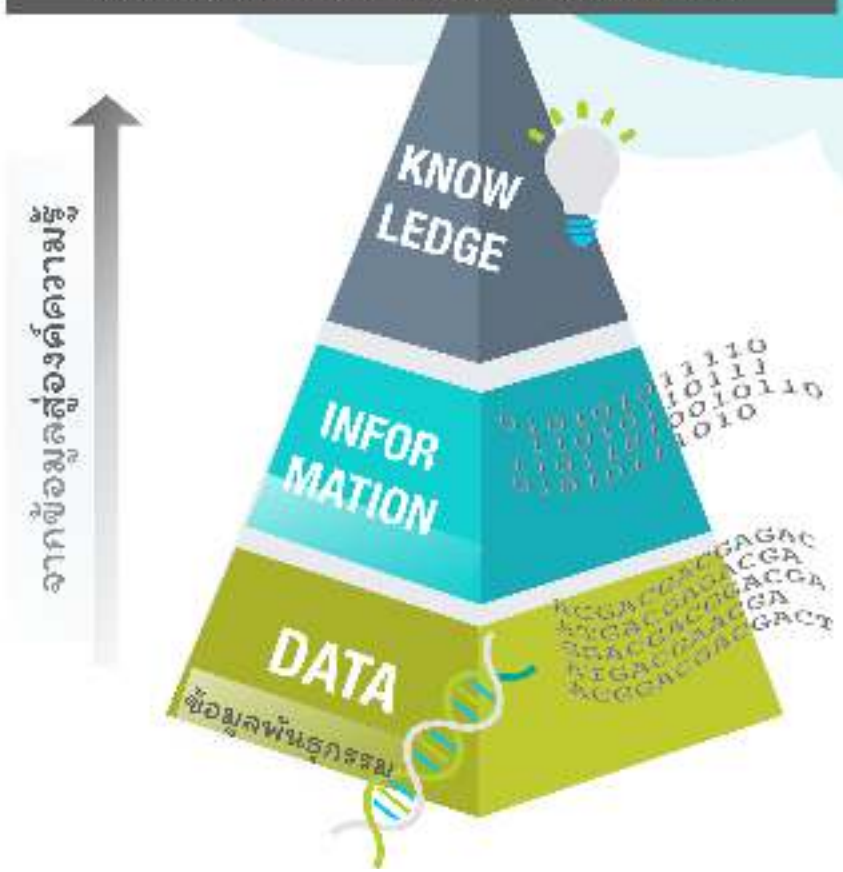
Contact: Dr. Somboon Otarawanna, MTEC

MTEC a member of NSTDA
NSTDA

BIOINFORMATICS

Precision Medicine

โครงสร้างพื้นฐานทางชีวสารสนเทศ
เพื่อการแพทย์แม่นยำในประเทศไทย



3. Knowledge portal

- Online web portal for querying valuable information

2. Big data analytics

- Software for large-scale genomic data processing

1. Computing infra

- HPC infrastructure
- Genomic databases for Thais

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สวทช NSTDA

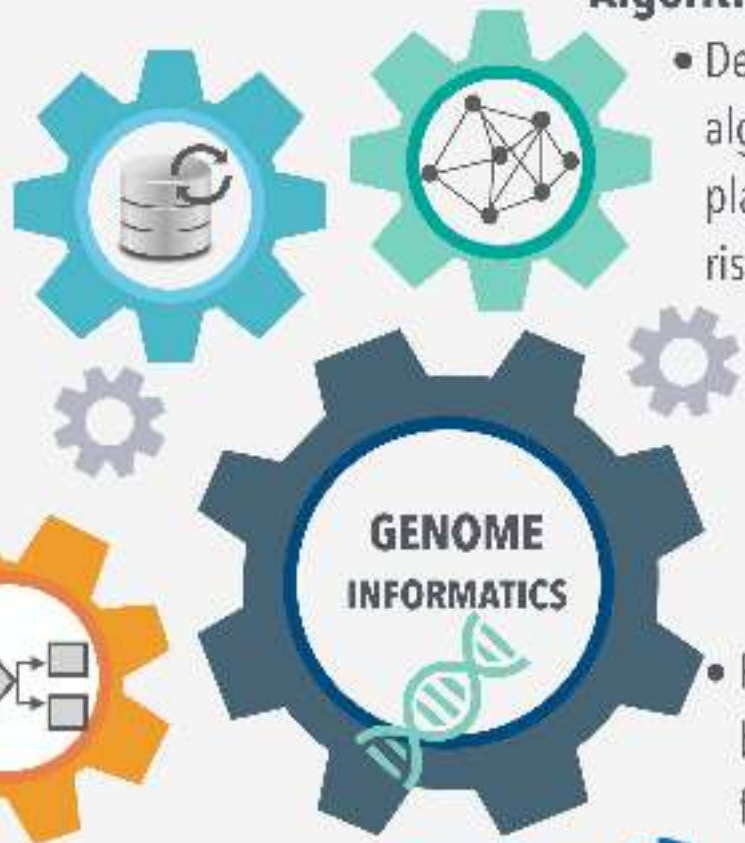
กิจกรรมหลักในการพัฒนาโครงสร้างพื้นฐานทางชีวสารสนเทศเพื่อการแพทย์แม่นยำ

Human -Omics Resources & Data Management

- Storing and managing human-omics data and other related information so that new knowledge can be synthesized

Algorithm Development

- Developing efficient algorithms for identifying plausible mutations, disease risk assessment etc.



Customized Bioinformatic Workflows

- Joining multiple tools to create suitable computational pipelines for analytics aspects of Precision Medicine

Web-friendly Interface

- Providing web access to standard bioinformatic workflows and portal for querying information/knowledge with graphical interface

สวทช NSTDA

Contact: Dr. Sissades Tongsima, BIOTEC

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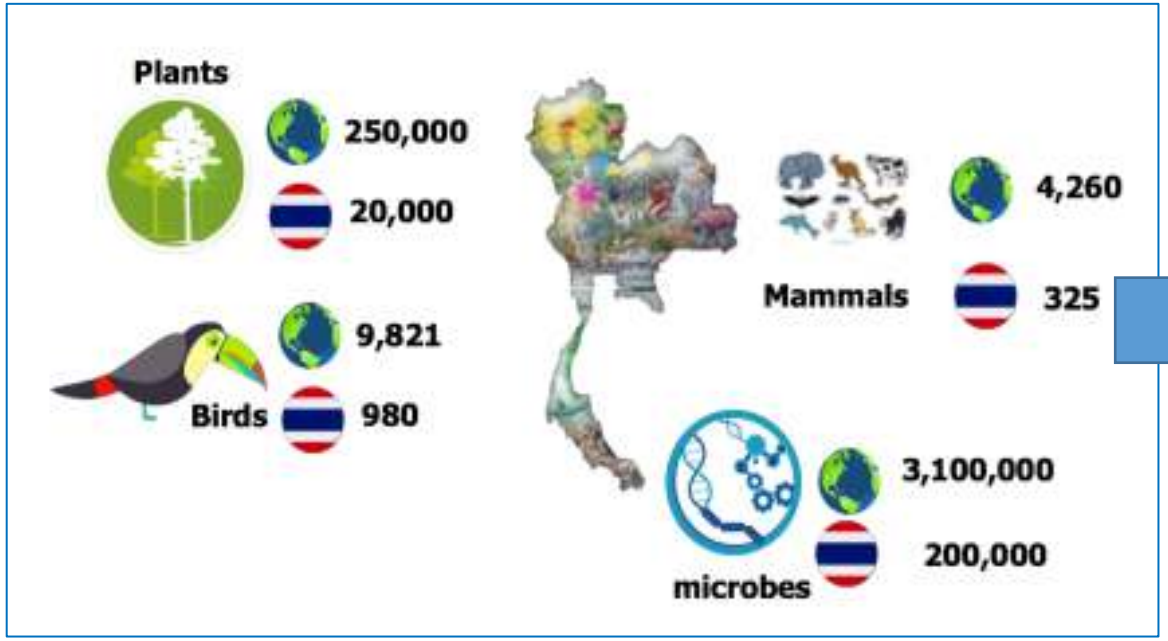
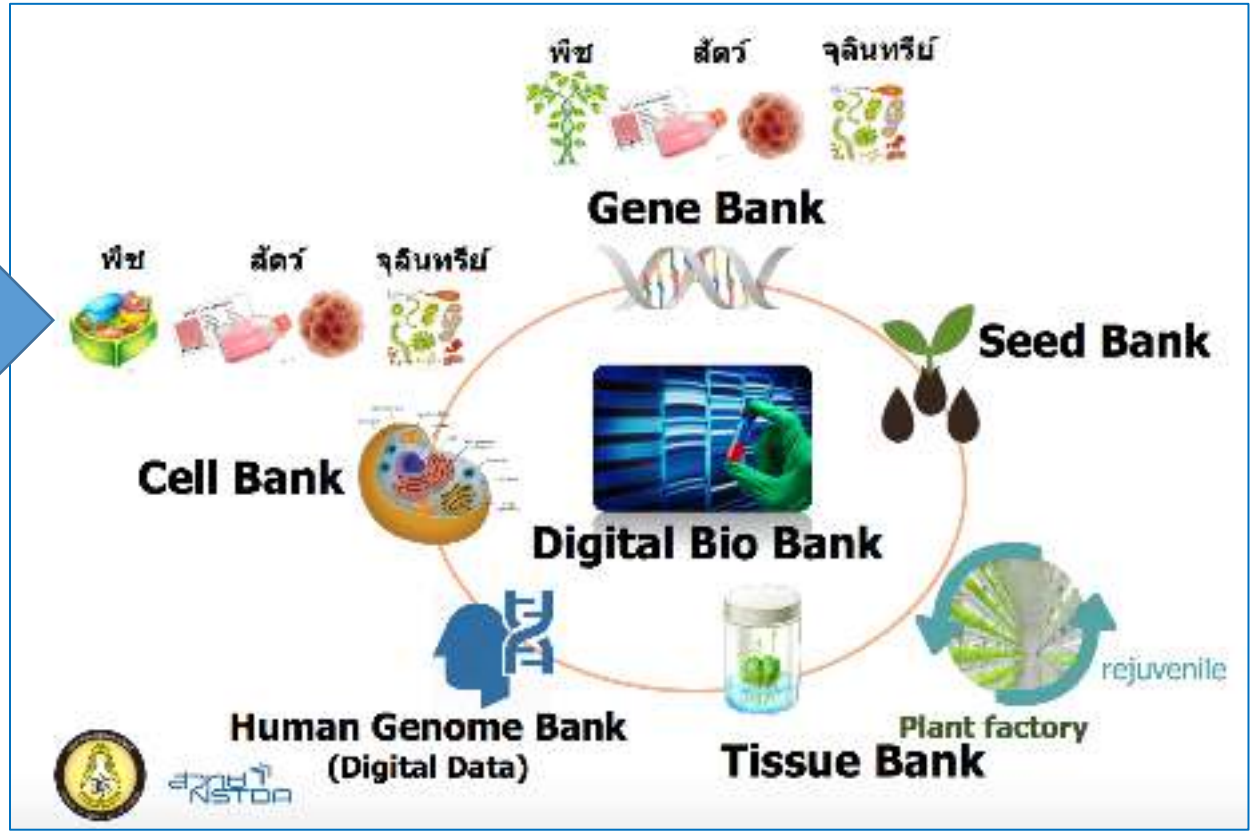
National BioBank

Thailand's Biodiversity: 10% of the world



How to maintain rich biodiversity in Thailand?

National Biobank for conservation, research, and utilization



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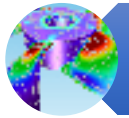
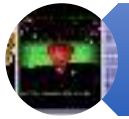
User Applications

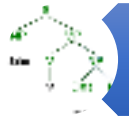

Finite element analysis

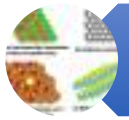

Computational fluid dynamics


Molecular dynamics


Bioinformatics


Water resource simulations


Natural language processing


Density functional theory


AI & data analytics

Computing Characteristics

Stencil & finite difference method

N-body problem

Sparse matrix

I/O & memory intensive computing

Dense matrix operations

Tensor computation

Graph computing

NSTDA Computing Infrastructure

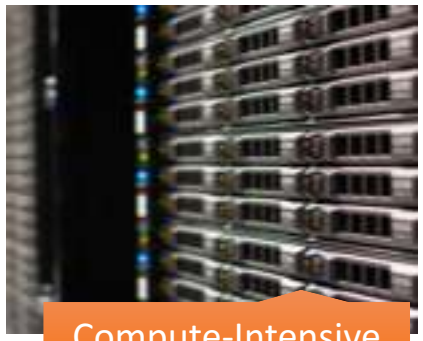

Compute-Intensive nodes


Memory & IO intensive nodes


GPGPU nodes

NSTDA Computing Infrastructure

Compute core = (2 x 20c) x 85 = 3,400
Memory/Node = 192 GB



Compute-Intensive nodes

Compute core = (8 x 24c) x 12 = 2,304 cores
Memory/Node = 3,072 GB (3.072 TB)

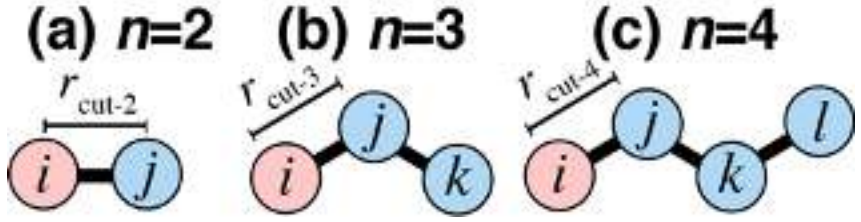
Memory & IO intensive nodes

24 NVIDIA V100 GPUs
24 x 5,120 = 122,880 CUDA cores
168 TFLOPS

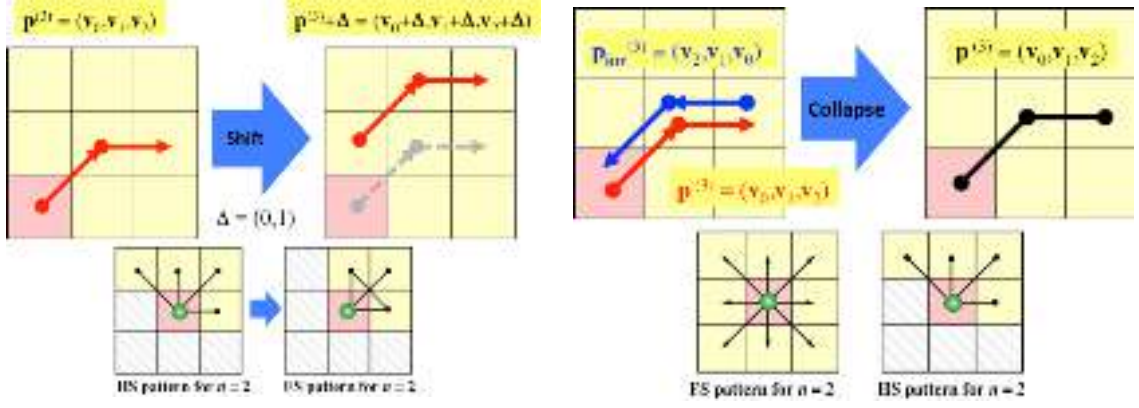
GPGPU nodes

Development of Shift/Collapse (SC) Algorithm

- A fast and scalable computation and communication algorithm for many-body potentials molecular dynamics (MD) based on general ***n*-tuple computation**

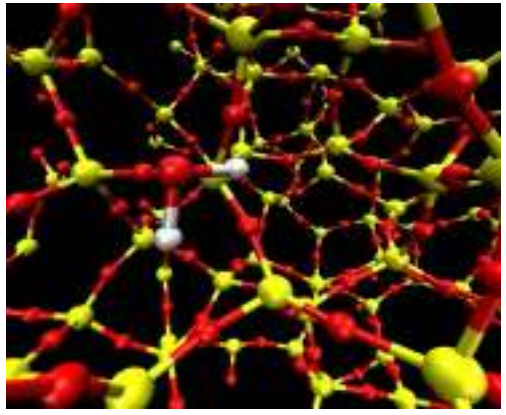


- SC algorithm utilizes ***shift*** & ***collapse*** operations to rearrange computation pattern **for optimal computation & communication**

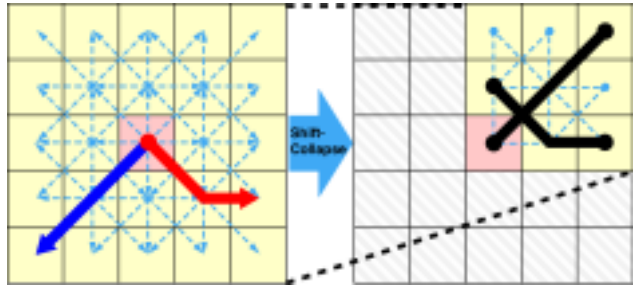


Translation (shift) invariance

Reflection (collapse) invariance



Steered Reactive-MD simulation of hydrolysis in amorphous silica using *n*-tuple computation



SC computation pattern for 3-body interaction

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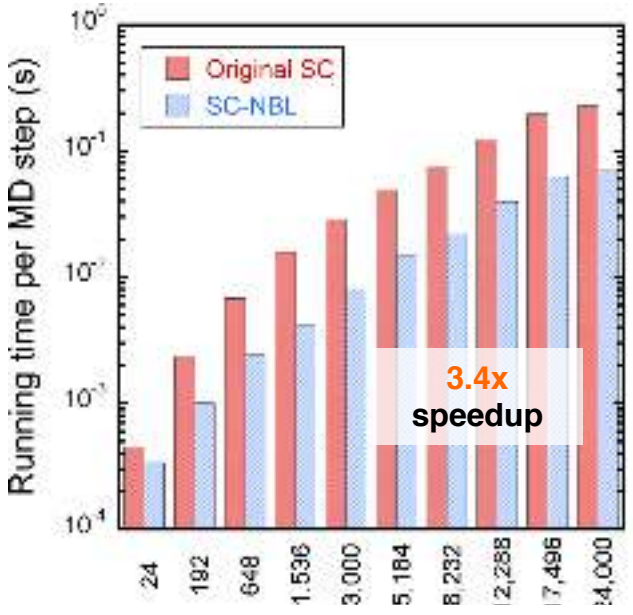
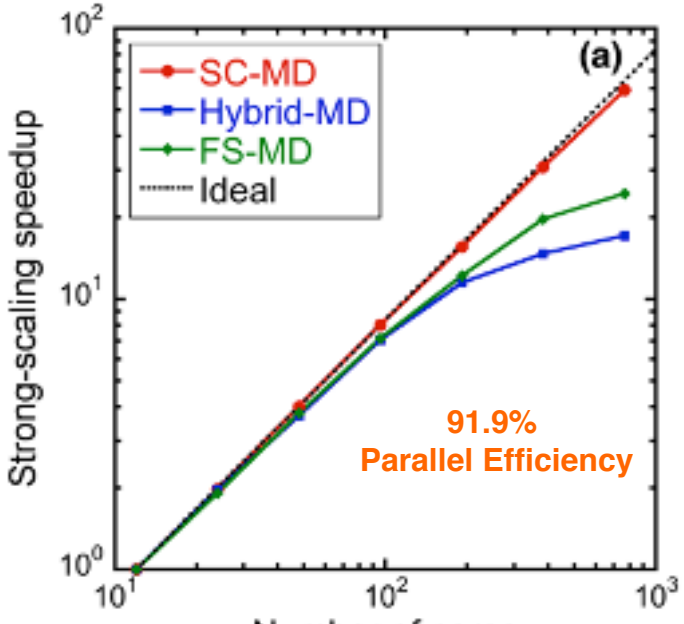
Scalability on Massive-Scale Supercomputer

- 25-million atom benchmark on Mira: BlueGene/Q supercomputer at the Argonne National Laboratory
  - **91.9%** strong parallel efficiency on **16,384 BG/Q nodes** (**1,048,576 MPI tasks** on **262,144 cores**)
  - **90.3%** weak parallel efficiency on **49,152 BG/Q nodes** (**3,145,728 MPI tasks** on **786,432 cores**)
- **9.1x speedup at small granularity** (24 atoms/core) over previous method



(Kunaseth *et al.*, submitted *Comput. Phys. Commun.*)



(Kunaseth *et al.*, **SC13**)

PI: Dr. Manaschai Kunaseth, NANOTEC

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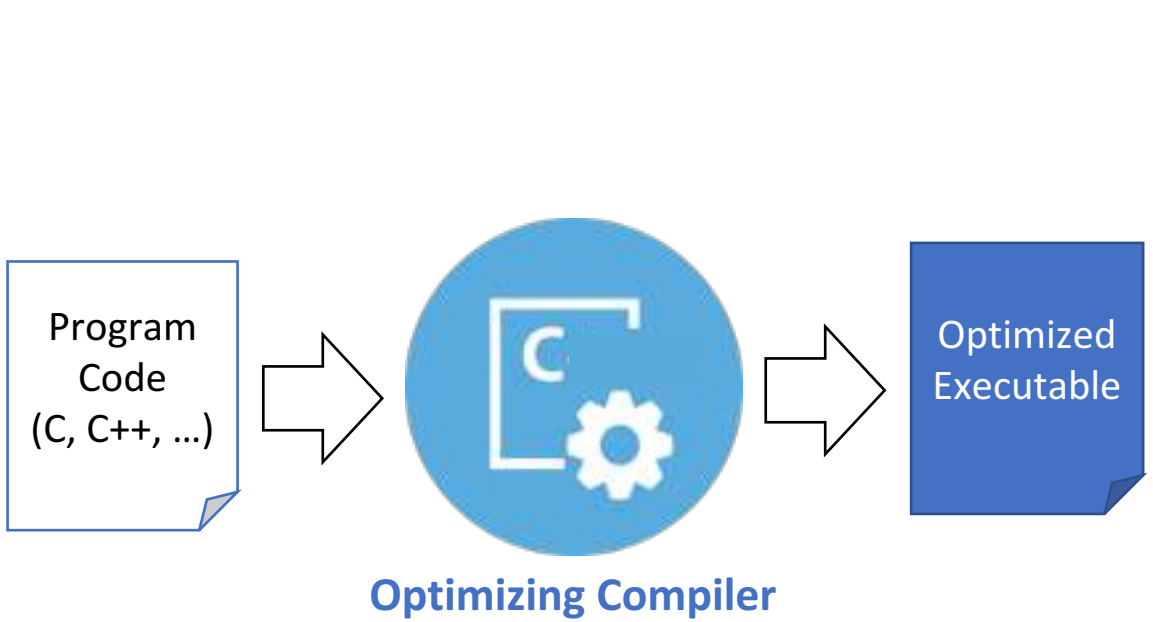
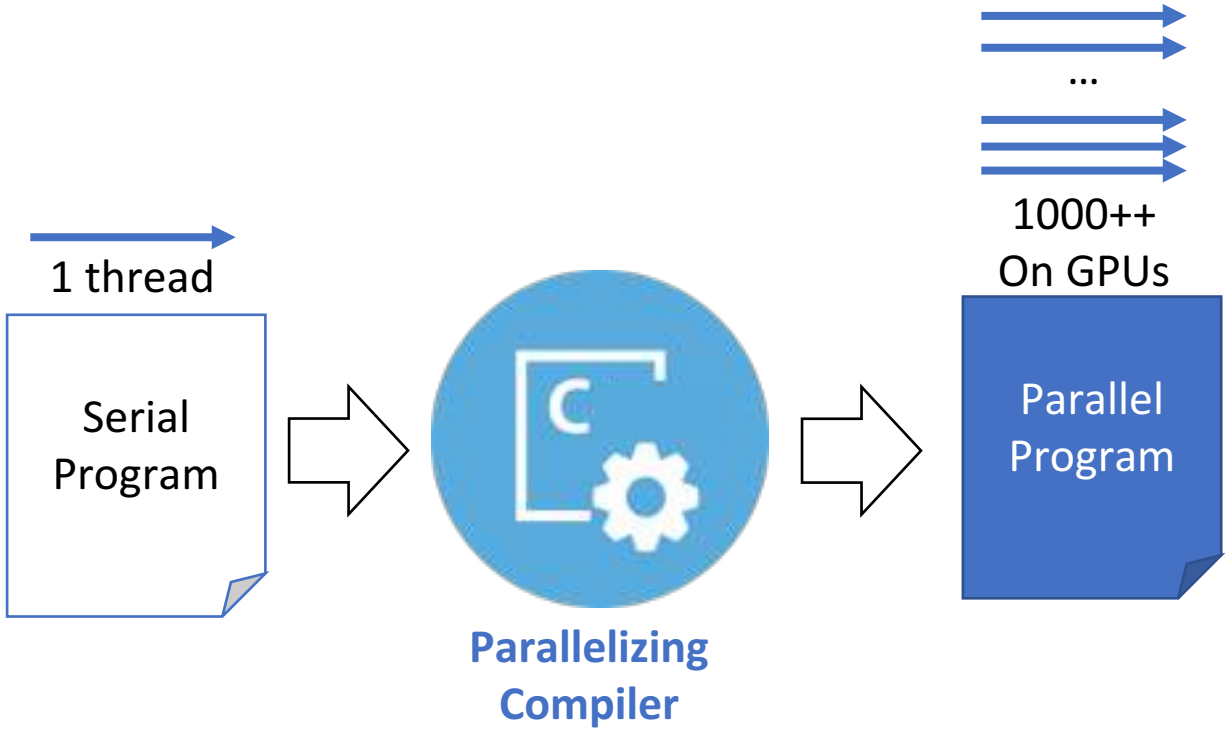
Optimizing / Parallelizing Compiler for GPUs

- **Optimizing Compiler:** **Automatically improve program performance through code transformation.**
- **Parallelizing Compiler:** **Convert serial program to run on GPUs.**





PI: Dr. Putt Sakdhnagool, NECTEC

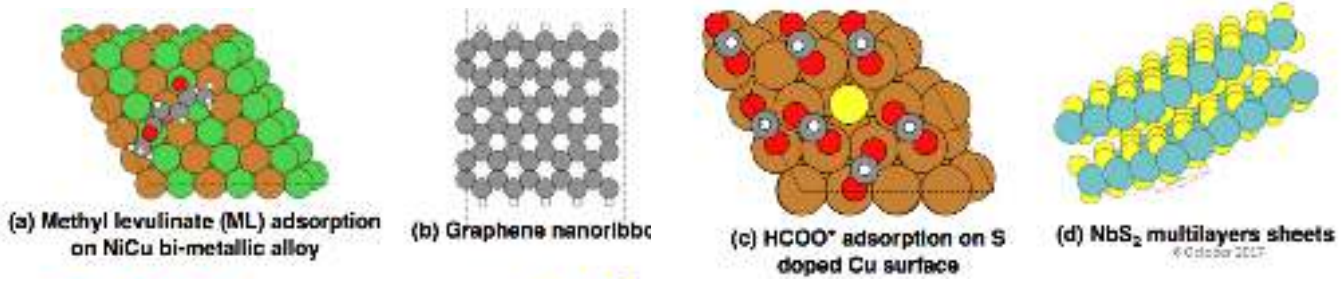
Automated VASP Performance Tuning (AVPT)

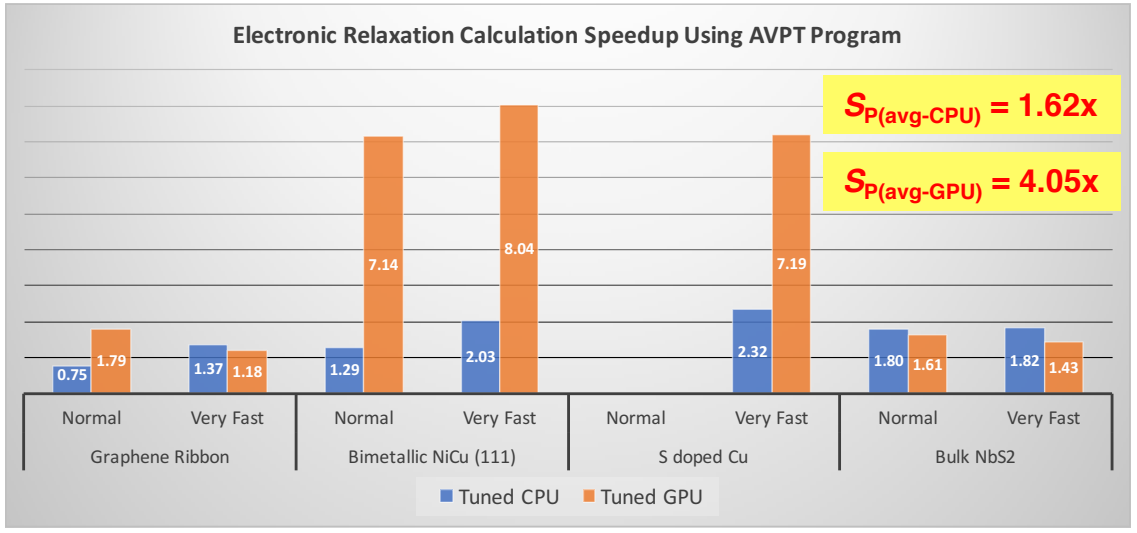
- Tuning performance related parameters of DFT simulations using VASP:
  NSIM, NCORE, NBLK, ALGO

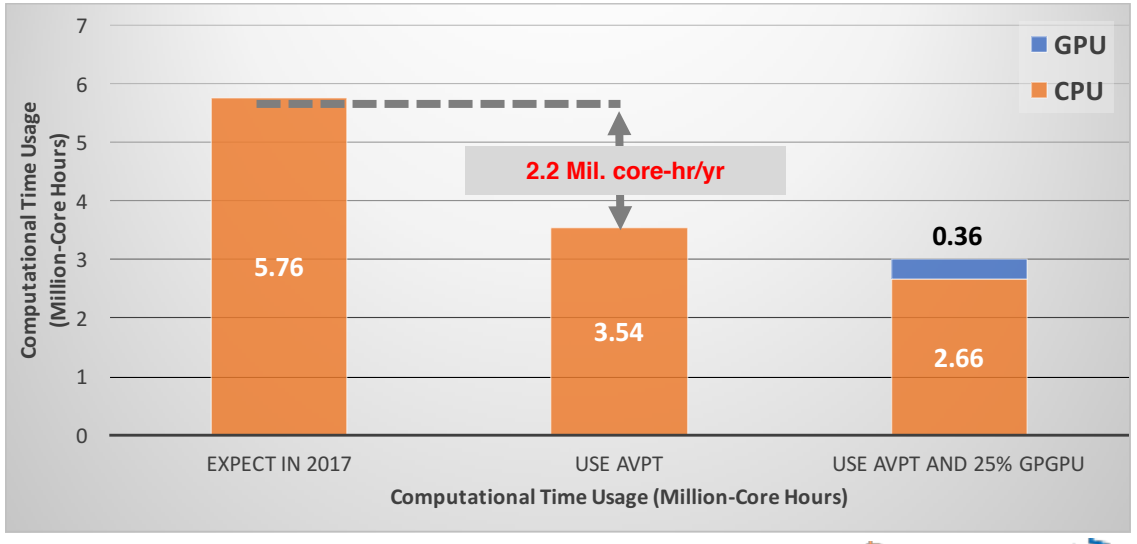
```
NSIM = 4,8,16,32
ALGO = Normal,Very fast
NCORE = 1,2,4,8,16
NBLK = 256,512,1024
TEST_TYPE = CPU_SHORT_PERFORMANCE
```

Generate

```
============================
Benchmark recipe: N = 120
============================
     NCORE  NBLK       ALGO  NSIM            Bench_Type
0        1   256       FAST     4  CPU_SHORT_PERFORMANCE
1        1   256  VERY FAST     4  CPU_SHORT_PERFORMANCE
2        1   512       FAST     4  CPU_SHORT_PERFORMANCE
3        1   512  VERY FAST     4  CPU_SHORT_PERFORMANCE
4        1  1024       FAST     4  CPU_SHORT_PERFORMANCE
5        1  1024  VERY FAST     4  CPU_SHORT_PERFORMANCE
6        2   256       FAST     4  CPU_SHORT_PERFORMANCE
7        2   256  VERY FAST     4  CPU_SHORT_PERFORMANCE
8        2   512       FAST     4  CPU_SHORT_PERFORMANCE
9        2   512  VERY FAST     4  CPU_SHORT_PERFORMANCE
10       2  1024       FAST     4  CPU_SHORT_PERFORMANCE
..     ...   ...        ...   ...                   ...
110      8   512       FAST    32  CPU_SHORT_PERFORMANCE
111      8   512  VERY FAST    32  CPU_SHORT_PERFORMANCE
112      8  1024       FAST    32  CPU_SHORT_PERFORMANCE
113      8  1024  VERY FAST    32  CPU_SHORT_PERFORMANCE
114     16   256       FAST    32  CPU_SHORT_PERFORMANCE
115     16   256  VERY FAST    32  CPU_SHORT_PERFORMANCE
116     16   512       FAST    32  CPU_SHORT_PERFORMANCE
117     16   512  VERY FAST    32  CPU_SHORT_PERFORMANCE
118     16  1024       FAST    32  CPU_SHORT_PERFORMANCE
119     16  1024  VERY FAST    32  CPU_SHORT_PERFORMANCE
```







PI: Dr. Manaschai Kunaseth, NANOTEC

Conclusions

- HPC and DA research in NSTDA are diverse and well-mature
  - **fundamental research** that are recognized at international stage
  - **Applied research** that are useful and beneficial for Thailand's economy
  - **S&T service** to industrial partners and customers
  - **In-house platforms & methods** development

- NSTDA computing Infrastructure is a key enabling facility for NSTDA research integration, collaboration