



**VIỆN KHOA HỌC & CÔNG NGHỆ TÍNH TOÁN TP. HCM**

Institute for Computational Science & Technology at HCM City



**Innovation through computing - Sáng tạo qua tính toán**



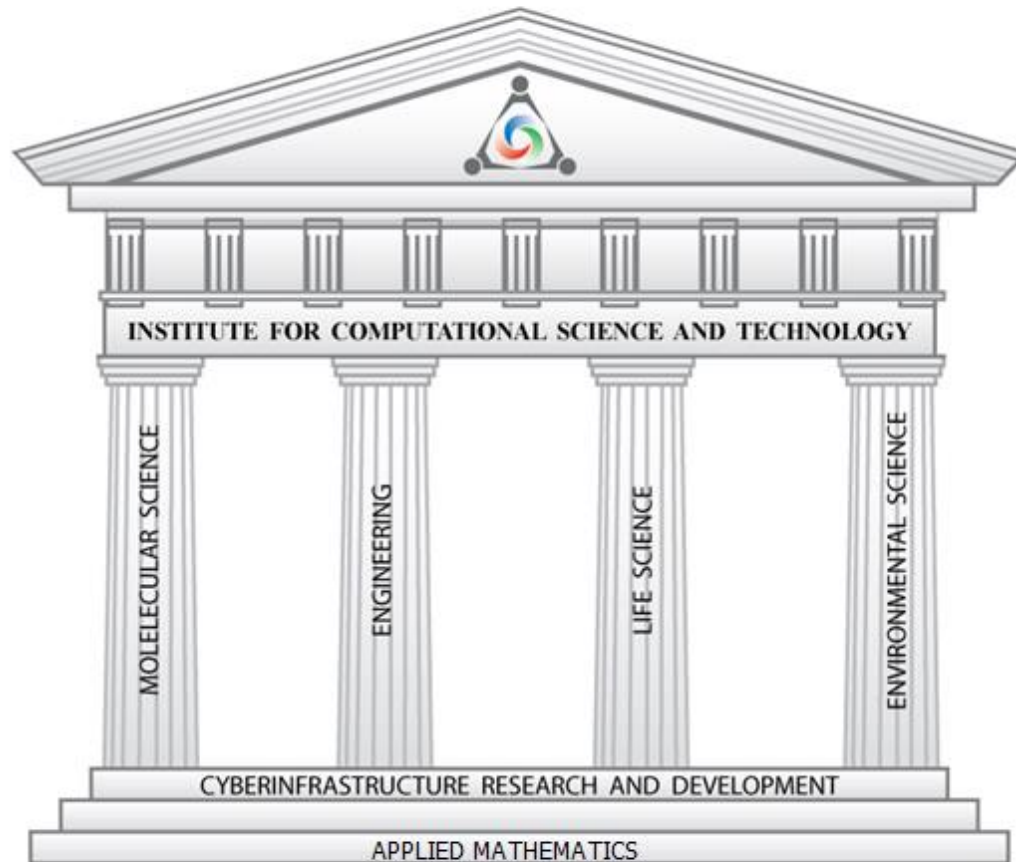
# Grand Opening Ceremony



December 18<sup>th</sup>, 2008 marked the beginning of ICST



# Research & Development Activities

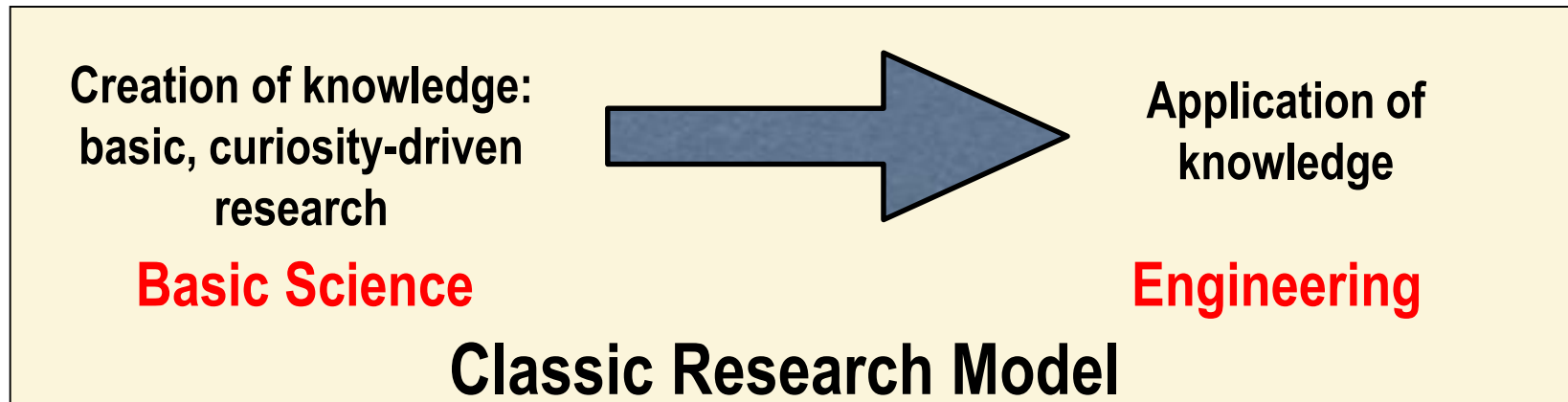


***Mission:*** To advance research, innovation and education in Computational Science and Engineering with the strategic aim for entering the global knowledge economy



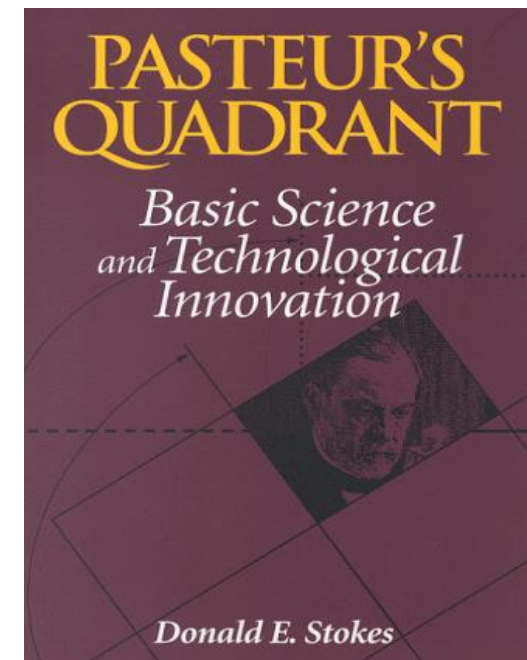


# Pasteur's Quadrant Research Model



## Mission-oriented research model

Focus on New Knowledge Creation?	Yes	Bohr	Pasteur
	No		Edison
		No	Yes
		Focus on Application?	



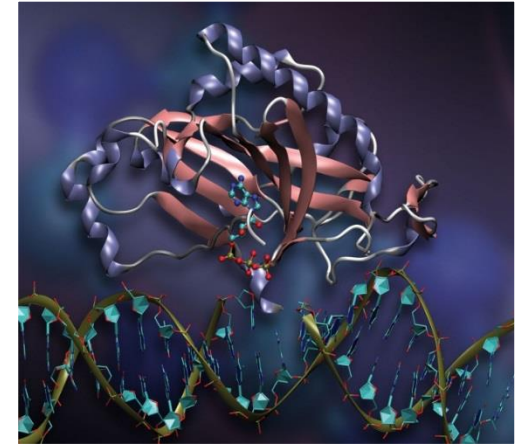


## Focus

- Computer-Aided Drug Design
- Fundamental Understanding of Biological processes
- Bioinformatics

## Current Projects

- Screening and design of drug candidates against Alzheimer's disease, diabetes, breast cancer, HIV and influenza
- Protein folding, unfolding and misfolding
- Method development: Coarse grain modeling
- Evolution of influenza A virus, Comparative study of human cancer genomics



## Members:

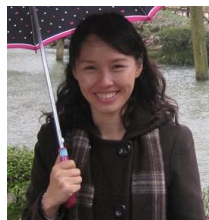
Le Viet Hung, PhD  
Son Tung Ngo  
PD Quoc Huy  
Nguyen Quoc Thai  
Nguyen Thi Kieu Thu  
Tran Minh Nhut  
Nguyen Truong Co  
Vuong Van Quan  
Pham Dang Lan  
Phan Minh Truong  
Nguyen Trung Tin  
Nguyen Hoang Linh  
Vu Thi Mui  
Van Dac Thanh  
Nguyen Van Hung  
Tran Tan Tien



Prof. Ly X. Mai  
Lab Director



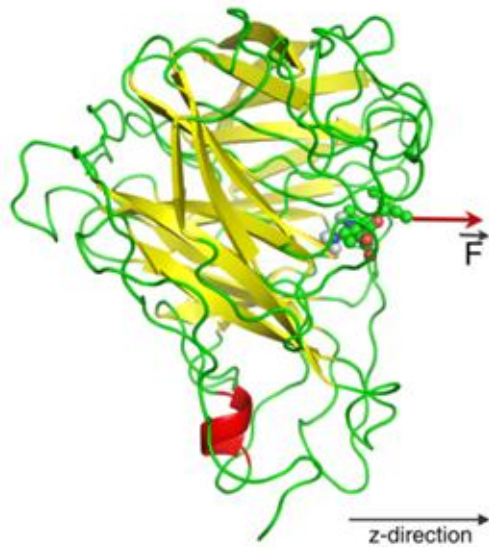
Prof. Thanh N. Truong



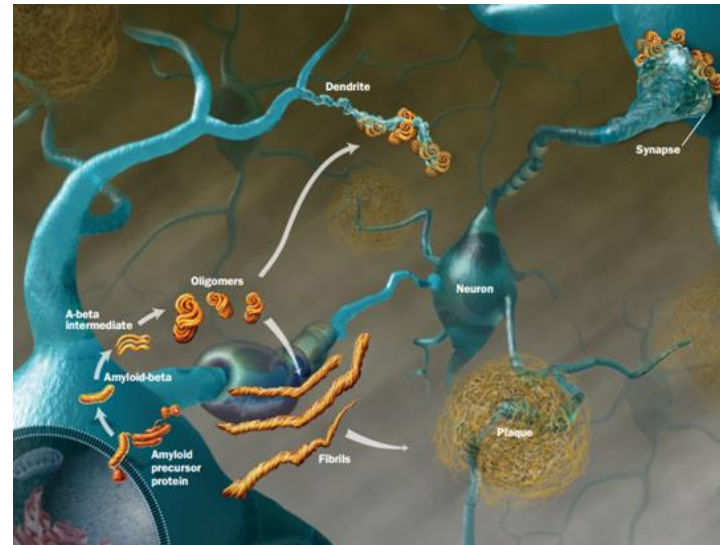
Dr. Ly T. Le



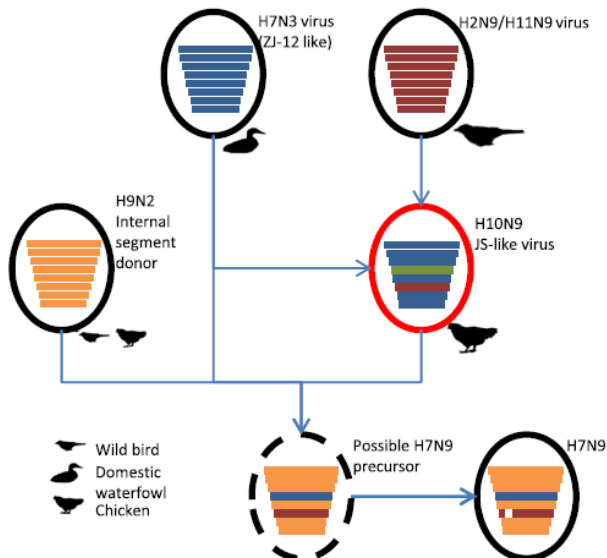
# Research activities



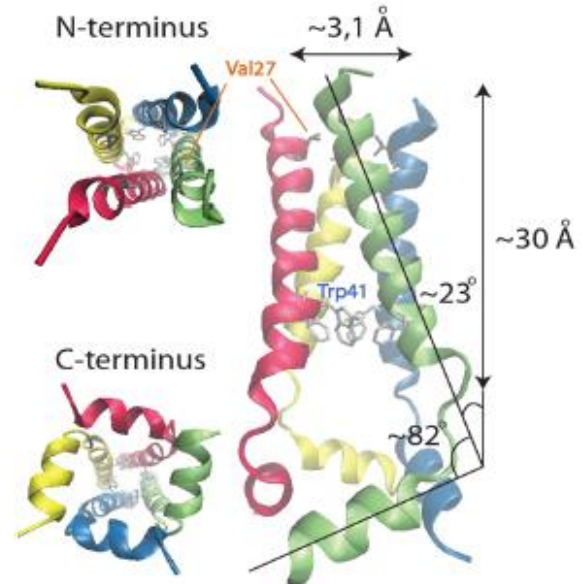
Steered MD for drug design



Understanding Alzheimer's disease



Evolution of Influenza H7N9 Virus



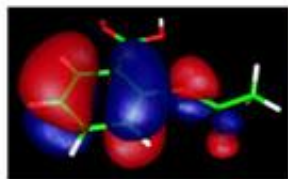
Analysis of M2 channel structures



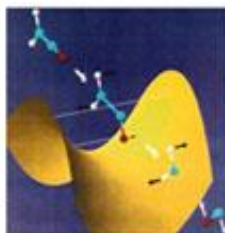
# Molecular Science and Nano-materials Laboratory



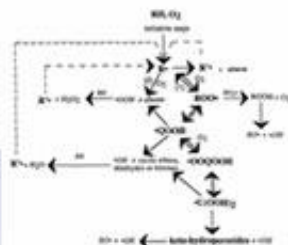
Prof. Tho M. Nguyen  
Lab Director



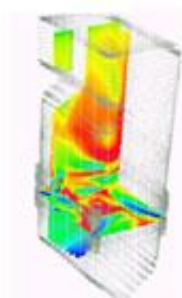
Quantum Chemistry



Kinetics & Dynamics

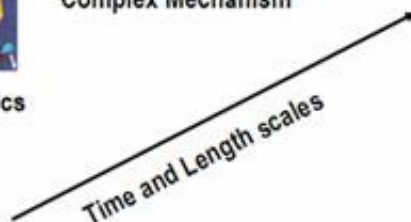


Complex Mechanism



Power Generation

CFD Simulations



Prof. Thanh N. Truong



Dr. Lam K. Huynh

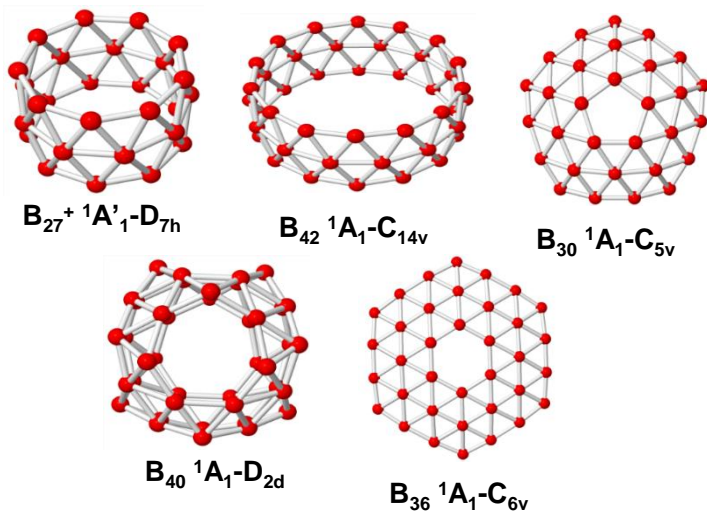


Dr. Nguyen-Nguyen Pham

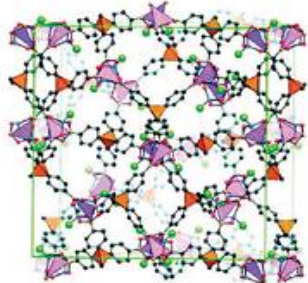
## Members:

My-Phuong H. Pham, PhD  
Tam Minh Nguyen  
Hung Tan Pham  
Duc Manh Nguyen  
Long Duong Van  
Nguyen Thi Ngoc Tuyet  
Phan Thi Thu Thuy  
Loc Quang Ngo  
Minh Van Duong  
Xuan Thanh Le  
Tam-Thanh V. Mai  
Thoa T.-P. Nguyen  
Thong N.-M. Le  
Vu Hoang Nguyen  
Uyen Que Ly

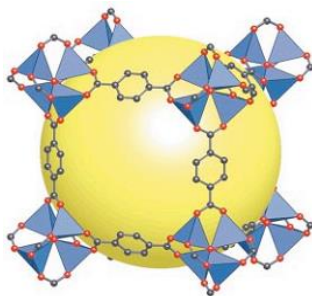




Novel Nano Metal Clusters for  
Catalysis and Hydrogen Storage

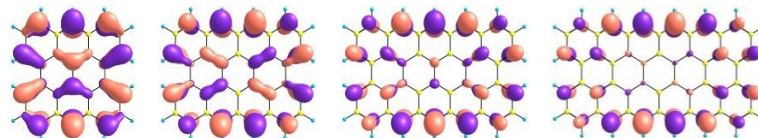


COF 202

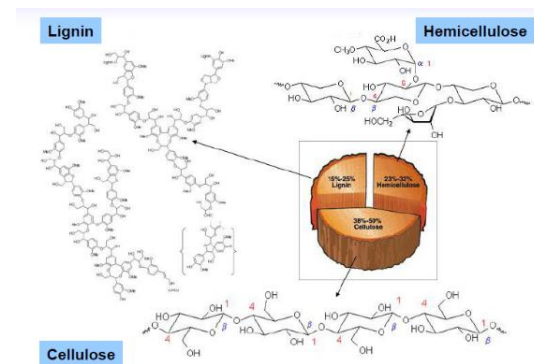
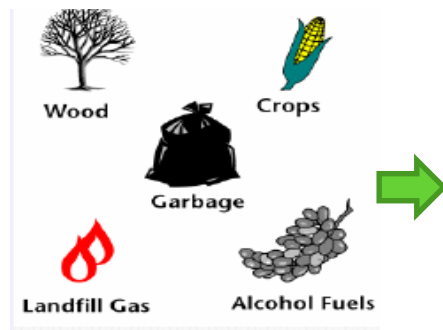


Structures and Activity of Porous  
Framework Materials

Chemistry is on edge



Graphene as new material for  
electronic and spintronic devices



Combustion of biomass

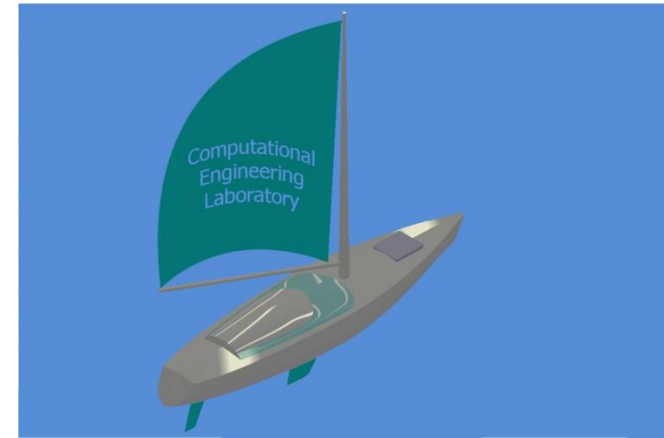




**Focus:** Applications of numerical modeling and simulation methods to discover new scientific knowledge relevant to engineering problems and to enhance technological competitiveness.

## Objectives:

- Achieve world-class expertise in computational methods in engineering sciences and technology
- Produce marketable software for computational engineering applications
- Help industry take advantage of computational engineering tools to enhance their market position
- Contribute to the sustainability of the Institute.



## Personnel

Dr T. Tran (Advisor)



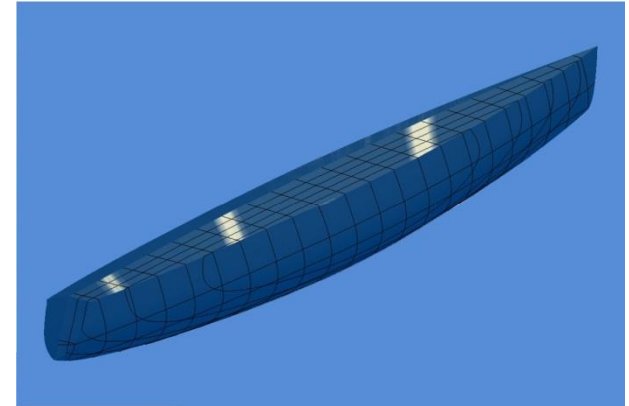
Dr Nhu Tran  
Tuan A. Nguyen  
Hung Q. Nguyen  
Thu-Hong T. Ho  
Duong B. Nguyen  
Nghia-Binh Tran Nguyen  
Dr Thanh X. Ho



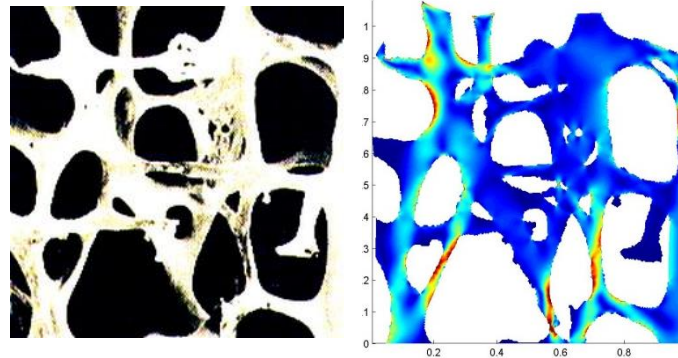
# Research Activities



Multi-physics  
computational systems  
provide coupled solution  
procedures, e.g. aero-  
elasticity problems



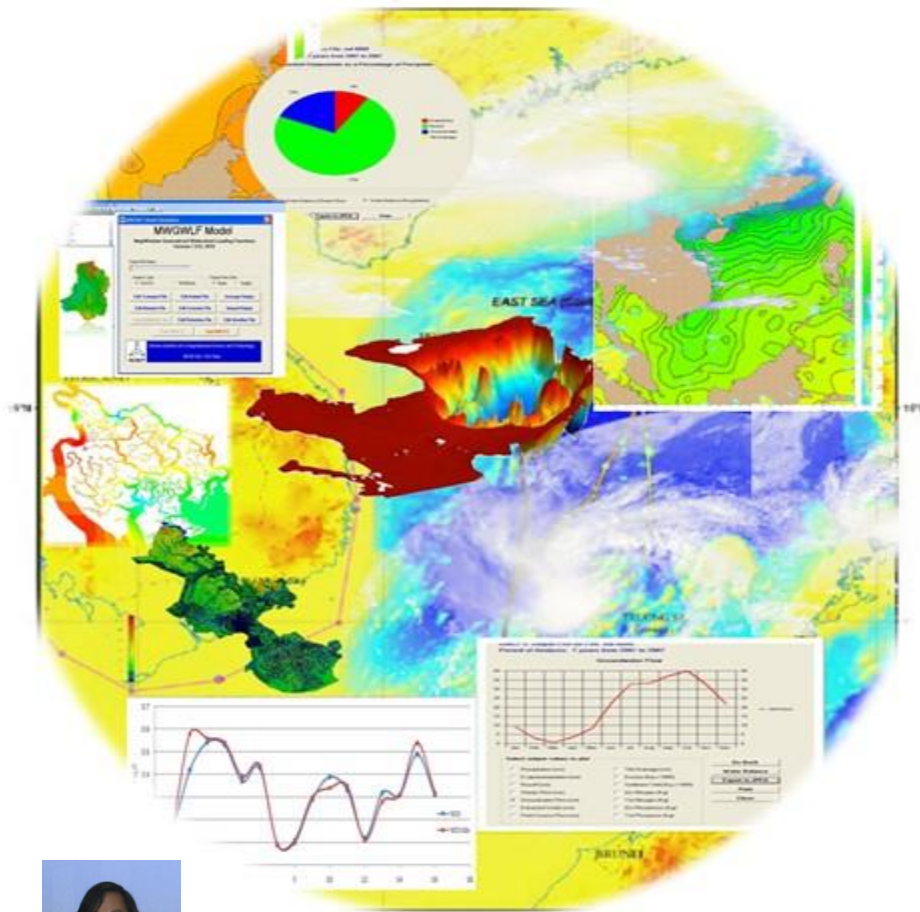
More efficient design and  
analysis process



Modern computational  
methods allow better coupling  
of multiple governing scientific  
principles



# Environmental Science Laboratory



Prof. Thinh V. Nguyen



## Members:

**Tuan Huy Nguyen, PhD**  
**Hong-Ha Thi Nguyen, MS**  
**Long Dinh Le, MS**

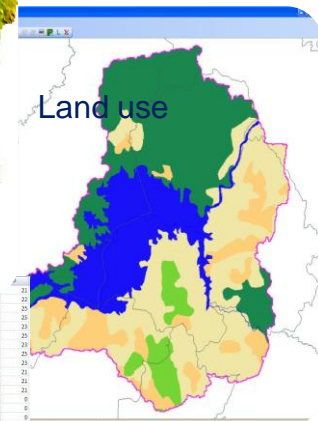
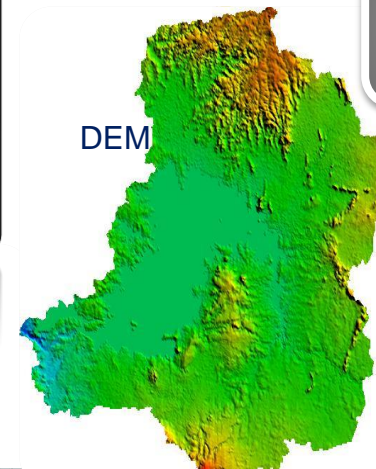
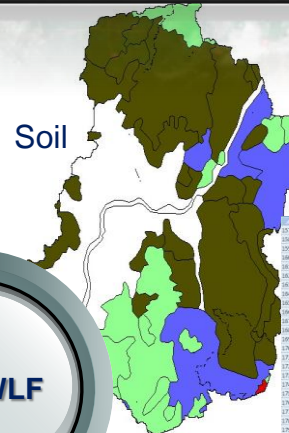
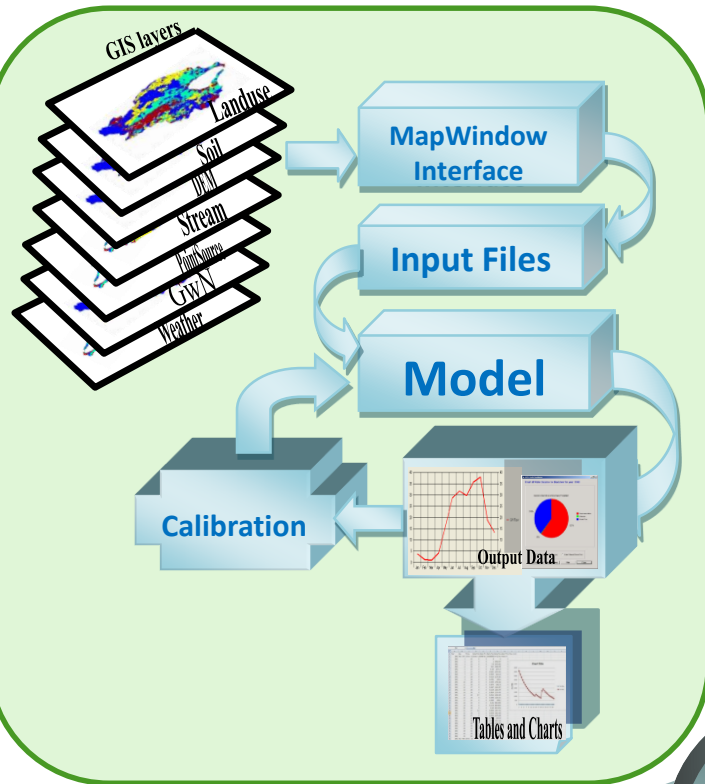




# Research Activities



## GIS-Based Watershed for VIETNAM



**Input data**  
Dem, Landuse, soil,  
stream, point source,  
weather, GwN, GwP

**MWGWLF**

**Flood Forecasting**

Water  
Balance  
Nutrient  
Loads

**Soil Condition for Farming**





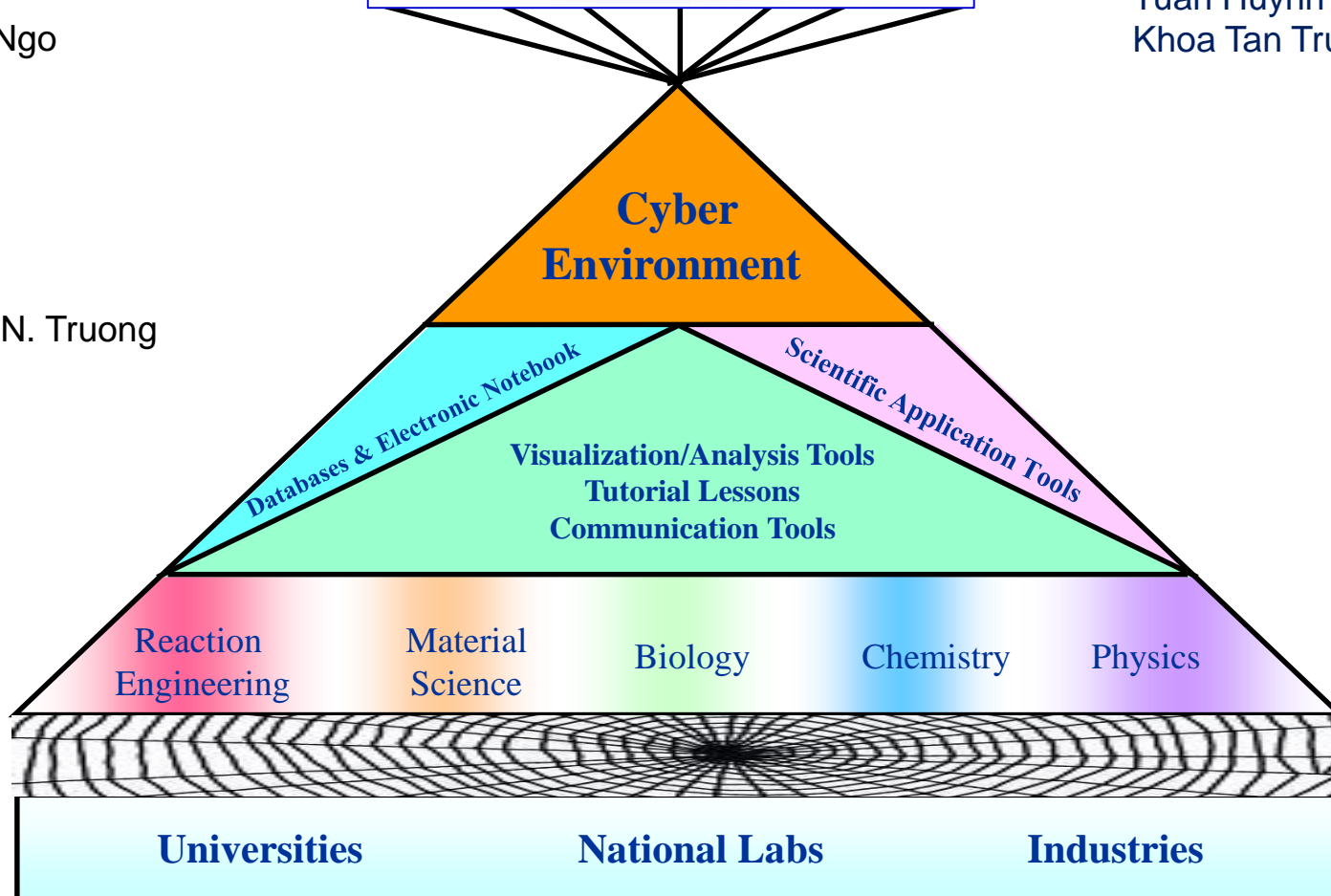
Dr. Chi Duc Ngo  
Lab Director



Prof. Thanh N. Truong



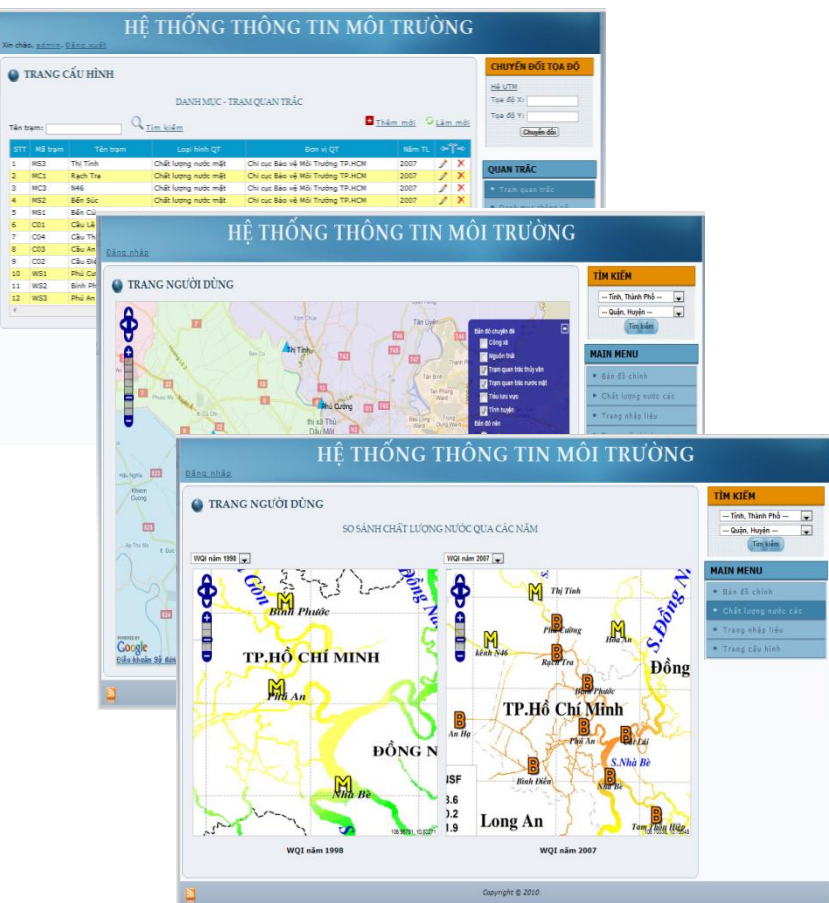
**Members:**  
Hai-Luu Tran  
Tuan Huynh  
Khoa Tan Truong







# Research Activities



## Web-based Information Management System for Environmental Data

**Science Community Laboratory**

Home Challenges Tools Notes Partners Resource About

ZINC Lib My Cards (0)

Pick one you think that may bind stronger to the disease target. Click SUBMIT after placing your bet

Chemical structures for selection:

- Structure 1: CCN(CC)C1CCCC1
- Structure 2: CC1(C)C2=CC(=CC=C2)C(=O)N1
- Structure 3: CC1(C)C2=CC(=CC=C2)C(=O)N1

Buttons: BACK, Collect, NEXT

GET NEW SET SUBMIT

**VERSUS**

**Disease:** Malaria

**Receptor:** Cyclin-dependent protein kinase PfPK5

**Ligand:** N-(2,5-dimethylpyrazol-3-yl)-2-(3-ethyl-2-oxo-benzimidazol-1-yl)acetamide

**Binding Energy:** -8.50 kcal/mol

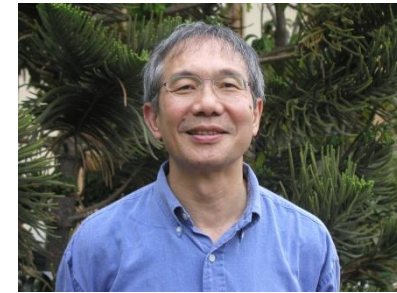
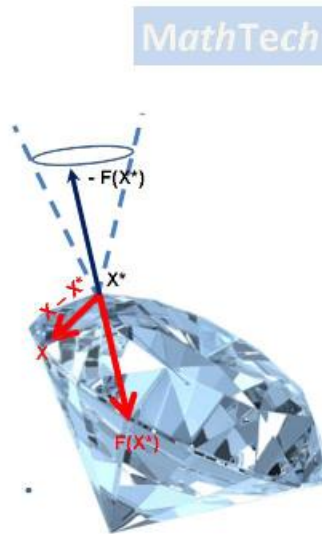
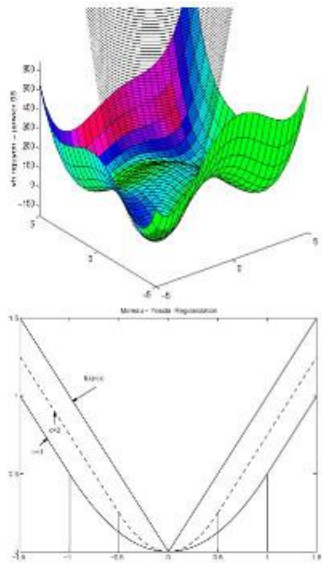
**Ranking:** 497/1099

**Player:** Harold Javid

CHANGE PLAYER

## Cloud-enabled Research and Education Environment for Drug Discovery





Prof. Emeritus Hien Van Nguyen  
Lab Director



Prof. Dr.Sc. Jean-Jacques Strodiot

Equilibrium problems such as **optimization**, **variational inequalities**, **fixed-point** and **saddle-point problems**, and **non-cooperative games** as particular cases based on concept introduced by John F. Nash (Nobel prize in economics in 1994)



Dinh Nguyen Anh Trung, MS

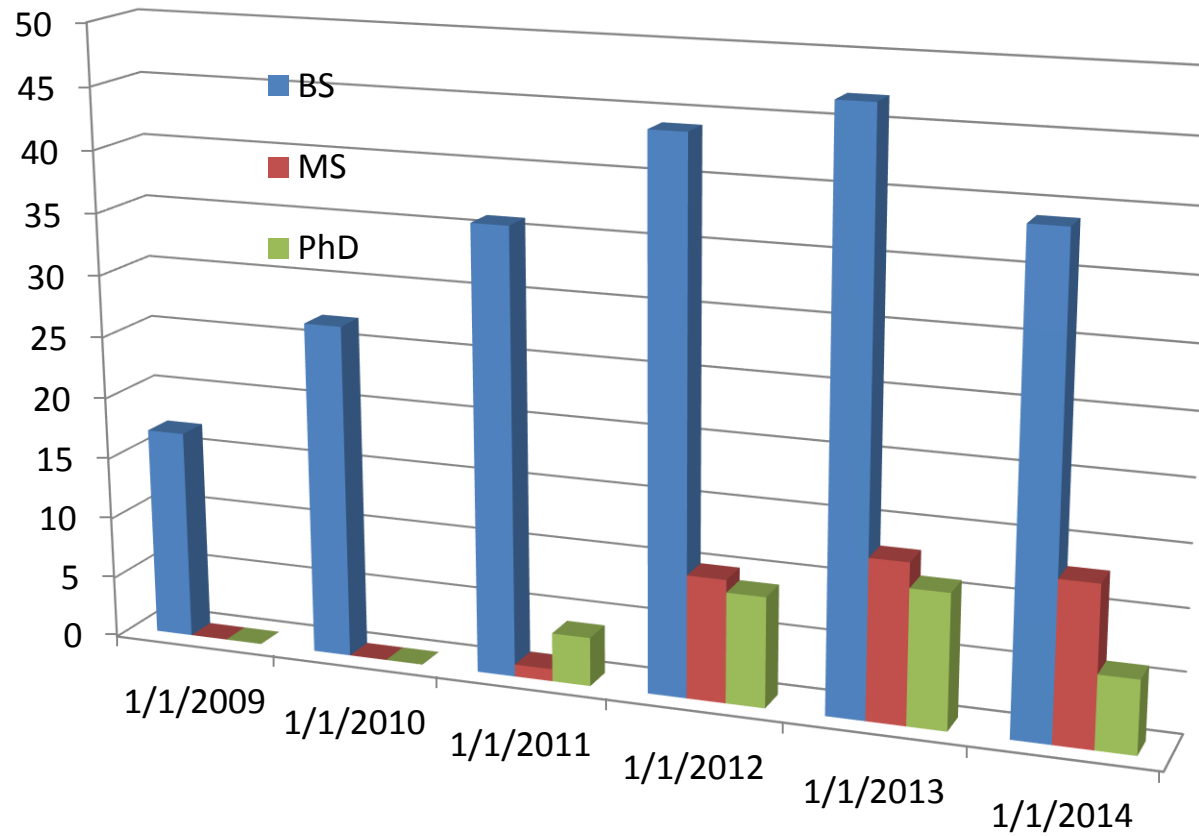


Thi Thu Van Nguyen, PhD

VuongTu Phan, MS



# Research Personnel

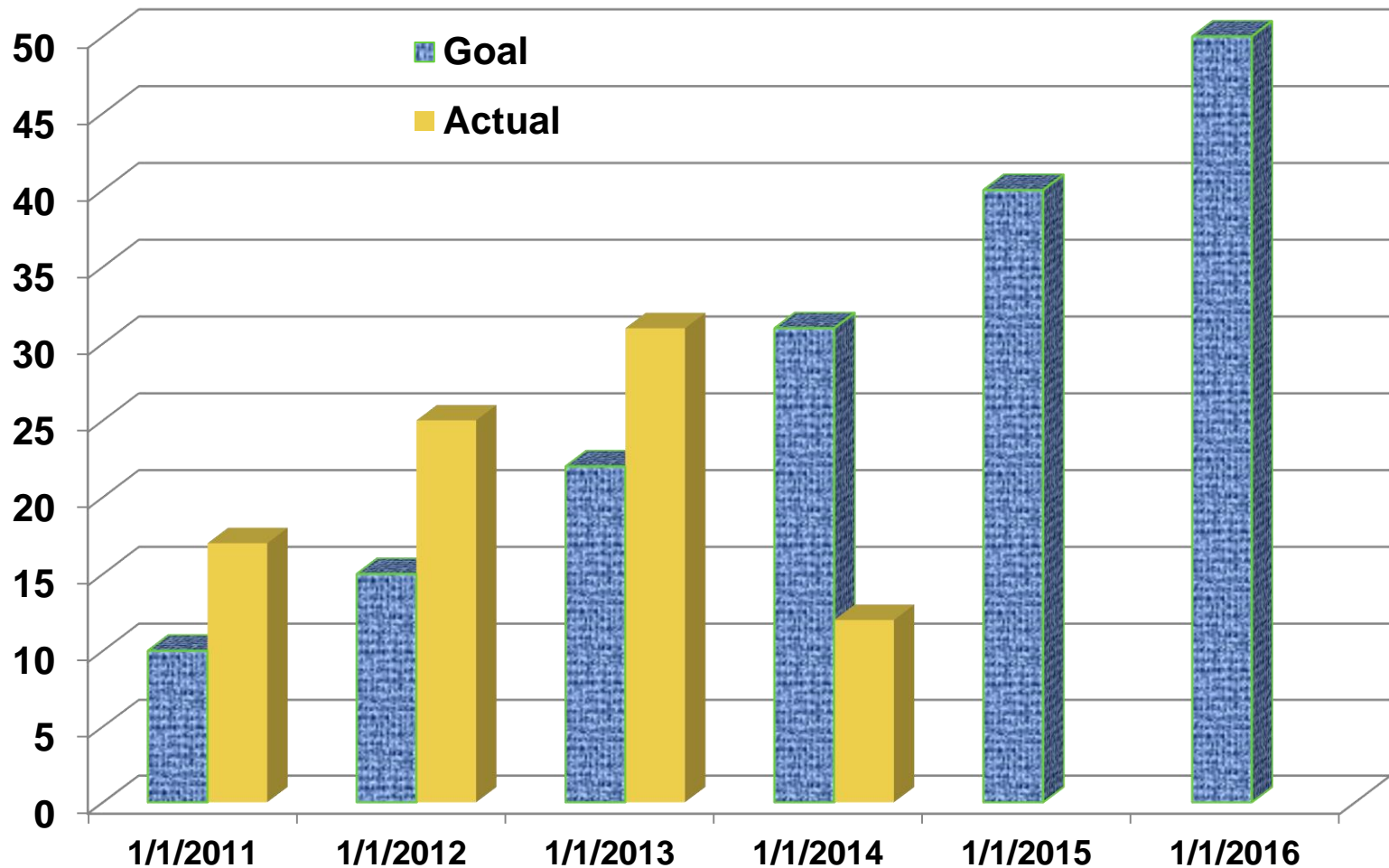




# Research Outcome



## Number of Publications in International Scientific Journals







# Education and Training



- Collaborating with other universities to organize a number of Summer Schools
- A number of researchers obtained MS degrees at local universities
- A number of researchers obtained PhD graduate fellowships in Europe, Australia, and USA.



# Strategies for 2015-2020

## Research



Continue to improve research capability and infrastructure.

Increase its reputation for research and education in computational science and engineering .

## Education & Training



Collaborate with universities to create a sandwich PhD program.

Summer schools in Computational Science & Engineering.

## Technology Incubator







# Three trees make a forest



Tree



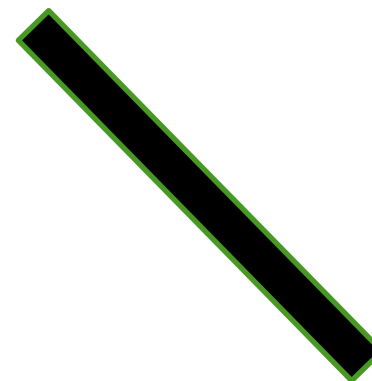
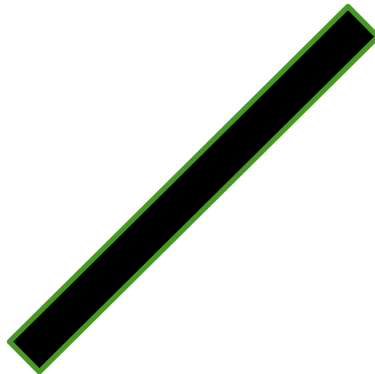
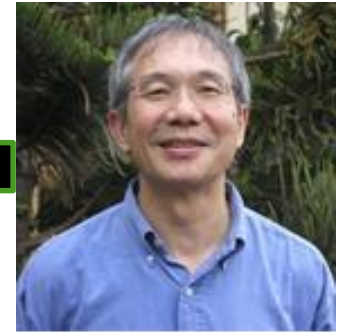
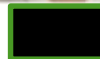
Forest

**Canh 6 - 6-6-2006**



木

# ICST Tree of people





***Thank You***