HPC and Cloud Computing in Nanyang Technological University

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2nd December 2009

Presentation Outline

- Brief introduction to NTU
- High Power Computing Needs at NTU
- HPC @ NTU
- HPC Cloud


NTU Campus

Our heritage

- Established in 1955 as Nanyang University, the first Chinese-medium university outside China
- 1981: Nanyang Technological Institute set up with 3 engineering schools
- 1991: Birth of NTU, incorporating National Institute of Education, an autonomous institute of NTU
- 2005: 50th anniversary - Set up of 3 new Schools
  - Art, Design and Media
  - Humanities and Social Sciences
  - Physical and Mathematical Sciences
- 2007: Formation of a college structure
  - College of Engineering
  - College of Business
  - College of Science
  - College of Humanities, Arts & Social Sciences

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Facts & Figures

- Total student population – More than 31,000
- International students make up 20% of undergrads and 60% of graduate students
- Total staff strength – about 2,700 faculty and research staff from over 55 countries
- About 50% faculty are international
- Alumni strength – about 120,000
- NTU is a research-intensive university with globally acknowledged strengths in science and engineering.

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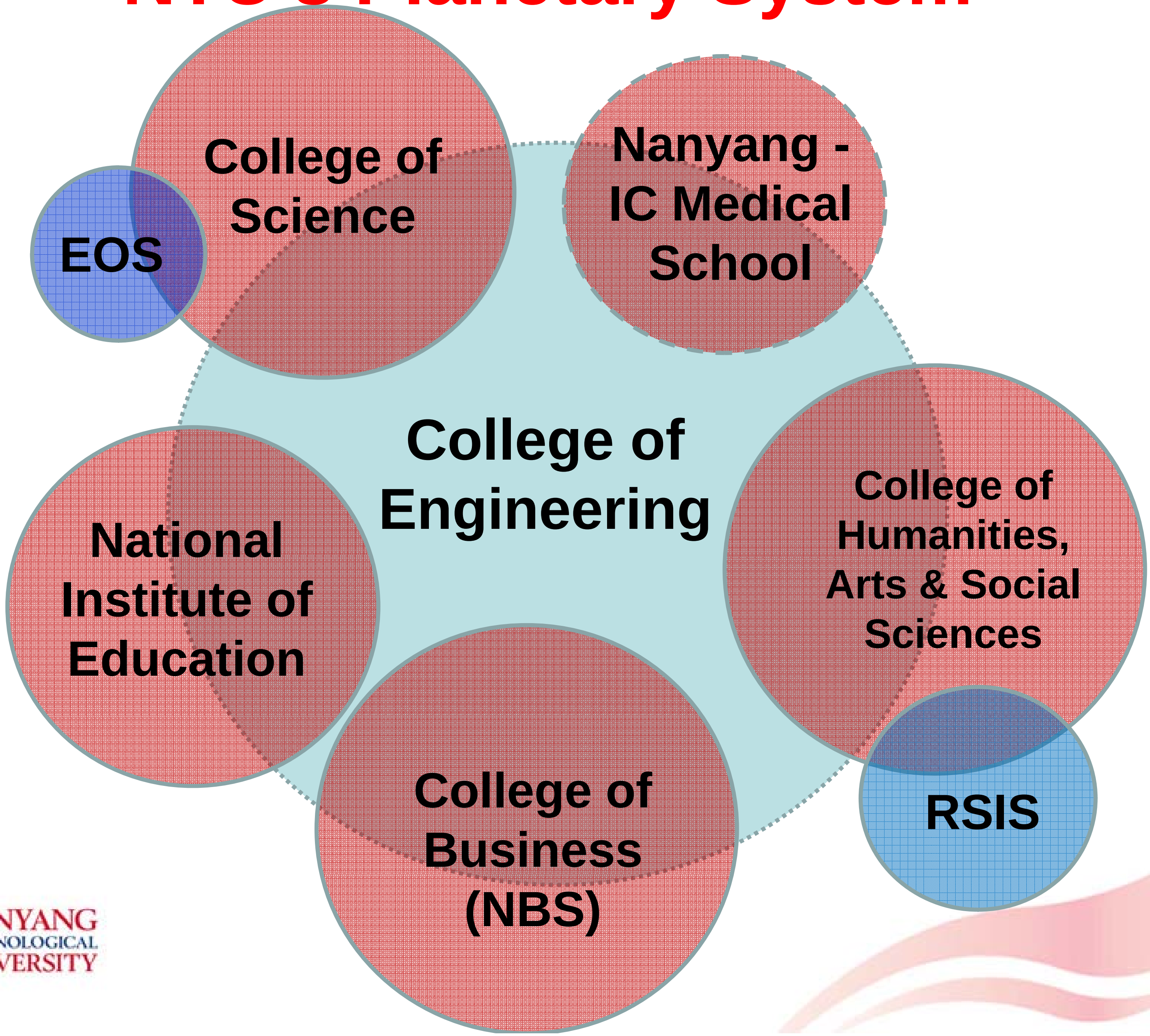
NTU's Planetary System



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High Power Computing Needs at NTU

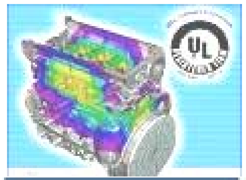
Environment & Energy

- Seismic Analysis
- Membrane Processes
- Reservoir Analysis
- Energy Conversion Systems

Finance

- Economic Analysis
- Actuarial Analysis
- Asset Liability Management
- Portfolio Risk Analysis
- Statistical Analysis

Engineering

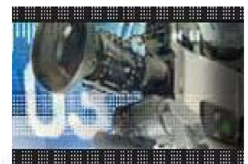


- Mechanical/ Electric Design
- CFD Studies
- Failure Analysis
- Aerospace Engineering
- NanoTech

Life Science

- Drug Discovery
- Protein Folding
- Medical Imaging

Digital Media



- Bandwidth Consumption
- Digital Rendering
- Gaming

Earth Science

- Earthquakes
- Weather Analysis
- Seismic Analysis

Earth Science

Earth Observatory of Singapore

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Traditional, *ad hoc* responses to dynamic earth processes are not adequate for the next century or millennium

We need a pro-active approach to tackling the problems associated with natural hazards in Southeast Asia

The Earth Observatory of Singapore

Aims to be the premier institution in Southeast Asia for understanding and addressing Earth processes that pose threats to human life, happiness and progress

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Earth Observatory of Singapore (EOS)

- Officially opened on 19 February 2009, it is the region's flagship institute for earth sciences research and innovation
- Awarded S$150 million by Singapore National Research Foundation and Ministry of Education

EOS is dedicated to the understanding of basic processes that produce natural hazards such as **earthquakes & tsunamis, volcano activities** and **climate change**

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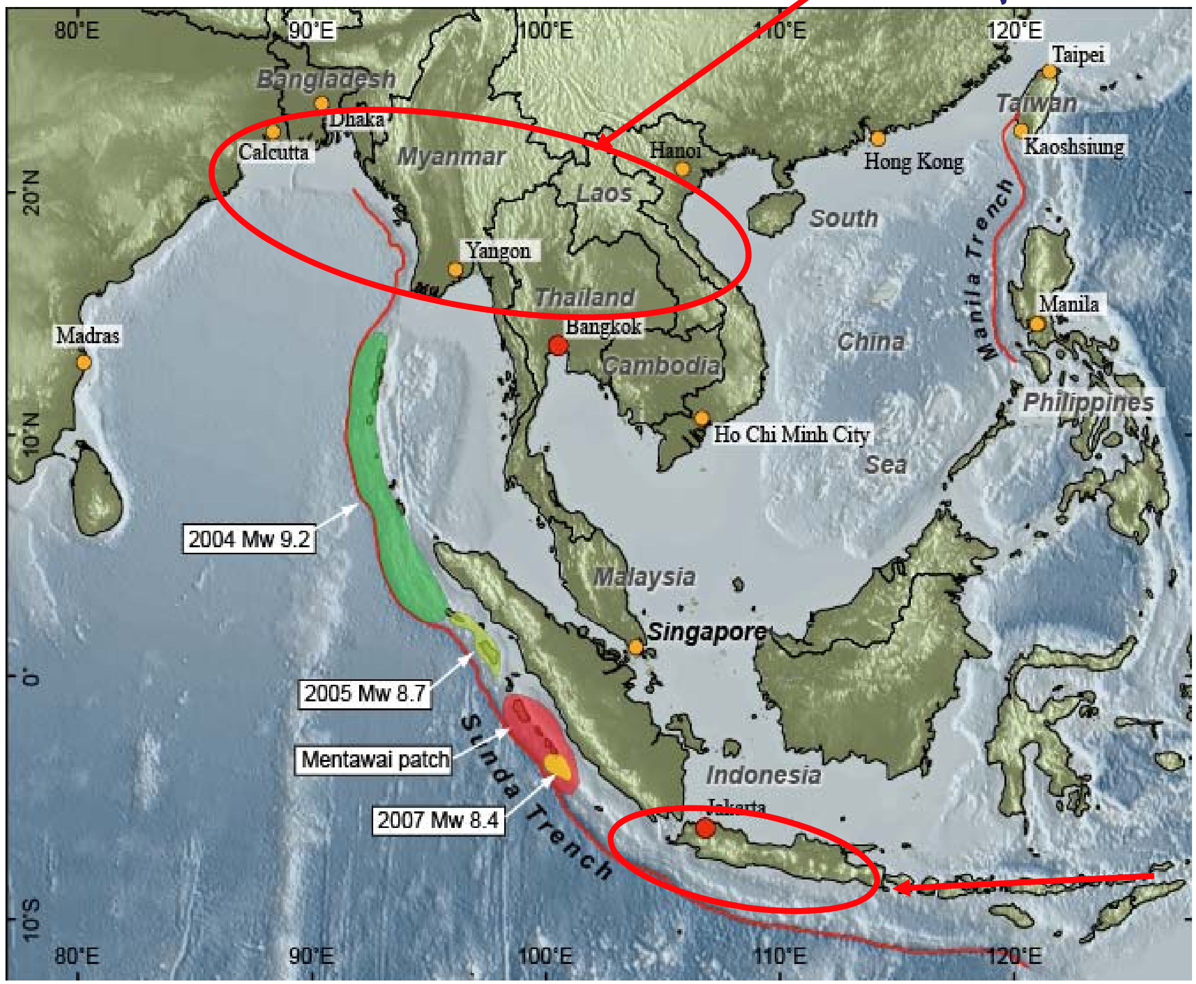
Region of Interest

Myanmar, northern Vietnam

Where are the other seismic and tsunami problems in Southeast Asia?



Java, Bali

EOS scientists will conduct systematic studies of these and other active regions

Among other things, the work will provide basic input to the Singapore-ETH Global Earthquake Model project

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Integrative Catastrophe Risk Management

- Natural Disasters
  - Hazard Assessments - Earthquakes / Tsunamis, Wind Storms / Floods, Volcanoes (connecting EOS with engineering)
  - Loss Estimates and Financial Engineering for risk transfer
  - Public Policies on Risk Mitigation, Emergency Response and Post-Disaster Reconstruction (science, technology & society)
- Manmade Disasters
  - Non-Traditional Security Issues
  - Pandemic, Terrorism, etc
- Security and Sustainability in Urban Living
  - Protective Technology for Safety and Security – protection against multi-hazards

Sustainable Living

- Environment and Water
- Energy
- Clean Tech Hub
- Urban Living

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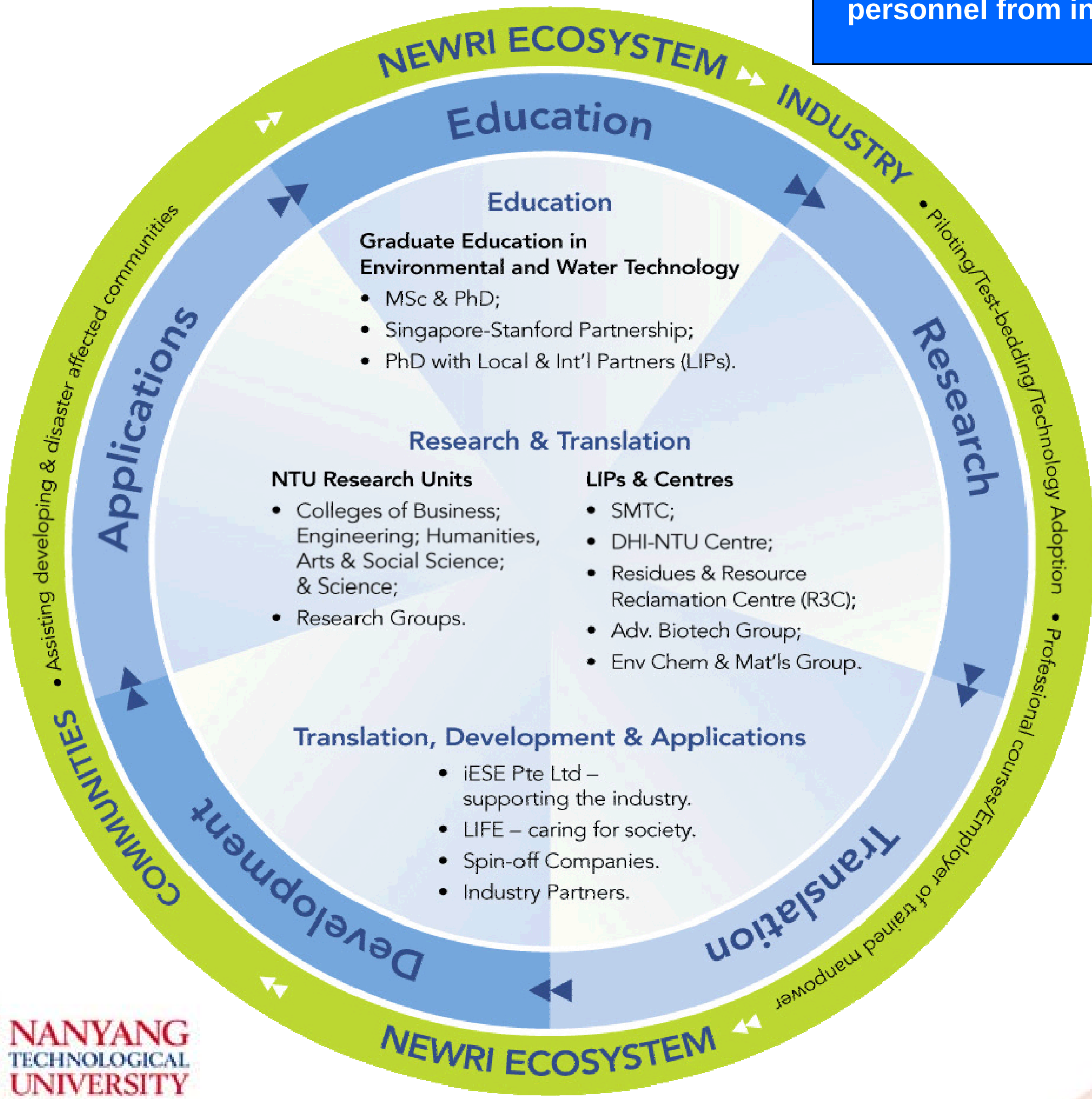
Environment and Water

NEWRI

NEWRI

- Chairman (Provost)
- Executive Director
- Members: Senior faculty, key personnel from industry

← International Advisory Panel



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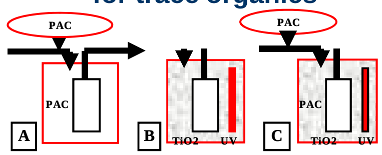
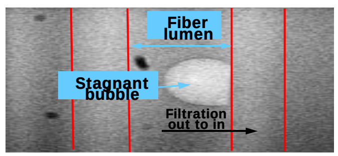
Nanyang Environment & Water Research Institute

Singapore Membrane Technology Centre

Hybrid membrane processes for trace organics

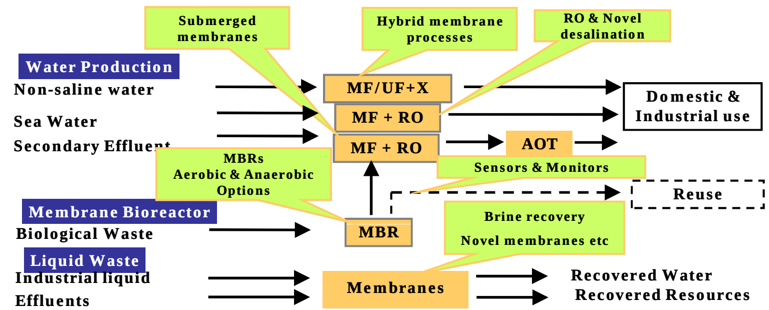


Observation of bubbles in Fiber Lumen by X-rays @Singapore Synchrotron

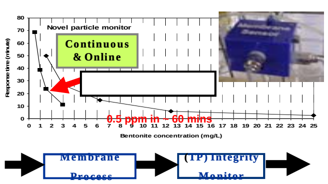


Bubbles formation in the permeate causes a loss of performance

Areas of interest in the SMTC include water production and waste water reclamation with membranes.

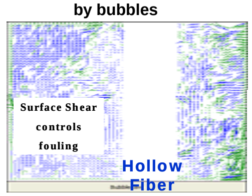


Integrity Monitoring

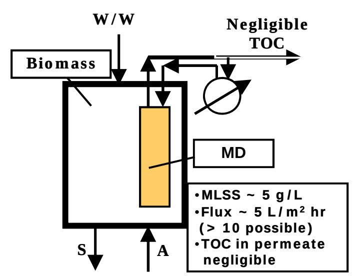


Particle Image Velocimetry

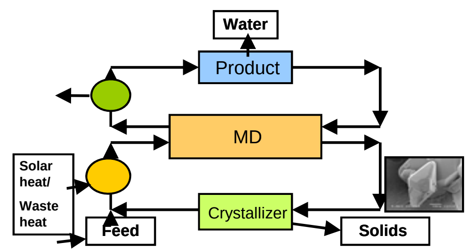
Surface shear on hollow fibres induced by bubbles



Membrane Distillation Bioreactor



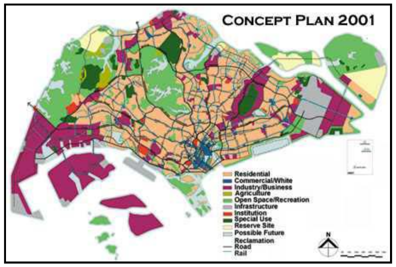
Membrane Distillation Crystallization for RO brines

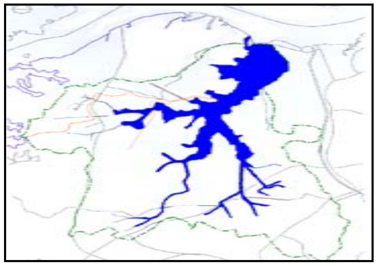


- Low (Atmospheric) Pressure and Low Grade Heat
- High purity water and potential solid product
- Very high recovery at respectable flux

A Centre for investigations on urban environmental issues

Urban Water Resources and Water Quality





- 3D water quality reservoir model coupling major biological, physical and chemical processes in Kranji reservoir

- Dynamic rainfall-runoff model for simulation of runoff quantity and quality from contributing catchments

Outfall and diffusion of discharge plume

Physical model study of the plume discharge from a denser fluid into a reservoir of fresh water. The predominant current is from left to right. This is an inverse model for discharge of wastewater through an ocean outfall.

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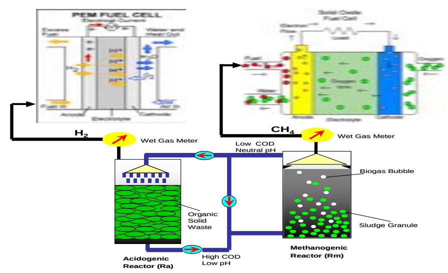
Nanyang Environment & Water Research Institute

Residues and Resource Reclamation (R^3) Research Centre

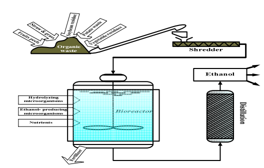
Co-production of Bio-H_2 and Bio-CH_4 from Food Waste

- Co-production of bio-H_2 and bio-CH_4 from organic solid waste using the second-generation of the hybrid anaerobic solid–liquid (HASL-II) bioreactor
- HASL-II can quickly and completely convert substrates into bio-hydrogen by controlling C/N ratio and partial pressure of H_2
- H_2 and CH_4 are used to drive Proton Exchange Membrane Fuel Cell (PEMFC) and Solid Oxide Fuel Cell (SOFC) to generate electricity



Bio-ethanol Production from Green Wastes

- In the proposed ethanol bio-production process, the biopolymers of green waste are converted into ethanol due to the simultaneous activities of hydrolyzing and ethanol-producing microorganisms
- Anaerobic hydrolyzing microorganisms are isolated from natural sources and guts of tropical wood-eating insects, like termites and caterpillars, to convert green waste into sugars as substrate for ethanol production



Cluster 1
Conversion of residues into energy

Cluster 2
Remediation of contaminated environment

Cluster 3
Conversion of residues into reusable / new materials

Nanyang Environment & Water Research Institute

Lien Institute For the Environment (LIFE)

Nanyang Technological University (NTU) and Lien Foundation have joined hands to establish the Lien Foundation – NTU Environmental Endeavour. The Endeavour is made up of two arms: the Lien Institute for the Environment (LIFE) and LIEN AID. Both will work hand-in-hand to develop, implement and promote affordable, socially and culturally acceptable technologies and practices for the betterment of living conditions in developing countries. LIFE capitalizes on technology for everyday challenges in developing communities.

A Real Crisis

1.1 billion people lack access to safe drinking water (58% in Asia).

2.6 billion people lack access to adequate sanitation services (71% in Asia).

80% of illness and death in the developing world is water related.

Lack of water forces 100 million children to miss out on an education.

60% of all earthquake casualties are a result of unreinforced buildings.

In the October 2005 Pakistan earthquake alone, 3.3 million were made homeless.

Sources:
World Health Organization
United Nations Environment Programme
Stockholm Environment Institute
International Centre for Urban Safety Engineering

Prospective Beneficiaries

Bringing the solutions where they are needed most. The young are the community's future and hope. Providing them clean water and a safe home is important.

Water Filter

Membrane technology developed to filter water. Filtering raw well water making it fit for consumption. A module is being monitored in Medan, Indonesia.

Water Sanitation Systems

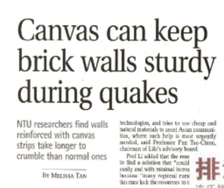
Provision of appropriate onsite systems can mitigate spread of water-borne diseases. Collaborative projects with LIEN AID are in: (a) Phnom Penh, Cambodia, (b) Hanoi, Vietnam, and (c) Sekayu, Indonesia.

Brick wall strengthening

An easy technique consists of sticking canvas strips across the brick wall to provide the restraint against abrupt collapse during earthquakes. Occupants can take advantage of the extra seconds for timely evacuation. This can mean the difference between life and death.

Rammed Earth

Low-cost and environmentally sustainable construction material. Used for community centre in Lam Plai Mat, Thailand, in collaboration with LIEN AID.



Canvas can keep brick walls sturdy during quakes

Strait Times, 16 June 2007

排污去臭送爱心

连氏援助组织为柬贫民建卫生中心

Lianhe Zaobao, 6 August 2007

Energy

ERI@NTU

Objectives of ERIAN

- Advance science and technology that aimed at *improving efficiency of current energy systems* while maximizing synergistic effects of *alternative energy sources*
- Foster a *multidisciplinary* and *collaborative environment* for scientists, engineers, and social scientists to interact and promote relevant energy solutions and policies for the future
- Enable interactions with policy, economic, and research development authorities as well as the industry through collaborative *knowledge creation and technology transfer* in areas of strategic importance to Singapore

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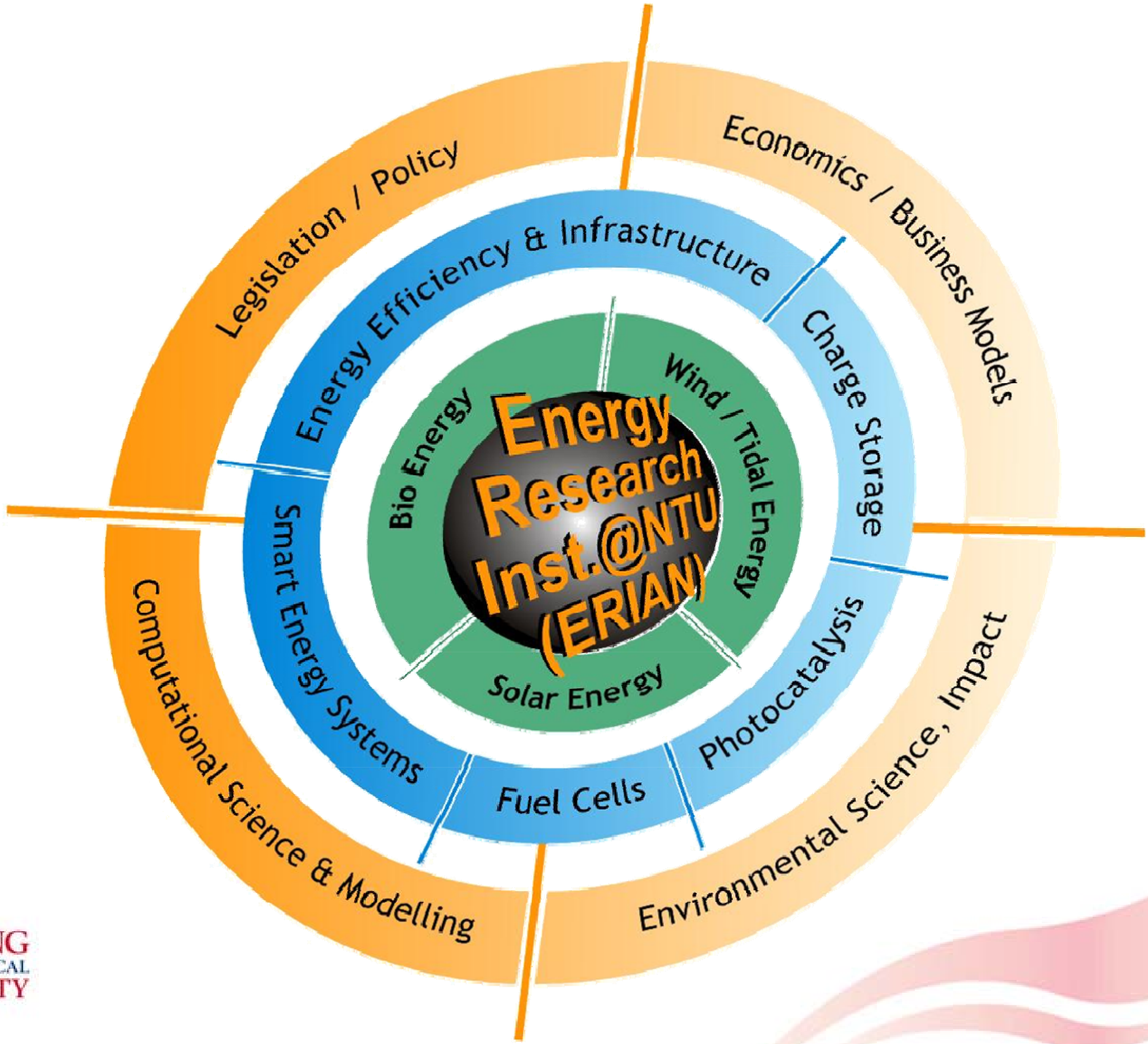
Research Areas



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Major Initiatives with EDB

- With support Economic Development Board (Singapore), a new ***Center for Sustainable Energy Research (CSER)*** has been set up.
- CSER (~$62 million funding) will be a subset of ERIAN and will cover:
  - 1. Advanced Fuel Cell Centre
  - 2. Charge Storage Centre
  - 3. Wind / Tidal Energy Research Centre
- Besides CSER, ERIAN aims to launch major efforts in Bioenergy and also enlarge its current efforts in Photovoltaics.
- Other areas including Thermoelectrics, Geothermal, Nuclear, Smart Energy Systems, Energy Security, Economics / Business Models … are being discussed as part of the ERIAN ecosystem.

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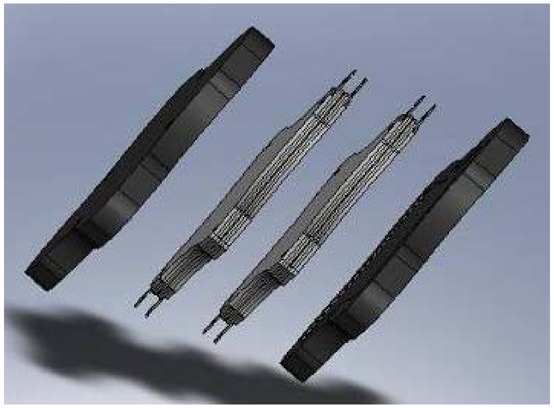
1. Advanced Fuel Cell Research Centre

- Research focuses on two types of fuel cells, i.e., Solid Oxide Fuel Cells and Proton Exchange Membrane Fuel Cells, which include direct methanol/ ethanol fuel cells and micro fuel cells.

- Key partners: Rolls Royce Fuel Cell Systems, GasHub, Horizon Fuel Cell, P21, A*STAR institutes, TP, DSTA,



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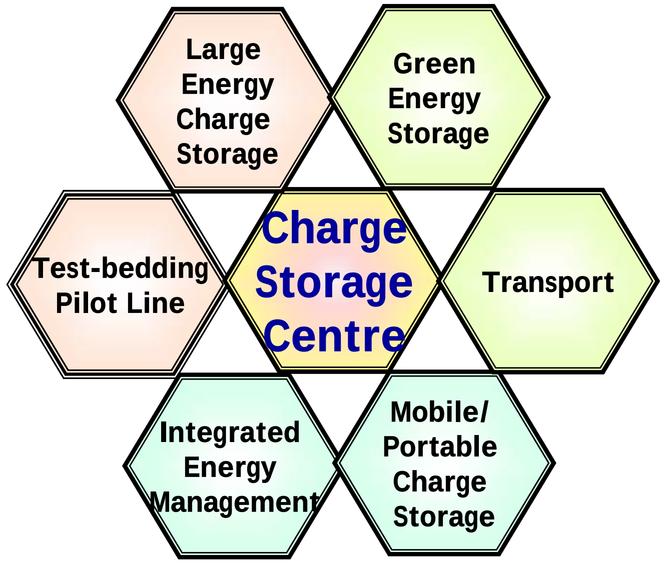
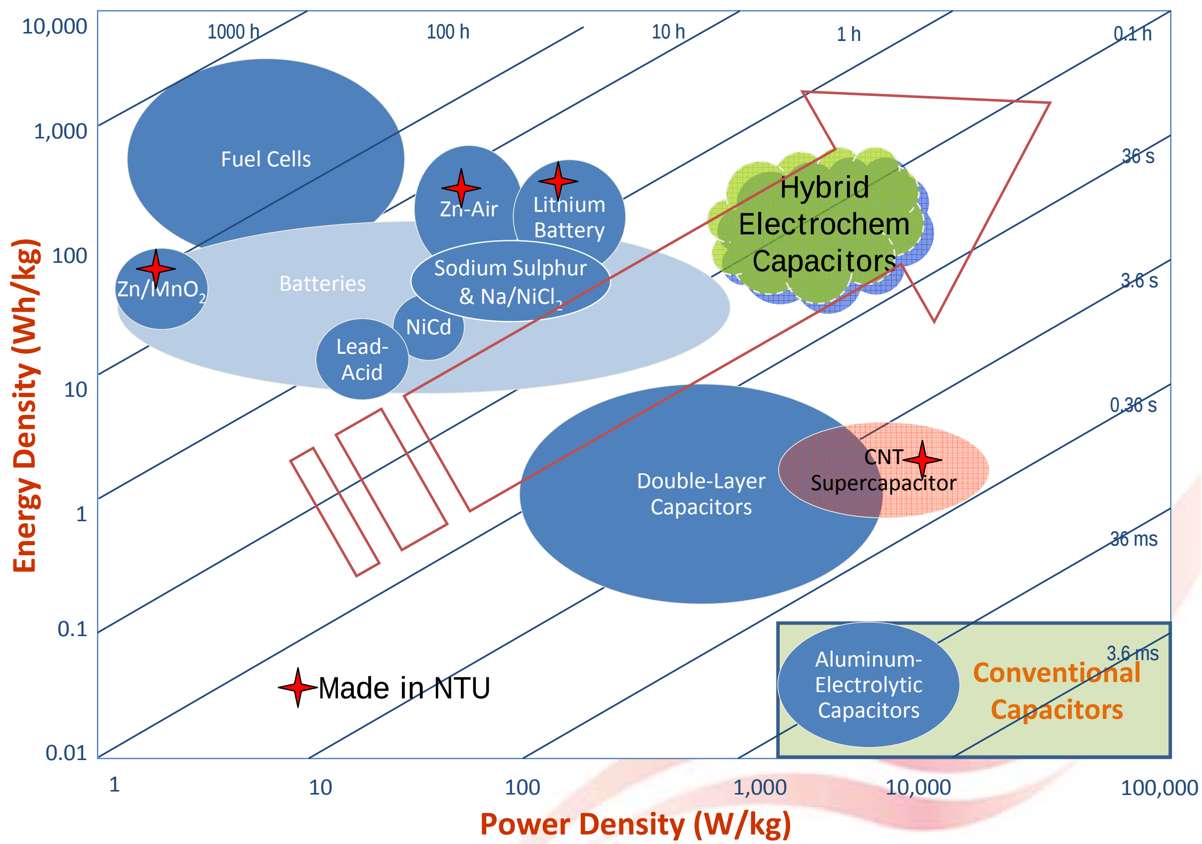
2. Charge Storage Centre

- Centre to focus on new battery technologies for applications ranging from mobile electronics, electric vehicles, and also integrated green energy storage

- Key partners: Bosch, Sony, Bayer, BASF, Varta





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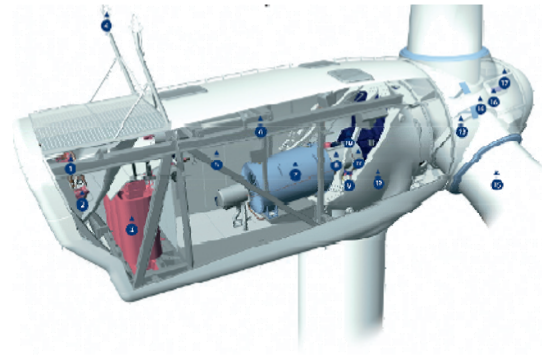
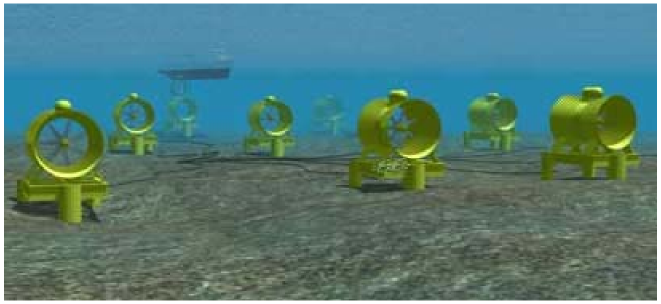
3. Wind / Tidal Energy Centre

- Centre to focus on turbines, generators, Computational Design/ Optimization, power electronics, grid integration, hybrid systems





- Key partners: Vestas, Atlantis – agreements signed in 2008

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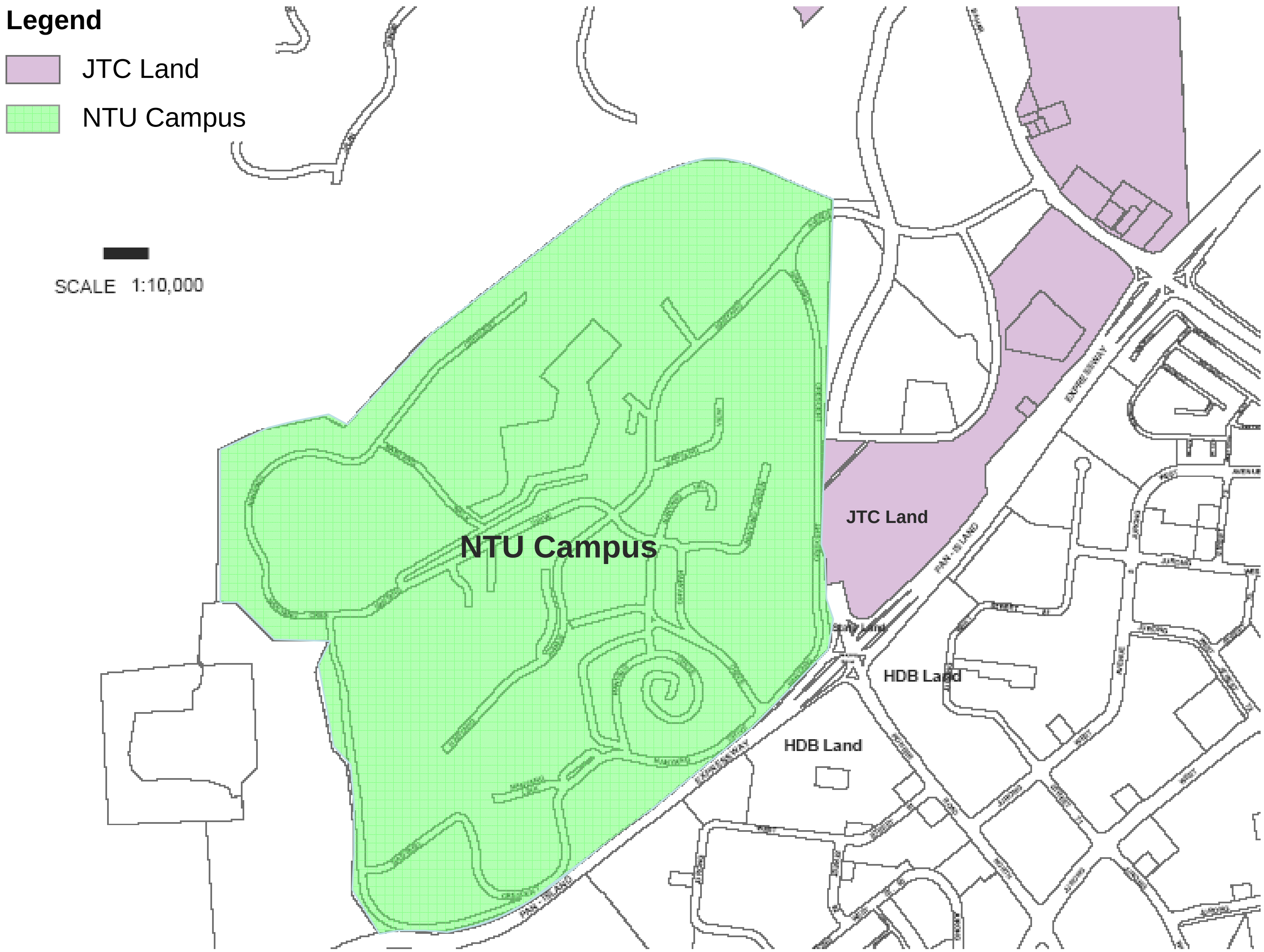
CleanTech Hub

Singapore's Second Science Park

<u>NTU partnering industry:</u> JTC-NTU Business/Science Park – Environment, Water and Clean Energy

Business/Science Park: 40-hectare

NTU: 200-hectare



THE STRAITS TIMES.

Home > Breaking News > Singapore > Story
Nov 4, 2008

Clean Tech Park gets greenlight

By Tania Tan, In Stockholm

IN A boost to the environmental R&D drive here, Singapore's first business park devoted to clean technologies has been given the green light.

A 10-hectare plot in Jalan Bahar in northwest Singapore will be the site of the new Clean Tech Park, which will house a cluster of about eight buildings.

Companies focusing on green R&D and products will be the main tenants.

- The 55ha (~0.55 km^2) plot in Jalan Bahar (next to NTU): house companies that specialise in industries like solar power, water, fuel cells
- The project will be about achieving new lows - 'low waste, low energy and low carbon emissions'

Artist
impression

CLEANTECH HUB

Urban Living

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Evolution of our Skyline

Timber, stone and masonry era with houses and mansions

Horizontal

Low density and energy consumption

Highly unsustainable

Continuous space

Age of concrete and steel skyscrapers

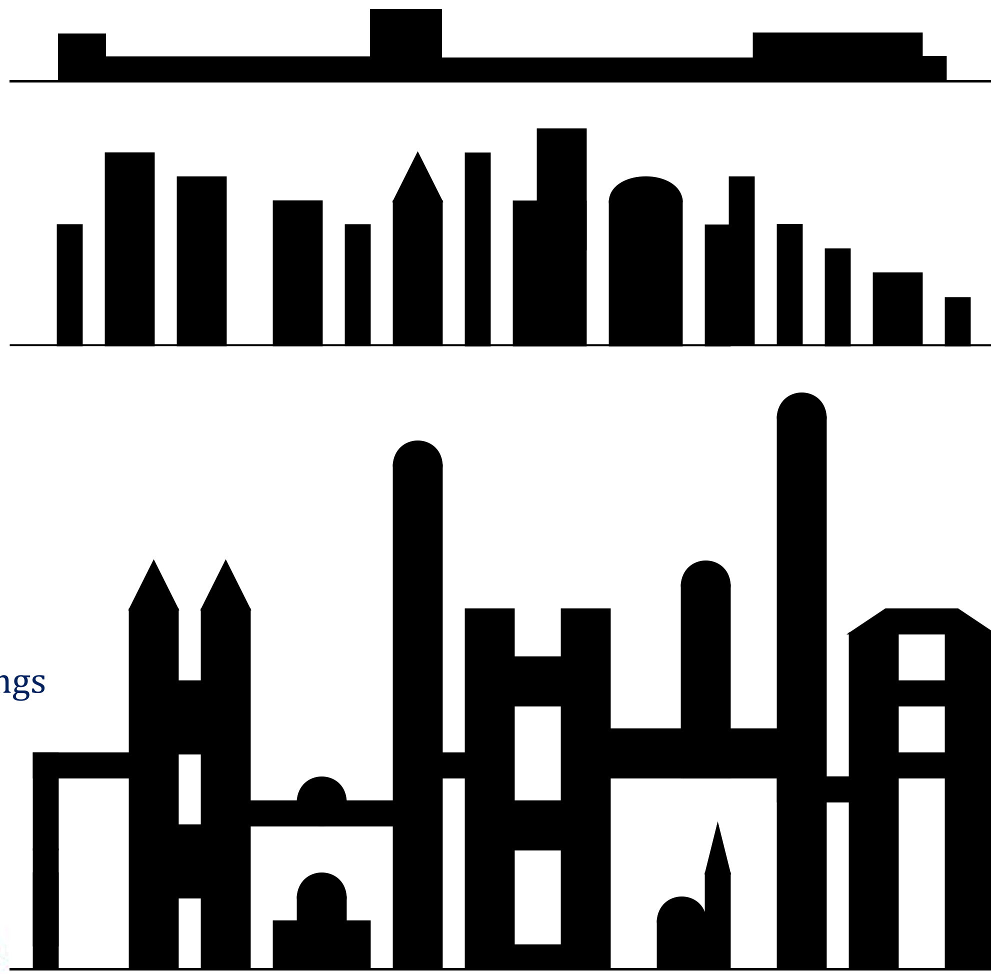
Vertical

Moderately Unsustainable

high density and energy consumption

D i s c r e t i z e d s p a c e

Time for high performance composite steel concrete hybrid intelligent buildings



3D Hybrid linked

Largely sustainable

higher density but low energy consumption

Continuous communities

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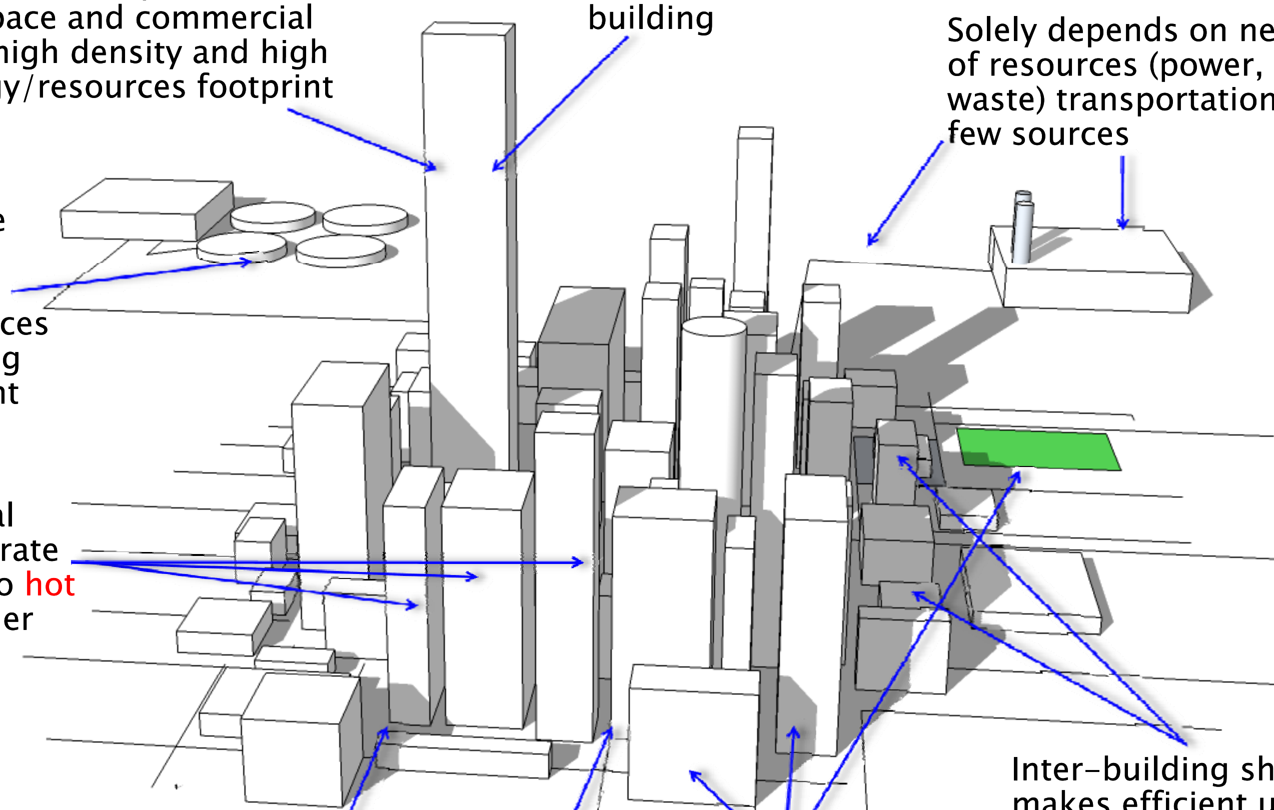
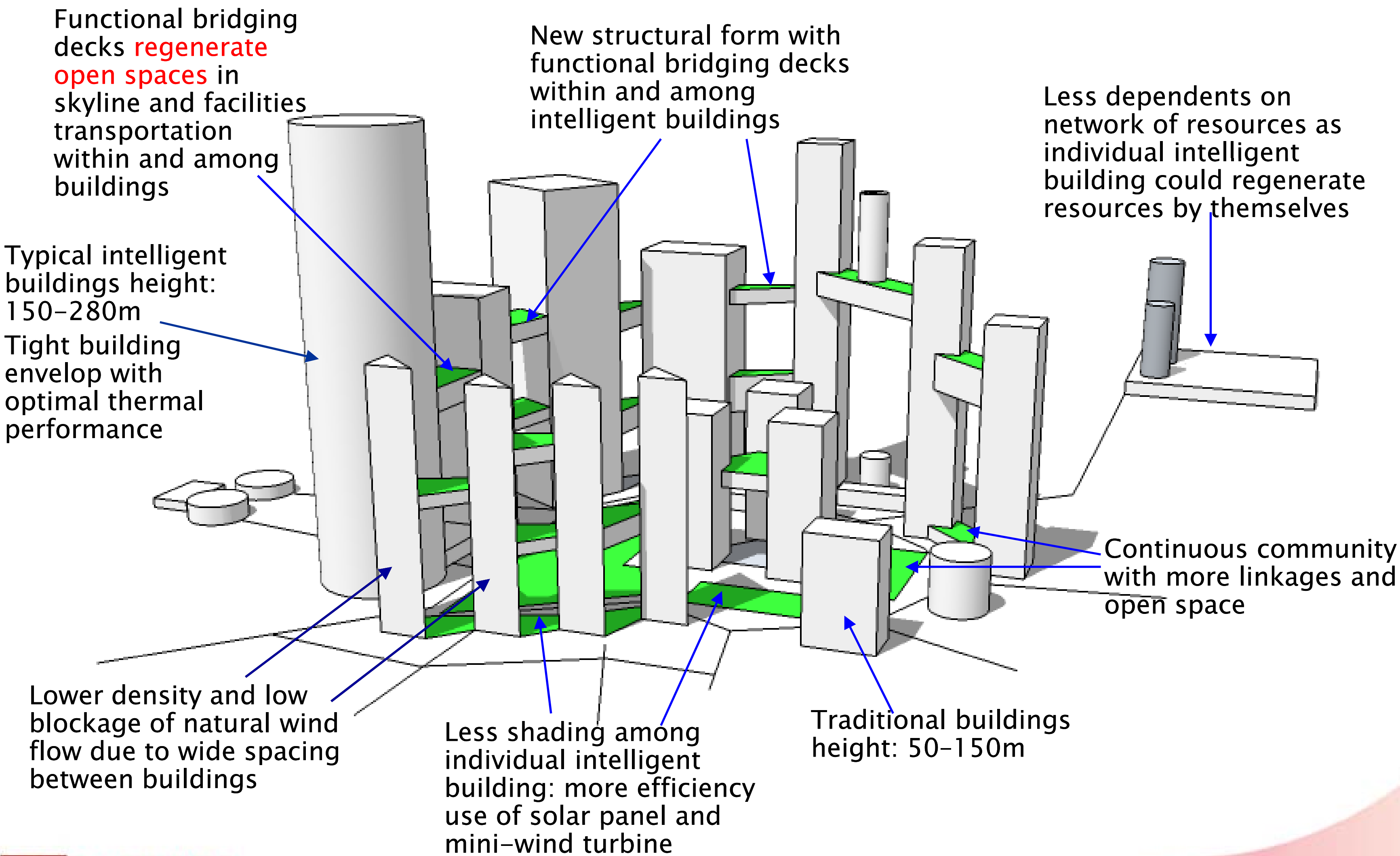
Traditional Upward Development of our Skyline



New Linked Hybrid Skyline (space in the air)



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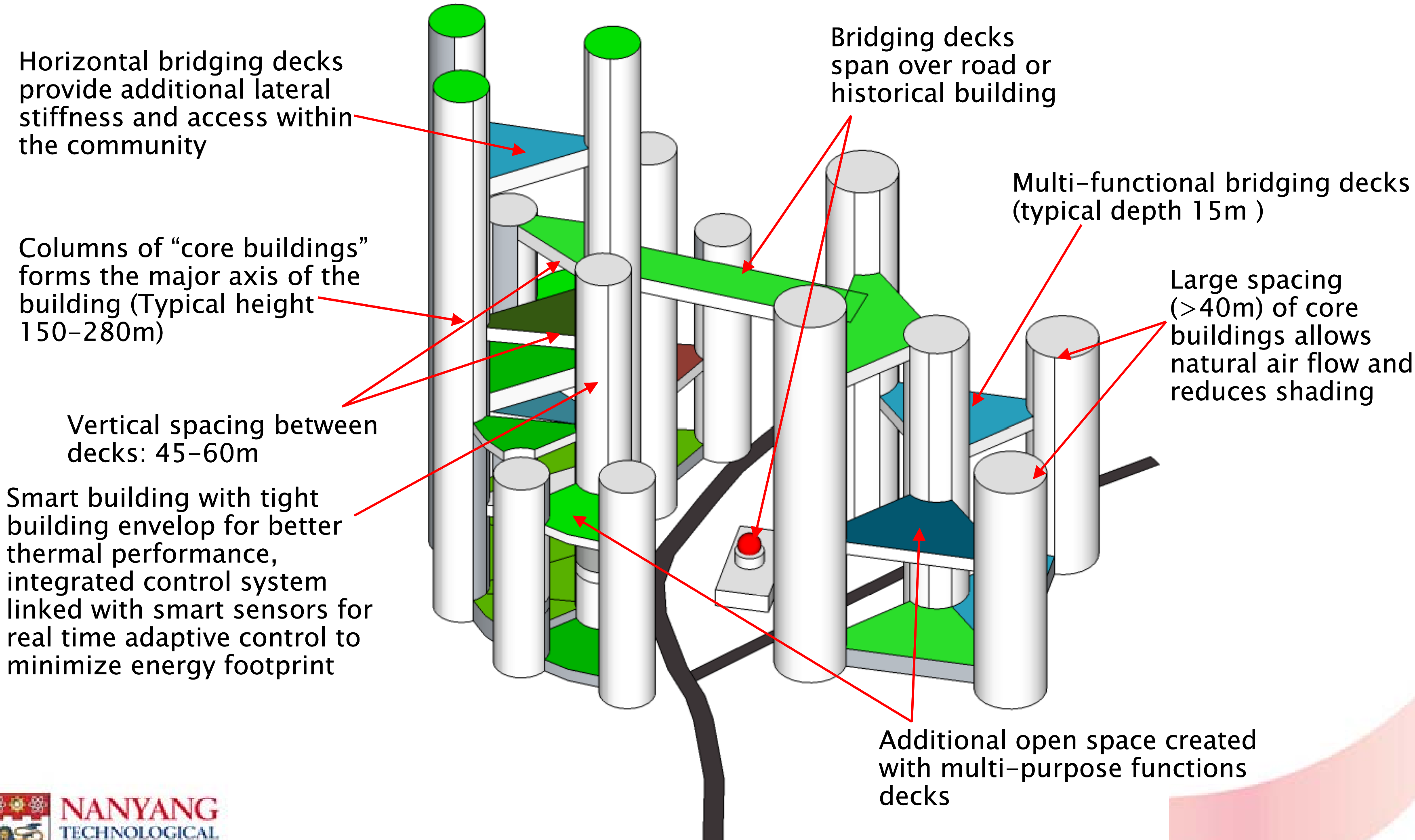
A typical Intelligent Building: Sustainable Community within a Building



Interactive Digital Media

IMI

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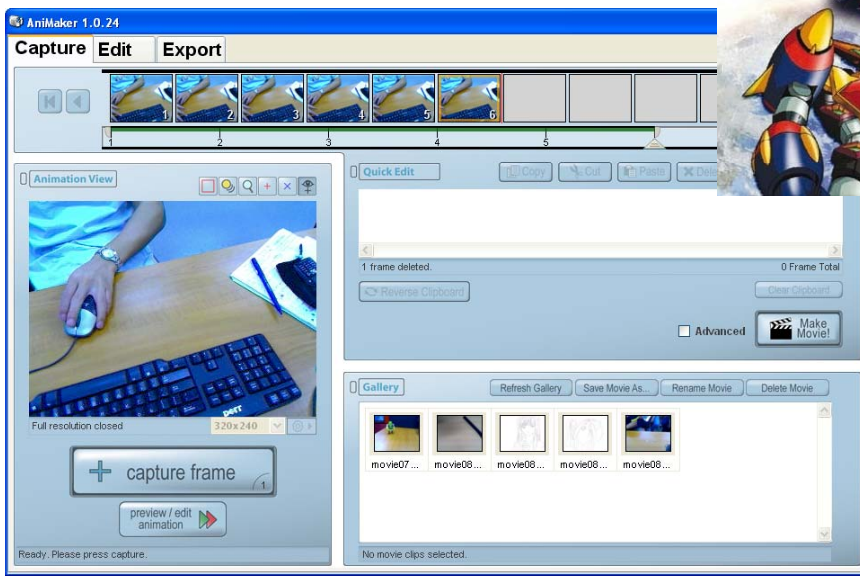
Institute for Media Innovation (IMI)



- Institute for Media Innovation created in 2008
- Top university in Singapore in research awards in IDM
- Applying IDM to entertainment, education, health and lifestyle

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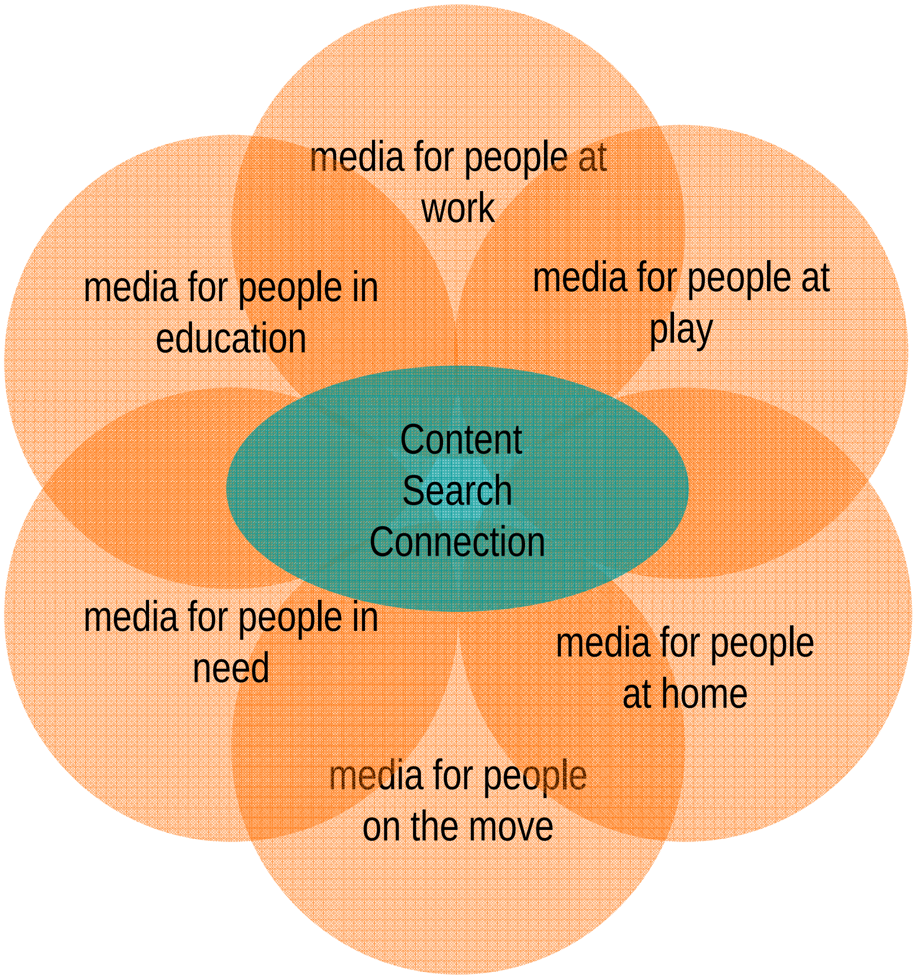
IDM Scenarios & Technologies



- Storytelling, narrative
- MM search methods
- Media networking
- CG, animation
- Game engine, simulation
- Virtual Reality, Augmented R.
- D-cinema
- Artificial Intelligence, Ambient Intelligence
- Image Analysis, comp. Photography
- Learning science

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High Performance Computing

HPC @ NTU

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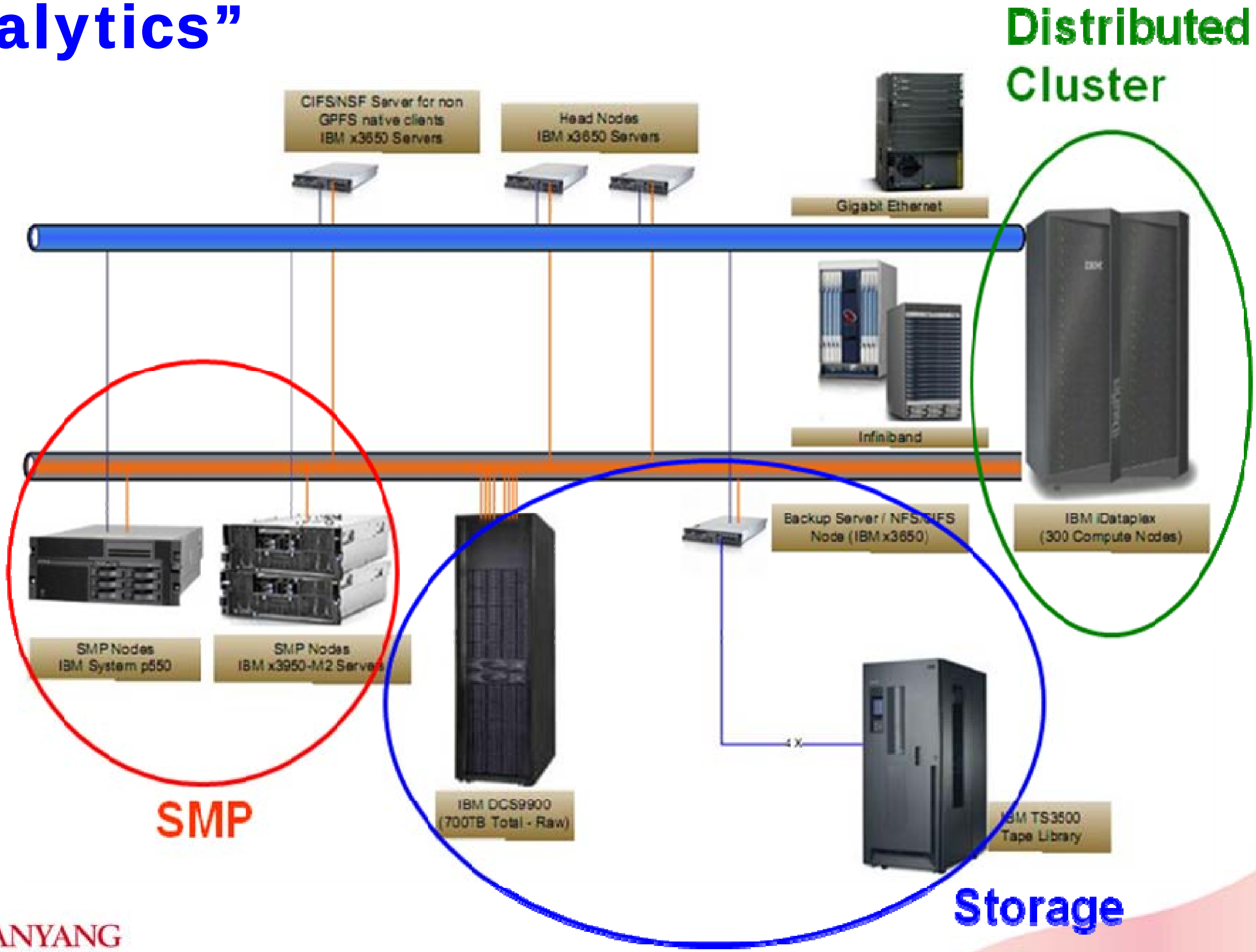
NTU's HPC System – "Nanyang Analytics"



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Overview of "Nanyang Analytics"

Intel X5570 Nehalem processor platform, on IBM iDataplex and Storage

Implementation Overview:

- ✓ **300 compute nodes (or 2400 cores) of dx360 M2 (2-socket processor node on IBM iDataplex platform), capable of performing 28 Tflops at 266.88Mflops per watt – 390th in TOP500 and 29th in GREEN500**
- ✓**IBM DCS9900 Storage (600TB) for high performance computing**
- ✓**System Power6-550 Server and x3950 M2 for 8-way SMP nodes**
- ✓**Voltaire Quad Data Rate (QDR) Infiniband backbone network**
- ✓**IBM General Parallel File System (GPFS)**
- ✓**Rear Door Heat Exchanger (water cool rack)**

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Green DC

1. New HPC DC setup in July <u>2009:</u>
   Currently uses **<u>25%</u>** of space capacity of 123m^2.

2. High Server Density with large heat foot-print
   - 4 x iDataplex Racks, about 85% fully loaded per Rack
     (approximately 110,500 BTU/hr max per iDataplex Rack)
   - 2 x Enterprise Storage Racks, at least 60% fully loaded
     (approximately 51,000 BTU/hr for each of our storage Racks)
   - 2 x Enterprise storage Racks, which contains our switches, SMP, P-series server
     (approximately 22,000 BTU/hr for each of our enterprise Racks)

3. Total Heat dissipation is approximately **<u>590,000 BTU/hr</u>**
   or approximately **<u>172.9 KW/hr.</u>**

4. Approximately 140Watt/psf using ambient cooling temperature of 25 ^{o}C.

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Green DC

Consequence of High Heat Dissipation without proper cooling methods

1. Exit Temperature from Servers can be 40^{o}C and above.

2. If DC is not sufficiently cooled, higher inlet temperature for the equipment is expected, causing faster fan speed which consumes more electricity and added acoustic signatures of equipment

3. Local Hotspots around the high density compute-nodes racks will be created if there are imbalance airflows

4. Consequence is that the equipment may not perform at its optimal reliability and performance

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Green DC

Solution – Rear Door Heat Exchanger:

- Liquid cooling is 75%-95% more efficient than air cooling by a CRAC
- Can eliminate rack heat exhaust
- No electrical or moving parts and low acoustic signature
- Chilled water
- Reduce Data Centre air-conditioning operational costs by operating at ambience temperature of 24-26^{o}C
- Remove up to 32KW per iDataplex Rack

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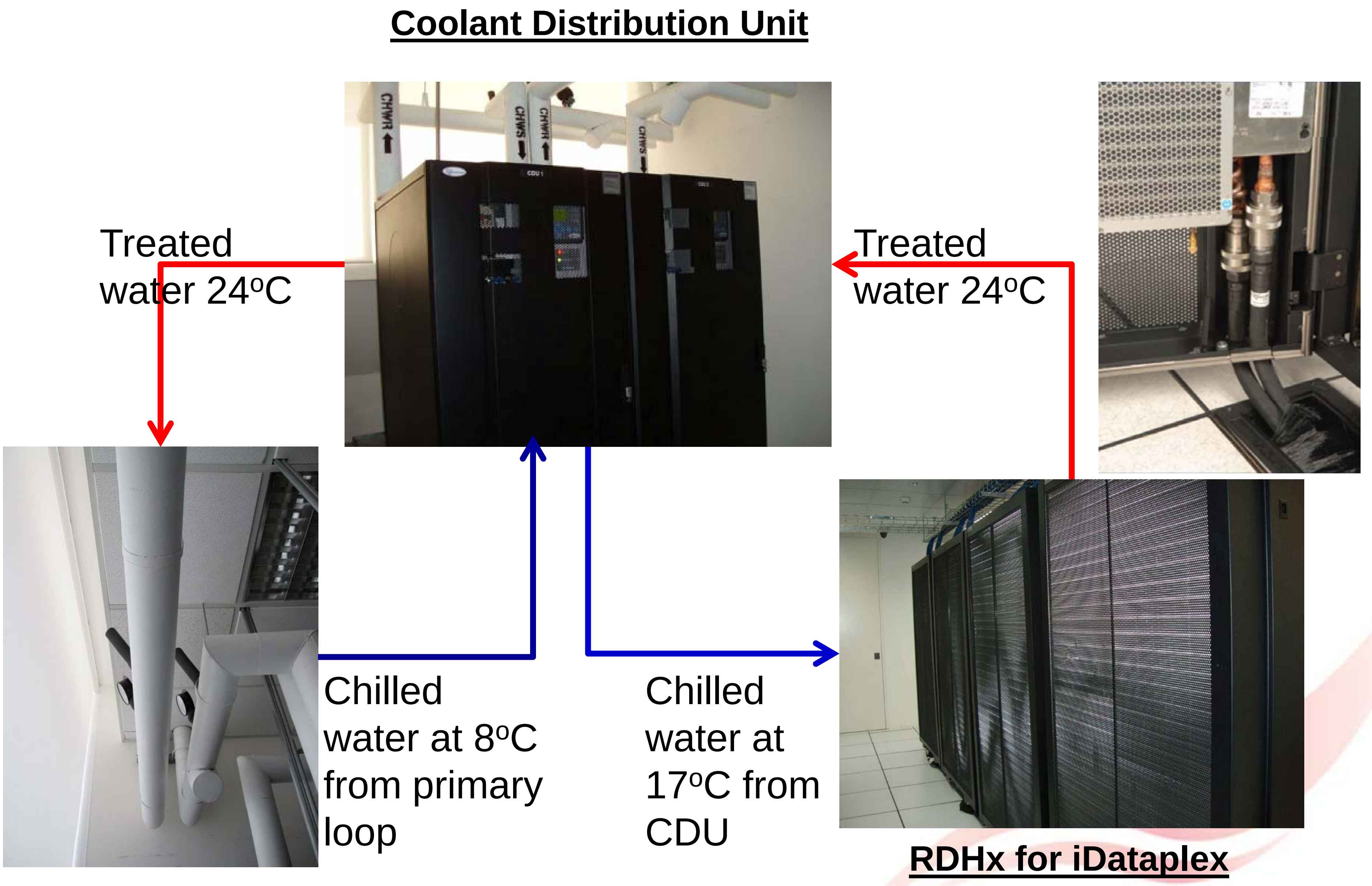
Rear Door Heat Exchanger



3 “Concerns” about water-cooled DC

- I am concerned about having chilled water in my data center.
  - IBM has over 40 years experience with chilled water in the data center. It started with the main frame. That expertise is used to design the RDHx solution.
- Is there any redundancy at and inside the Cooling Distribution unit (CDU)
  - Yes! The only moving mechanical part, which is the valve pump, CDU comes with a redundant 2-way valve pump
- In the tropics, there is always this possibility of condensation, how can we eliminate this issue?
  - There is an automatic temperature control feature at the CDU that controls the temperature of the water from the CDU to the Racks. The different in temperature between the ambience and the chilled water can be tweaked to eliminate the condensation issue.

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Comparison of Electrical Utility Cost

Precision Cooling vs Rear Door Heat Exchanger

Total Heat Load: **170KW**
Utility Cost: **0.1929**

Description	Precision Cooling (7 units)	RDHx (Cool Blue) (8 units)
Total Power Consumption of cooling devices	70 KW	10.4 KW
Electrical Power (KW) (7am – 11pm)	1120 KW	701.91 KW*
Electrical Power (KW) (11pm – 7am)	560 KW	428.29 KW*
Estimated Electrical Bill per Month (30 days)	S$ 9722.16	S$6540.48
Estimated Electrical Bill per Year	S$118,286.28	S$79,575,85
Savings		**+ $38,710.43**

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* The figures will be lower with a more efficient chiller system

HPC Scaling Test

Project title: **Regional Climate downscale modeling in Maritime Continent**

Short description of the test-runs:

- We set up two MPI runs:
  - The first one requires less computational power with lower domain resolution at 20km. We did performance scaling using less than 256CPUs (8, 16, 32, 64, 128, 256 CPUs)
  - The second one requires higher computational power with higher domain resolution at 5km. We did performance scaling using up to 1024CPUs (128, 256, 512, 1024 CPUs)

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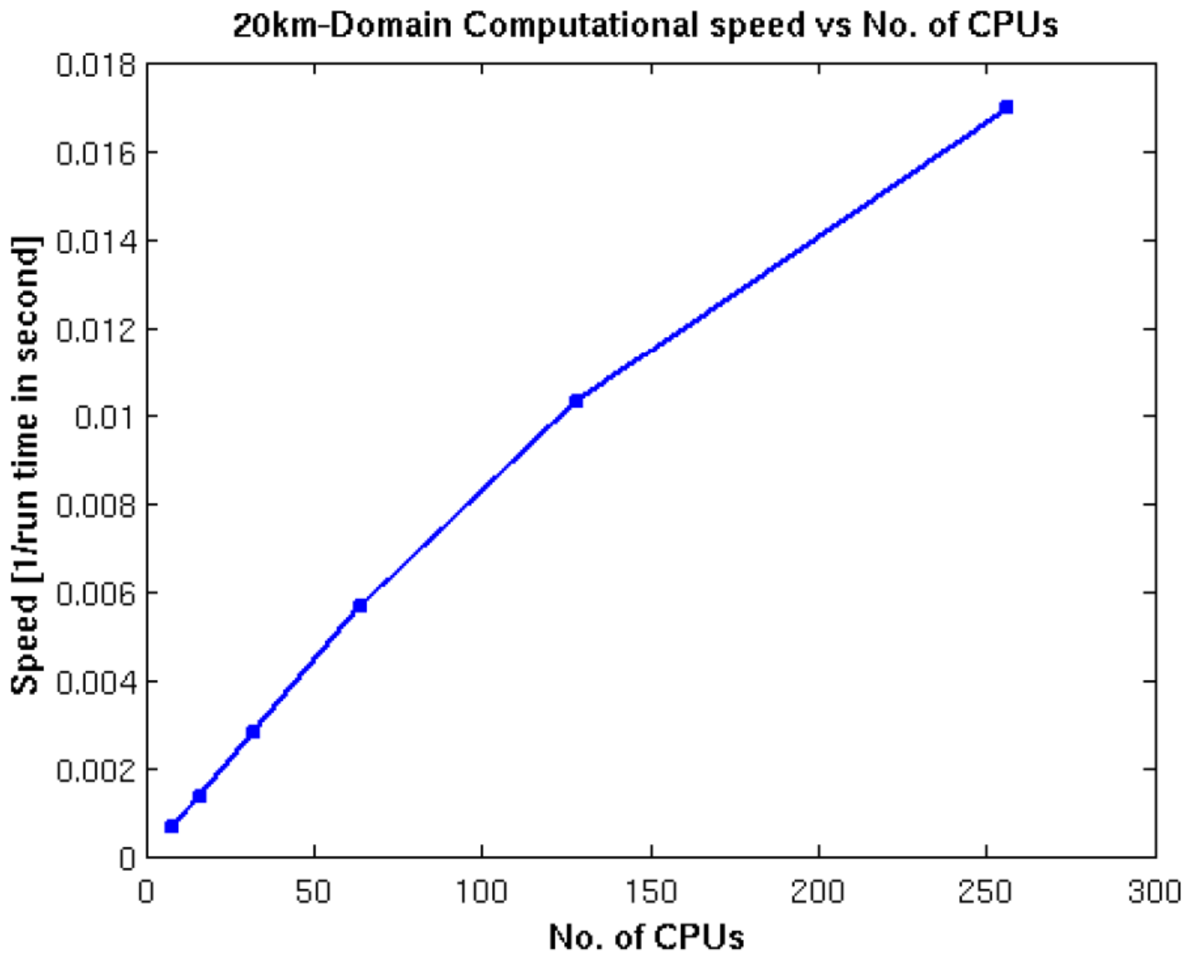
Computational time vs no. of CPU:

Small domain experiment

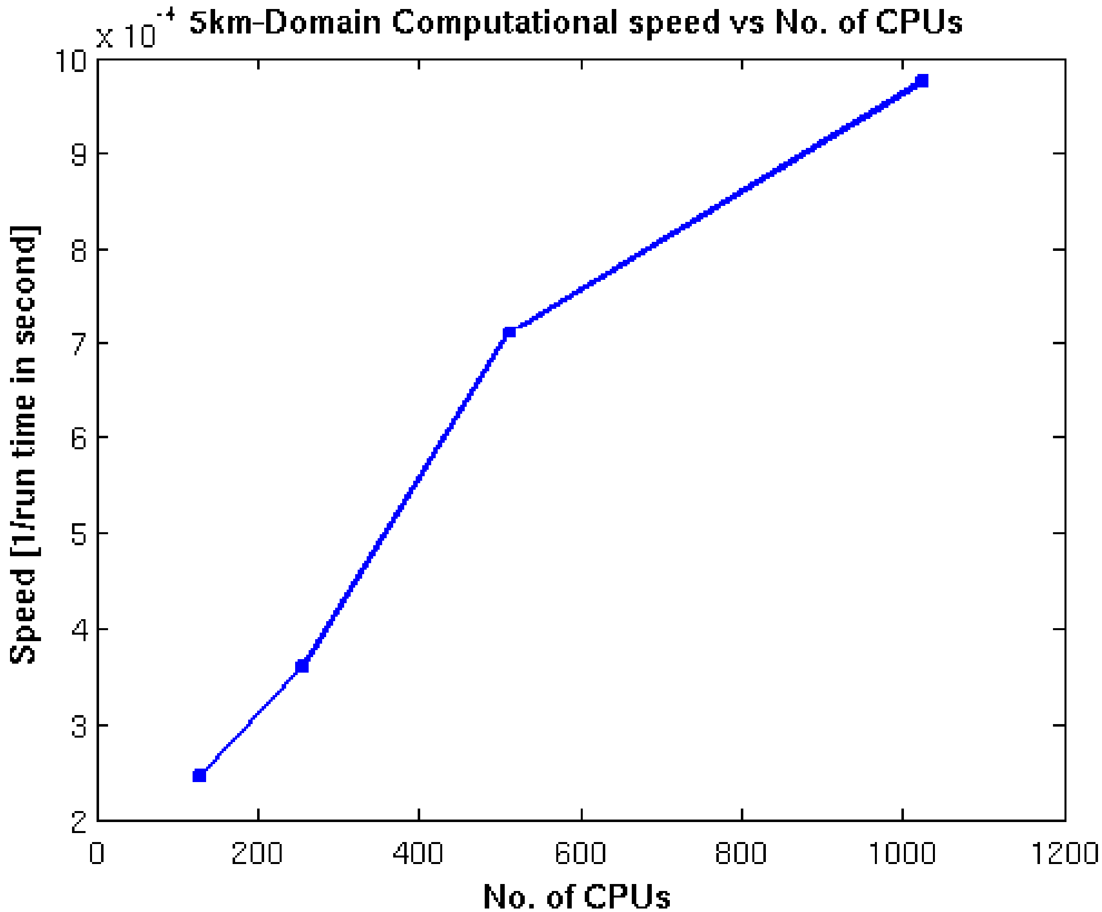
No. of CPU	Computational time(second)
8	1531
16	741
32	354
64	176
128	97
256	59



Computational time vs no. of CPUs

large domain experiment

No of CPUs	Computation Time(second)
128	4068
256	2772
512	1399
1024	1031



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HPC Cloud

Convergence of HPC and Cloud

What is Cloud Computing?

Cloud Computing can be referred to as IT as a service, in the same way as a utility company delivers electricity, to the end users for their specific and unique consumption. The challenge is whether Cloud Computing can deliver cheaper, faster, superior user experiences.

Benefits of Cloud Computing

- Elastic capacity
  - Usage of Computing resources will be more optimised
  - Virtual Machines with customised RAM and CPU can be provisioned easily accordingly to user requirement
  - Resources can be scheduled to meet various cycles of demand with scheduling and optimization of existing hardware via virtual machines
- Pay-per-use model
  - Actual usage can be easily measured as the computing is provided on demand
- Platform abstraction
  - With the inherent use of stored templates, different OS, templates and specific hardware requirements can be made available to meet user demand whether it is virtual machines or bare-metal machine. The templates can be made available and customised to different types of Research Groups and Platform
- Economies of scale
  - Clouding Computing Initiatives usually accompanied consolidation of computing resources which will then provides users with various capacity of resources
- Built-in fault tolerance
  - Due to the segregation of the hardware and the platform and data, Computing platform can be easily diverted to from one failed hardware to another available computing resource very easily

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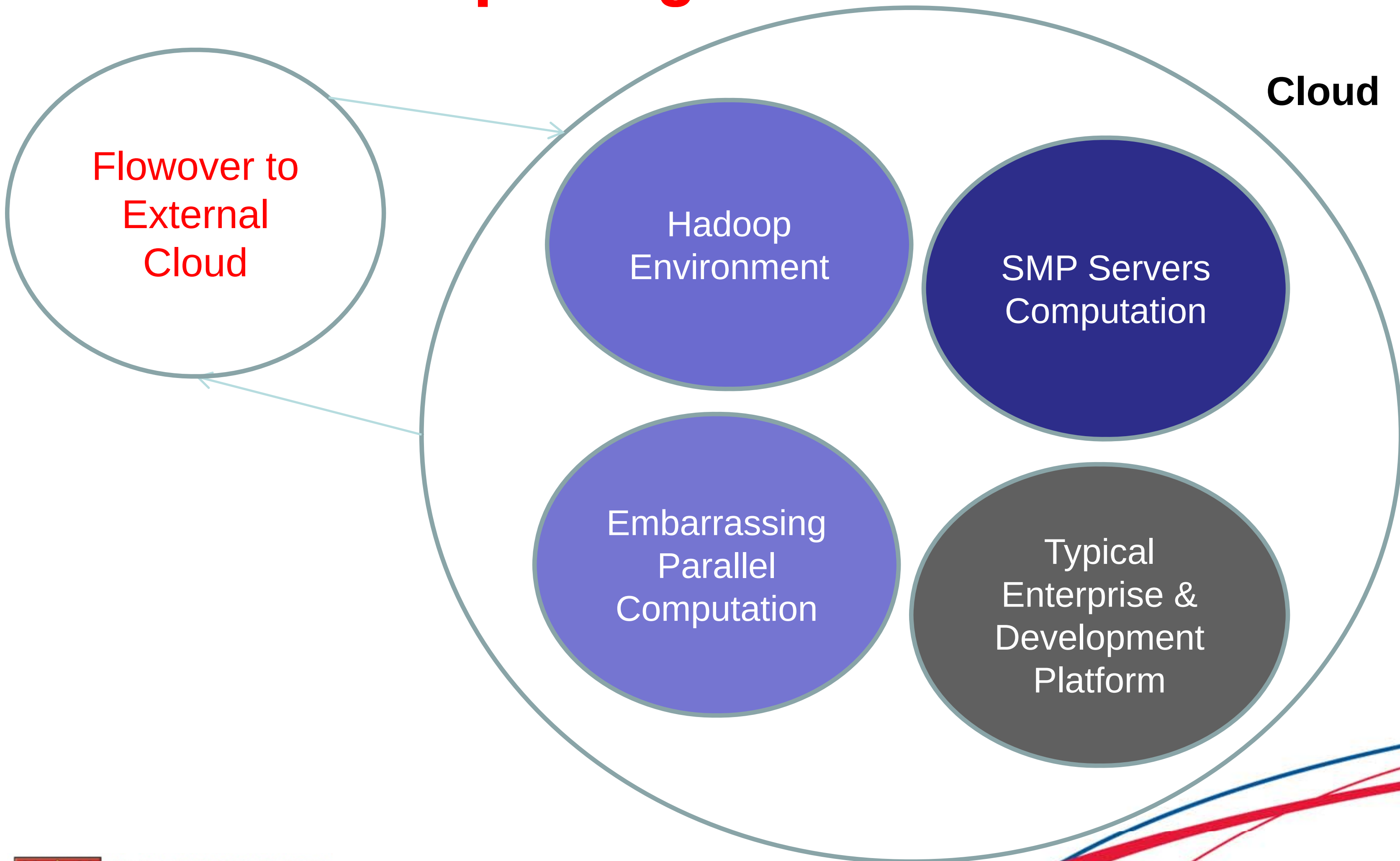
Current Embracement of Cloud

- Current Cloud Deployment is able to scale across the enterprise, supporting the ability to manage other heterogeneous resources.

- Some Frameworks and Platforms have been ported to Cloud. These include:
  - **Hadoop / Map Reduced Model Framework**
    - Has been hailed as being suitable for processing extremely large data sets in a highly parallel manner. However interconnect latencies and performance are not addressed adequately
  - **SMP Computation**
    - Bare Metal or Virtualised SMP with large memory and multiple can be customised easily on the Cloud
  - **Typical Enterprise & Development Platform**
    - Include Development, Web and other typical enterprise computing environment
  - **Embarrassing Parallel Computing Platform**
    - Computation with Parallel characteristics but interconnect latencies and performance are not essential requirements
  - **Flowover to External Cloud (Computing on Demand)**
    - If the Computation Resources are not sufficient within the environment, it should be able to flow over to an external cloud with a computing on demand concept

Current Embracement of Cloud on Computing Environment



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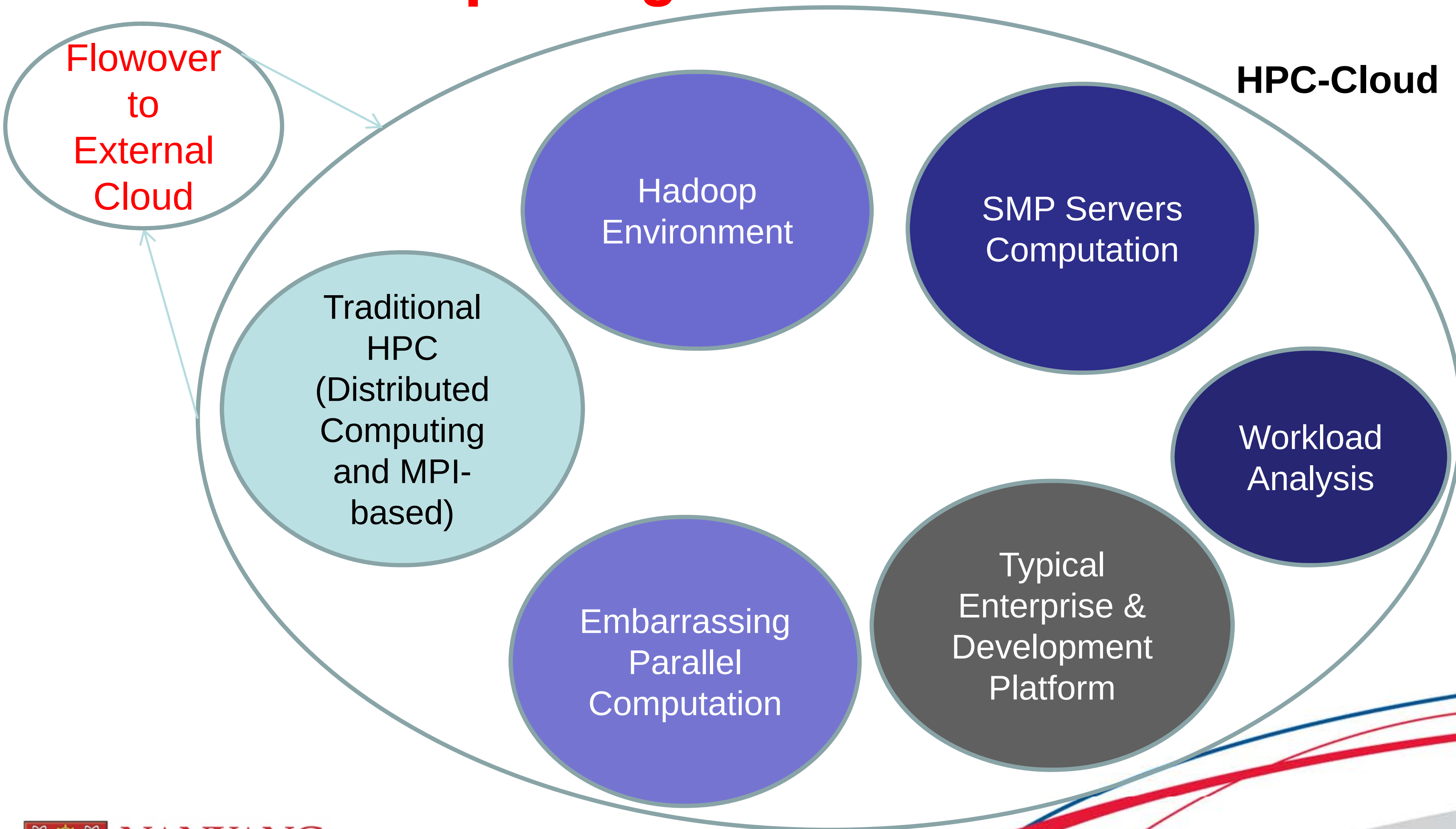
HPC-Cloud Unification

- HPC-Cloud Deployment is looked upon as a unification of the Traditional HPC Environment and The Cloud Framework. Besides what the Cloud can already do, HPC-Cloud should embrace 2 more computing environment
  - Hadoop / Map Reduced Model Framework
  - SMP Computation
  - Typical Enterprise & Development platform
  - Embarrassing Parallel Computing Platform
  - Flowover to External Cloud (Computing on Demand)
  - **Traditional HPC (Distributed Computing with MPI)**
    - Require very low latency and different interconnect protocol (Infiniband) for Optimal Performance
    - Require High-Speed Parallel File System for Optimised I/O performance
  - **Workload Analysis Computation**
    - Workload Analysis provides the HPC-Cloud the ability to respond to the feeds of data and customise more computational resources to support the computation
    - For example, suppose that a large earthquake is about to happen in the region, and data from the various probes in the vicinity increases substantially. The HPC-Cloud should be able to react to the increase feed by provisioning more computing resource to crunch data

Embracement of HPC Cloud on Computing Environment



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Challenges of HPC-Cloud Convergence

1. Different Interconnect Protocol Latency Requirements

- Traditional HPC requires Interconnect with ultra-low latency of 100 to 450 nanoseconds for most effective interconnect communication
- Traditional Enterprise Cloud latency can be 1ms to 40ms without adversely affecting the required interconnect communication performance requirements between nodes

2. Different Preferred Interconnect Protocol

- Infiniband Interconnect Protocol is preferred for HPC than hr Ethernet Protocol due to latency requirements
- Ethernet is the preferred Protocol for Traditional Enterprise Cloud as it is the most widely accepted interconnect protocol for enterprise computing.

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Challenges of HPC-Cloud Convergence

3. Different File System and Storage Requirements

- Traditional HPC I/O performance is optimised with Parallel File System with Infiniband Interconnect
- Traditional Cloud I/O performance can be met by the current non-parallel File System with System Storage Area Network on Fibre Channel Protocol or High-End NAS on Ethernet Protocol

4. Complexity of HPC System setup and provisioning

- HPC System are inherently complex due to the intensive customisation to ensure the various distributed hardware and resources work as an integrated system. This includes the Head and Compute Nodes, the Scheduler, the interconnect, Resource Managers, etc
- Traditional Cloud Computing Resources Provisioning are more straightforward and less complex

Benefits of HPC-Cloud Convergence

- High Performance Computing is getting pervasive in research and even corporate and enterprise environment due to the need to handle tremendous amount of information and data. It is necessary to incorporate HPC into the Cloud Infrastructure

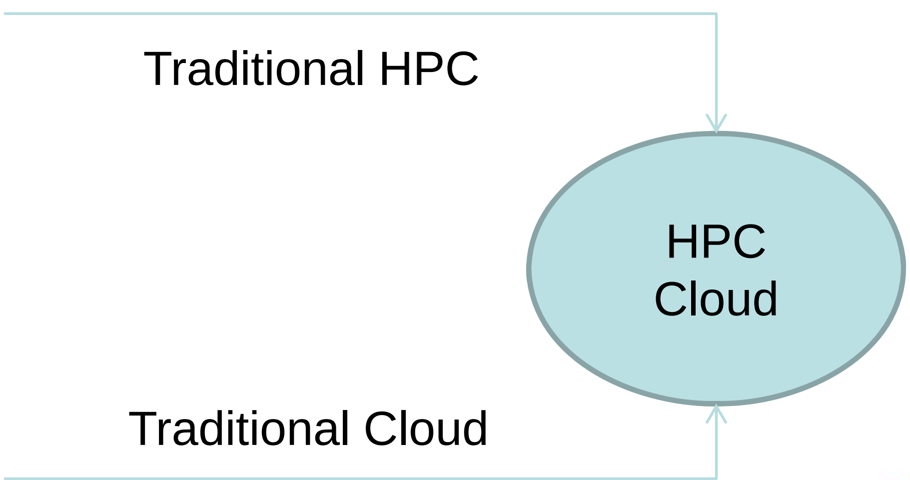
- With HPC-Cloud Convergence, it can provide a complete and encompassing computing resource, platform and framework as a service.

- All the benefits of Cloud and HPC can be derived from HPC-Cloud Convergence.

Paths to HPC-Cloud Convergence

- Currently, HPC-Cloud is a hot area of research due to the numerous challenges to the convergence of technologies. It will be very well received by the research and technical communities if a workable and deployable prototype can be built

- The Path to develop this HPC-Cloud convergence can be done with lots of application customisation. The starting point can be from the Traditional HPC framework or the Traditional Cloud Framework



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NTU's efforts on HPC-Cloud Convergence

- HPC@NTU Team is working on the design of the HPC-Cloud concepts. 2 Pilot Projects have been identified as test examples to study whether the prototype is viable and deployable in a production environment. The projects are:

  ✓ Non-MPI Computing Project : To assist ADM (School of Art, Design & Media) to conduct a research project on **4K Omnimax Movie**. Currently, the school does not have the resources to produce the 4K movie.

  ✓ MPI Project Project : To assist SCE (School of Computer Engineering) to carry out an MPI-based Research Project entitled "**Locating Water Cluster Transition State Structures Using Mimetic Algorithms**"

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Pilot Cloud for non-MPI project

Implementing HPC Cloud Computing on non-MPI project

- **Objective**
  - To implement HPC cloud computing on the 4K Omnimax movie. Currently, our School of ADM does not have the resources to produce the 4K movie.

- **User requirement**
  - Compute on 1% of the movie and perform bench marking. If time permits, bench marking will be performed on different OS (Linux, WCCS2003 and Window HPC 2008).

  - The MAYA plug-in such as smoke, mist, fire, etc, to be installed into the compute nodes.

- **Implementation**
  - ADM technical support and HPC technical team will work closely in implementing the MAYA distribution on HPC.
  - 20~30 compute nodes allocated for the pilot test.
  - Window OS will be implemented on all the nodes.
  - ADM will supply the trial licenses of the software such as MAYA and RUSH.
- **Procedures**
  - Users book resources through self service portal.
  - Cloud will provision a virtual private cluster, with one of the nodes as head node and the rest as compute nodes.
  - User RDP (remote desktop protocol) to the head node to run rendering job.
  - The processed movie file will be stored in GPFS.
  - User may need some time to download the movie file as it is quite huge.

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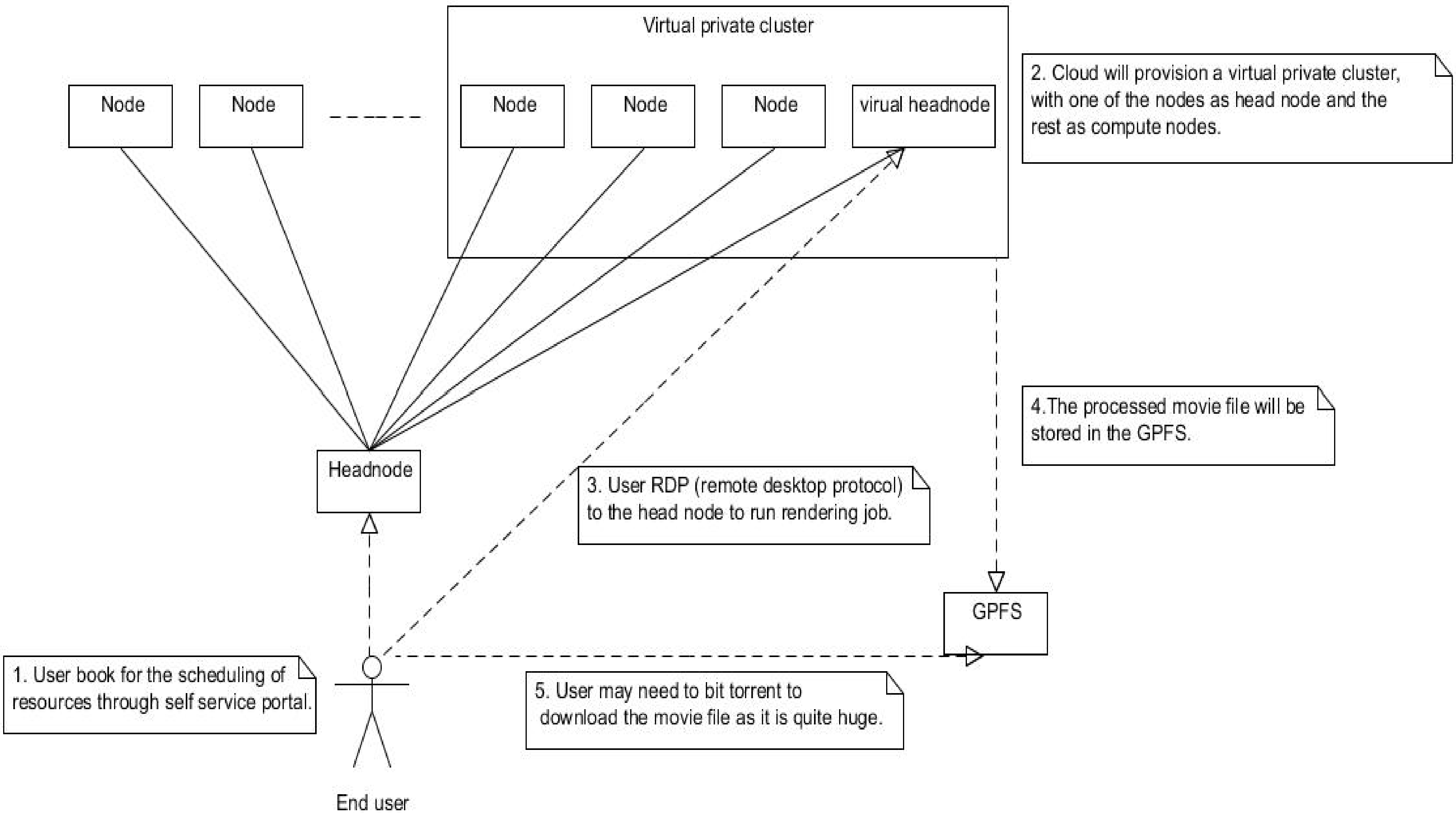
Implementing HPC Cloud Computing on non-MPI project



Pilot Cloud for MPI project

Implementing HPC Cloud Computing on MPI project

- **Objective**
  - To run an MPI computing task on HPC cloud. The project is entitled **"Locating Water Cluster Transition State Structures Using Memetic Algorithms"**

- **User requirement**
  - Require 15~20 nodes (8-cores/node).
  - Software such as Python 2.5, MATLAB 2008b or higher, Fortran Compilers F77 gFortran F90 F95, C/C++ Compiler, VASP, ChemShell, Amber, Chem3D, CPMD, LAMMPS, MMx, MOIL, MOPAC, Tinker, etc, to be installed.
  - Bench marking the performance.

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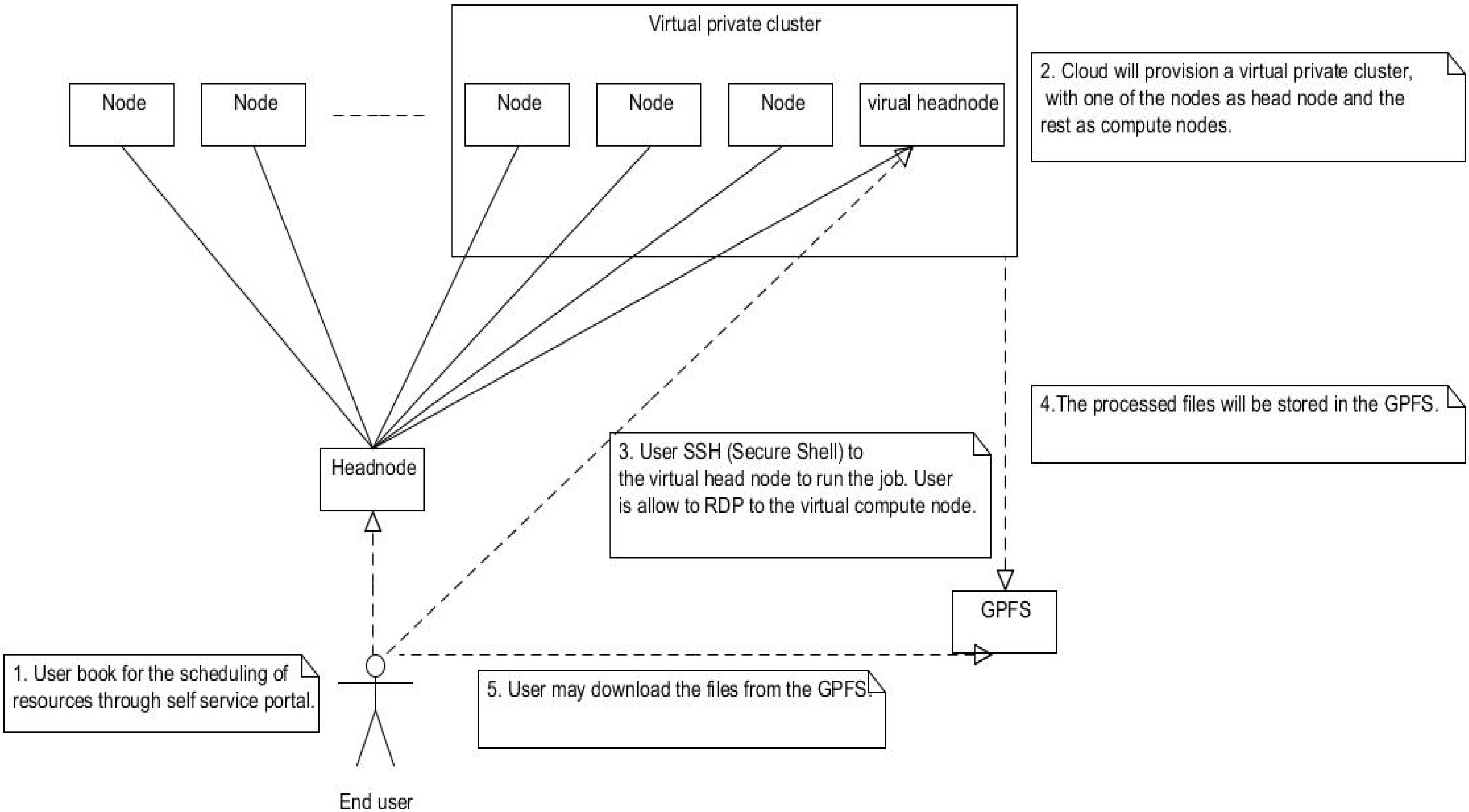
- **Implementation**
  - HPC technical team will work with SCE research staff to implement the customized cloud environment on HPC
  - 15 to 20 compute nodes allocated for the pilot test
  - Linux OS will be implemented on all the nodes
  - OPEN SOURCE and purchased software. SCE research staff will source for the required software
- **Procedures**
  - Users book resources through self service portal
  - Cloud will provision a virtual private cluster, with one of the nodes as head node and the rest as compute nodes
  - User SSH (Secure Shell) to the virtual head node to run the job. User is allow to SSH to the virtual compute node.
  - The processed files will be stored in GPFS
  - User may download the files from GPFS

Implementing HPC Cloud Computing on MPI project



Thank you

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