National R&D Framework

Research, Innovation & Enterprise Council

Ministry of Health

Ministry of Education

Ministry of Trade & Industry

Lee Hsien Loong
Chairman, RIEC
Prime Minister of Singapore

FUNDING AGENCIES & MINISTRIES

A*STAR Research Institutes

Polytechnics
Universities
Hospitals
Corporate Labs
Foster synergies in public-private partnership

Invest in basic science for future innovation

Attract and develop scientific talent

Support for technology commercialisation

Focus on research with economic outcome

Emphasise on competitive funding

5-year S&T Plans

National Technology Plan (1991-1995) S$2 billion

National Science & Technology Plan (1996-2000) S$4 billion


RIE 2015

Research ▶ Innovation ▶ Enterprise
A*STAR Mission

We advance science and develop innovative technology to further economic growth and improve lives

Chairman
Managing Director

BMRC
JCO
SERC
A*GA
ETPL

Support world-class basic and translational biomedical research capabilities, develop talent and engage industry for economic impact and innovative healthcare solutions

Promote and support multidisciplinary research

Support a wide spectrum of leading edge science and engineering R&D capabilities and nurture talent for innovation and industry development

Attract and develop scientific talent

Transfer of A*STAR technologies to industry
A*STAR’s Research Entities

**Science & Engineering Research Council**

- > 4,300 Researchers
- > 2,200 PhDs
- ~ 60 Countries

- Institute of Molecular & Cell Biology (IMCB) 1987
- Institute of Microelectronics (IME) 1991
- Data Storage Institute (DSI) 1992
- Institute of High Performance Computing (IHPC) 1998
- Institute of Materials Research & Engineering (IMRE) 1996

- Institute for Chemical & Engineering Sciences (ICES) 2002
- Institute for Infocomm Research (I²R) 2002
- Genome Institute of Singapore (GIS) 2000
- Institute of Bioengineering & Nanotechnology (IBN) 2003
- Institute for Bioengineering & Nanotechnology (IBN) 2003

**Biomedical Research Council**

- Singapore Consortium for Clinical Sciences (SICS) 2006
- Singapore Institute for Clinical Sciences (SICS) 2006
- Singapore Stem Cell Consortium (SSCC) 2006
- Institute of Molecular Biology (IMB) 2007
- Institute of Medical Biology (IMB) 2007
- Experimental Therapeutics Centre (ETC) 2008
- Singapore Immunology Network (SIgN) 2006
- National Metrology Centre (NMC) 2008

**Biopolis**

- Phase I (2003)
- Phase II (2006)

**Fusionopolis**

- Phase I (2008)
Alfred Huan

Executive Director of Institute of High Performance Computing (IHPC)
Executive Director of A*STAR Graduate Academy (A*GA)

Computational Science & Engineering
To Further Economic Growth & Improve Lives
Physics, Chemistry, Mathematics, Electronics, Material Science, Computer Science, Social Psychology, Cognitive Science, Economics ...

250 researchers; >80% with PhD
Study dynamics of fluid/heat flow and their interactions

Capabilities
- Multiphase flow
- Fluid structure interaction
- Multi-physics environment modelling

Application areas
- Green building
- Microfluidics
- Risk analysis
- Marine & offshore
- Oil & gas
Multiphysics simulations of interactive coupled systems

μSICS: a FSI computational framework

Robust and efficient flow solvers
- Compressible, incompressible flows,
- Free surface

Fast and reliable structural solvers
- Non-linear, large deformation
- Fractures, fragmentation, multi-body flow structure interactions

Advanced meshing capability
- Unstructured mesh generation for complex domains, parallel mesh generation
- Fast local feature-based mesh adaptation

Versatile and accurate coupler
- Advanced coupling approaches, accurate coupling algorithms

*μSICS developed from FLITE cores in collaboration with Swansea University
Urban Flow Simulations

Airflow over a HDB town: 531x477x100 (m)
22mil elements with μSICS

Blast in CBD area: 500x1000 (m)
~15 mil elements with μSICS
Parallel Performance

μSICS optimized for parallel performance
Simulation of droplet splashing on a thin liquid film

This 3D study requires large computational resources due to the development of liquid structure of very different length scales and topology change. Our results were carried out on SGI Altix UV 1000 machine

Mesh number: 8.6 × 10^8
Processors: 512 cpu
The speedup is linear up to Np=256. Then the speedup performance slightly drops below the ideal linear curve when Np=512

This work aids in the understanding of drop splashing and non-splashing control and the underlying mechanism governing flow development at different condition.
The Story

- To predict the transient wave loading forces on complex deck structure with beams.
- Target wave to reproduce a measured real ocean extreme wave.
- Giant domain required to sustain this huge wave: 3D and spreading energy in all directions.
- Extremely fine mesh in the vicinity of the deck structure for accurate force prediction.
- Massive CPUs required to reduce the simulation time within an acceptable range.

Mesh info

About 30 million hybrid cells
The Results

• 128 CPUs are finally used in all our simulations, due to its best cost efficient performance.

• The use of supercomputing resource in this project has enabled us to deliver an advanced numerical tool that is capable of predicting various environmental loads for offshore structures under extreme weather conditions.
Design and Analysis of Engineering Systems

Capabilities
- Structural reliability/performance
- Manufacturing process simulation
- Design of flexible structures
- Soft active materials & devices
- Nanostructure growth & properties

Application areas
- Thermal management solutions
- Maritime & offshore
- Microelectronics
- Aerospace
- Manufacturing & MRO
- Renewable energy
Large-scale MD for Mechanical properties of Metallic Glass

- Metallic glasses (MGs) for future structural and functional applications
- Large-scale MD simulations (up to 15 million atoms with 4000 cores)
- Excellent correlations to experimental results from collaborators at Caltech
- Demonstrate that computations bridge gap between macroscopic mechanical fracture processes and the corresponding mechanisms at the atomistic time and length scales

Sample works:

Flaw-sensitivity of MG nanopillars

Nano Letters 14, 5858–5864 (2014)

Size-dependent mechanical behavior of MG nanolattices

Coarse-grained simulation of Melanosome Lipid Bilayers

MD models for accurate representation of human skin melanosomes such as their biophysical structure, properties and functions

Constructed and validated atomic and coarse-grained models for the melanosome lipids (100,000 beads with 256 computational cores)

Properties including area per lipid, order parameter, density profile, bilayer thickness and diffusion coefficient for preliminary understanding of their molecular interactions and biomechanical behaviour

Snapshot of a typical lipid mixture at $T = 305K$

DPPC  Cholesterol  Palmitic acid (C16:0)
Communications using light-matter & wave-matter interaction

**Capabilities**
- Electromagnetic compatibility/interference
- Radio wave propagation
- Lightwave technologies
- Solar irradiance modelling

**Application areas**
- Low-power, high-bandwidth comms
- High-resolution/sensitivity sensing
- Structural flaw detection & imaging
- Biomedical devices
- Personal care, skin optics
- Meta-material antenna (satellite)
Parallel computing to advance nanophotonics technology research

- Objectives
  - To speed up the development of novel nanophotonics technology for data communications and sensing
  - Tool for fast and accurate novel theoretical prediction
  - As useful guideline and low cost tool for experiment

- Approach
  - Finite difference time domain method: fully vectorial 3D computational engine to solve electrodynamics problem on multi-core processors and multiple nodes of HPC system

- Results
  - Successfully modelled optical performance of real 3D experimental multiscale and complex multi-materials structures
  - Used 64 cores or 128 cores (impossible to run on 12 cores of Z800 HP workstation with 32G memory)
  - Very good agreement with characterization results
  
  **Modeling domain:** 151x151x268 cells
  
  **~15h on 64CPU for each simulation**
  
  **Nano Lett 15, 5796 (2015)**

  **Modeling domain for 9 periodic structure:** 481x57x394 cells
  
  **~8h on 128CPU for each simulation**
  
  **ACS Photonics 2, 385 (2015)**
Advance Materials/Chemical Science by Computation

Capabilities
- Properties of materials/chemicals
- Catalysis modelling
- Erosion and Corrosion
- Adhesion/permeability/coating
- Surfactant/emulsion
- Nucleation/crystal growth
- Phase diagram/diffusion kinetics
- Materials/chem informatics

Application areas
- Virtual material design
- Personal care/food beverage
- Chemical/pharma manufacturing
- Aerospace
- Electronics/semiconductor
- Marine offshore/oil & gas
- Building/construction
Our Capabilities

First Principles
DFT, Post-KS, HF, Reactivity, Electronic, Magnetic, and Optical Properties

Molecular Dynamics
All-Atom, Coarse-Grain Monte Carlo, Self-Assembly, Diffusion, Geometry, Thermodynamics, Kinetics

Meso Scale
Phase Field, Crystal Nucleation and Growth, Phase Transitions

Continuum
Bulk Properties, CALPHAD, Informatics, Phase Diagrams
Our Capabilities

**First Principles**
VASP, Quantum ESPRESSO, Gaussian, Materials Studio

**Molecular Dynamics**
GROMACS, LAMMPS, in-house code

**Meso Scale**
In-House Code

**Continuum**
Dictra, Thermocalc

Atomistic methods make use of extensive HPC resources

Meso scale and Continuum Methods don’t require extensive HPC power for MSE
Classical molecular dynamics simulation of large branched polymer electrolyte adsorption on oxide surface in cement solution for cement additive design

Number of atoms: ~1 million, with complex solution formula and charged surface. Number of cores: 4096 cores
Unit A of human estrogen receptor A

- Want to understand binding in Estrogen
- Prevent Endocrine disruptors like BPA

Details of Simulation
- 78,000 atoms
- CHARMM all-atom forcefield
- Gromacs 5.1 with CUDA 7.0

Performance on a Single Node
- CPU-only run (24 cores): 56 ns/day
- With 1x K40m: 85 ns/day
- With 2x K40m: 130 ns/day
- With 1x K80: 120 ns/day
- With 2x K80: 146 ns/day

Challenges
- Finding the best ratio between number of OpenMPI/OpenMP tasks
- CPUs are substantially slower
- More routines should be optimized for GPUs
Making computing more efficient, insightful & intelligent

Capabilities
- High performance computing
- Cloud computing
- Big data
- Geometrical modelling
- Complex systems modelling
- Intuitive interactive technologies

Application Areas
- MRO optimisation
- Real-time prognostics
- Urban planning & logistics
- Medical diagnostics & training
- Tutoring robots
High-Speed Sparse Matrix-Vector Multiplication (SpMV) on GPU

Sparse systems arise in many engineering problems:
- Fluid dynamics
- Structural mechanics
- Circuit analysis
- Graph analysis

System represented as $Ax=b$, where $A$ is sparse

Iterative algorithms for solving systems
- E.g. conjugate gradient method, GMRES
- Sparse matrix-vector multiplication usually a bottleneck in such solvers

**Motivation**
- Design and develop bit compressed sparse matrix-vector formats that compute SpMV efficiently on GPU with high speedup

**Approach**
- Designed efficient bit compressed formats called BRO that reduces memory bandwidth requirements of SpMV kernels on GPU
- Developed a family of BRO-CSR and BRO-ELL kernels that achieved high speedup on real-world matrices

**Achievement**
- Demonstrated speedup of SpMV on real-world matrices, of up to $2.7x$ for BRO-CSR to CSR and $2x$ for BRO-ELL to ELLPACK
- Showed that conjugate gradient method is faster by up to $1.4x$ when BRO-ELL/BRO-CSR is used
- ACM/IEEE *Supercomputing Conference (SC) 2013*
- IEEE Transactions on Parallel & Distributed Systems (TPDS) ‘14
Optimizing and Auto-Tuning Iterative Stencil Loops on GPUs

**Motivation**

- Stencils: important class of computations used in many scientific disciplines. E.g. Computational fluid dynamics, heat diffusion, electromagnetics, image processing
- Optimize and develop an auto-tuning method for iterative stencil loops that execute efficiently on GPUs with good speedup

**Approach**

- **Identified bottlenecks** in current implementations such as Nvidia SDK
- Developed **efficient memory staging method** for stencil computation
- Developed **model** of the performance characteristics
- Designed **auto-tuner** to identify optimal parameters with high execution efficiency on GPUs

**Achievement**

- Demonstrated speedups of between **1.4x to 2x** for single and double precision stencil kernels **compared to Nvidia’s implementation**
- Model-guided tuning approach can improve search times by up to 20x
- **IEEE IPDPS 2013**

“We have developed optimized and auto-tuned stencil implementations that execute efficiently on GPUs.”
Workflow Management & Adaptive Computing

Designed and developed workflow-enabled scalable data computation platform for large-scale data-intensive applications.

- Manage **big, distributed** nature of data for data analytics workflow applications in Hybrid Clouds.
- Automate the workflow process for data analytics with multi-objective optimisation: **budget + performance**
- **Adaptively** scale up and down resources

**Achievements:**
- Best Prototype Award: IEEE International Workshop on Scalable Computing for Big Data Analytics ’12
- 1st prize: IEEE Scale Challenge’13
- IEEE Transactions on Cloud Computing ‘13, FGCS’13
Scalable Complex System for MRT Disruption Scenario analysis

1st Prize IEEE Scale Challenge

- 90 MRT stations
- 3000 trains
- 2-7 million agents
- 1000 AWS VM instances

Large scale Complex System Data Modelling and Visualization

Reduce the cost by 10 times using our adaptive fault tolerance tech In Clouds
Develop advanced social computing and social informatics solutions to study people-centric issues and human behaviour

Capabilities
- Psychometrics & decision science
- Psychographic analysis & inference
- Study behaviour at individual, group and community levels
- Social media/network analysis
- Collaborative technologies

Application Areas
- Cognitive function monitoring
- Psychographic profiling
- Consumer insight
- Behaviour motivation
- Public communications
Capabilities for Multiple Domains
How does M&S enable our partners
better products, better processes,
better environment, healthier society...
"I am very surprised at the reality of the analysis results. We are going to apply this analysis method to our business."

"The higher level management in print head division is confident that Seiko Instruments Inc. can definitely generate great sales by using IHPC solver in future."

Seiko Instruments Inc

"Accurate temperature modelling during printing operation"

"Abrator tower for SOx/Nox reduction"
Near-field scanning + M&S replaces expansive far-field scanning
Benefits: performance & productivity increase by 10-20%

Design of high-speed modulator
Benefits: estimated R&D savings of 500%; 4-fold reduction in turnaround time

High-bandwidth visualisation for large facility design & validation
Benefits: reduce team design review by 70%
Cooler, Liveable Environment

- Esplanade concert hall
- Hawker Center
- Bus Interchange

Urban airflow over marina
Technology/Process that can save lives

- Heart valve engineering
- Mitral valve diagnosis
- 4D strain model
- Stent
Development of “Urban Microclimate Multi-Physics Integrated Simulation Tool" (UM-MIST)

Institute of High Performance Computing
Institute for Infocomm Research
Building Research Institute, HDB

POH Hee Joo, IHPC

Oct 2015
Aim: Creating Highly Liveable Residential Towns

Response to L2NIC – Create a Virtual Platform

- Planning & urban design
- Key environment factors
- Impacts to environment and liveability

Land & Liveability National Innovation Challenge
Integrated Research Approach

Integrate whole process (master planning, urban design & environmental modelling)

Multi Disciplinary Modelling Platform
- Noise
- Thermal
- Solar Irradiance
- Shadow
- Wind

Integrated process

Urban Digital Model
- Planning & Urban Visualisation

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Key Points

- **Multi-physics Simulation Tool Impact**
  - Novelty to perform multi-physics simulation on single digital platform
  - Large scale simulation process
  - Ease of interfacing with other modules
  - Competitive advantage over stand alone commercial package

- **Validation with ground truth**
  - Environmental data collection over 1 year period

- **Multi-agencies work together**
  - Integrated town planning, visualization and modelling
  - Sharing of agency research findings
  - Coordination on sensor data and simulation tool usage
  - Collective policy making
All these achievements/results were based on the older generation of HPC resources (up to 220 TFLOPs)

Going forward, we will be able to further advance science & technology as Singapore gets equipped with its first Petascale supercomputer
National Supercomputing Centre (NSCC) Singapore

- **National facility** with computing, data and resources
- Enable users to solve science & technology problems
- Stimulate industry to use computing for problem solving, testing designs and advancing technologies
- Linked by **high bandwidth networks** for high speed access to users anywhere
NSCC & STAR-N
OBJECTIVE

To establish a National Supercomputing Centre (NSCC); and a Science, Technology And Research Network (STAR-N); so as

– to support national initiatives, attract industry partnerships and enhance capabilities to solve problems of greater complexity

– to provide open access to HPC resources and services to public and private sectors
NSCC & STAR-N
ECONOMIC IMPACT

1. Supporting National R&D Initiatives
2. Attracting Industrial Research Collaborations
3. Enhancing Singapore’s Research Capabilities
National Supercomputer Centre

**National Supercomputing Centre (NSCC)**
- New 1+ PetaFLOP Supercomputer
- Recurrent investment every 3-5 years
- Co-investment (OpEx) from primary stakeholders

**Science, Technology & Research Network (STAR-N)**
- High bandwidth network to connect the distributed login nodes
- High speed access to users (both public & private) anywhere
- Support transfer of large data-sets (both locally & internationally)
- Build local & international network connectivity (Internet 2 USA, TEIN*CC To Geant, To Japanese Networks)
  - ASEAN, USA, Europe, Australia, Japan, Middle East

Joint Stakeholders

[NSCC logos]
[STAR-N logos]
NSCC Supercomputer

~1 PFlop System

- **1,288 nodes** (dual socket, 12 cores/CPU E5-2690v3)
- **10 Large memory nodes** (1x6TB, 4x2TB, 5x1TB)
- **Mellanox EDR Fat Tree**
- **128 nodes GPU accelerated**: Tesla K40

~10PB Storage

- **HSM, Tiered, Tier 3 cheap, non-spinning disks**
- **I/O 500 Gbps flash burst buffer**, 10x **Infinity Memory Engines (IME)**

Fast Connection

- **InfiniBand connection to all end-points (login nodes) at three University campuses**

Workflow pipeline (from sequencer to memory/storage) + interactive access built in

Just-in-time resource delivery i.e. interactive access for some workloads (genomics)

Warm water cooled
Global Connectivity as Anchor Participant of InfiniCortex Project
ありがとうございます

ありがとうございます