HKU Grid Point Project

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Thank You!

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- The UGC SEG grant was matched by a special grant from HKU

Computational Science

- **The "third pillar" of 21ˢᵗ century science**
- **Alongside <u>theory</u> and physical <u>experimentation</u>**
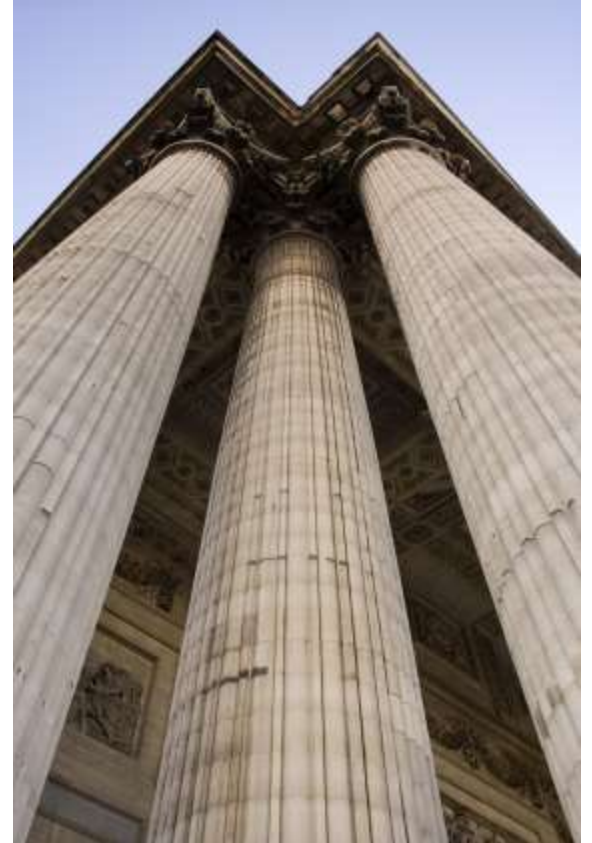
REPORT TO THE PRESIDENT
JUNE 2005

COMPUTATIONAL SCIENCE:
ENSURING AMERICA'S
COMPETITIVENESS

PRESIDENT'S
INFORMATION TECHNOLOGY
ADVISORY COMMITTEE

International Review of Research
Using HPC in the UK
December 2005

This document represents the conclusions of an international
Review Panel of experts in computational science and engineering.
The views expressed are entirely those of the members of that Panel.

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EPSRC
Engineering and Physical Sciences
Research Council

Deutsche
Forschungsgemeinschaft
DFG

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What's Computational Science?

- **Computational science is a rapidly growing <u>multidisciplinary</u> field that uses <u>advanced computing capabilities</u> to understand and solve <u>complex problems</u>**

Improvements in Algorithms Relative to Moore's Law
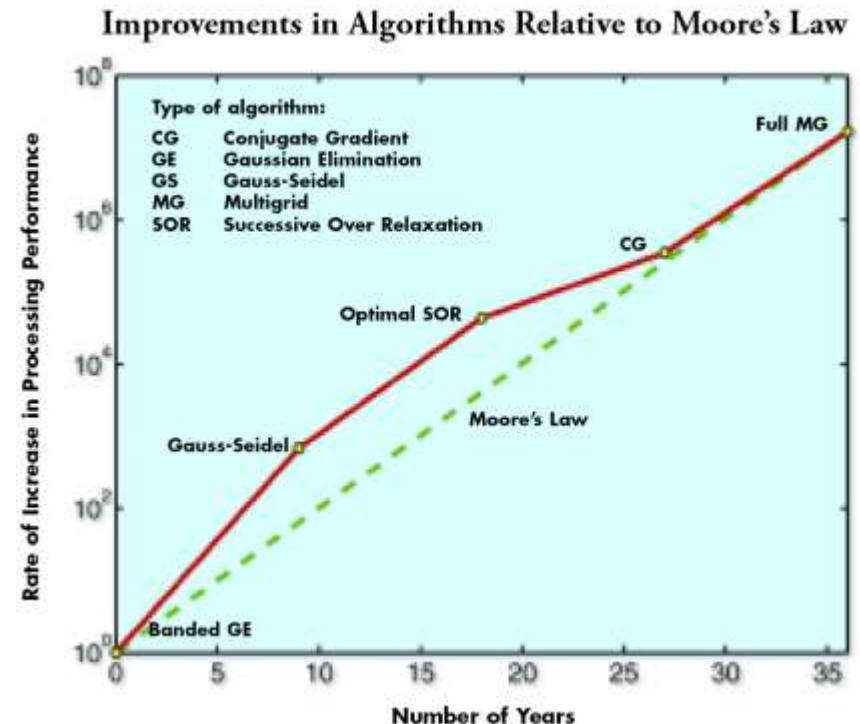
Example 1

- **The first great scientific breakthrough of the new century – the decoding of the <u>human genome</u> (2001) was a triumph of large-scale computational science**
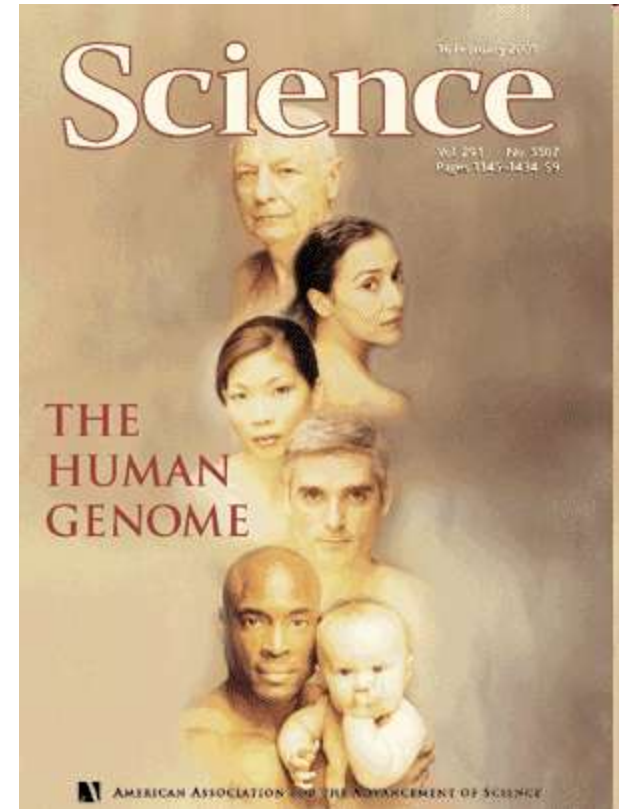
The sequencing of the human genome will impact all of us in diverse ways-from our views of ourselves as human beings to new paradigms in medicine.

Example 2

- **A Rubik's Cube can be solved in <u>20 moves</u> or less from any position – Google computer**
- **Possible moves: 43,252,003,274,489,856,000**
  - **It will take 35 years to compute on a modern PC**
- **In 30 years, mathematicians could only nail it to**
  - **18 < max. moves (the <u>God's number</u>) $\leq$ 52**
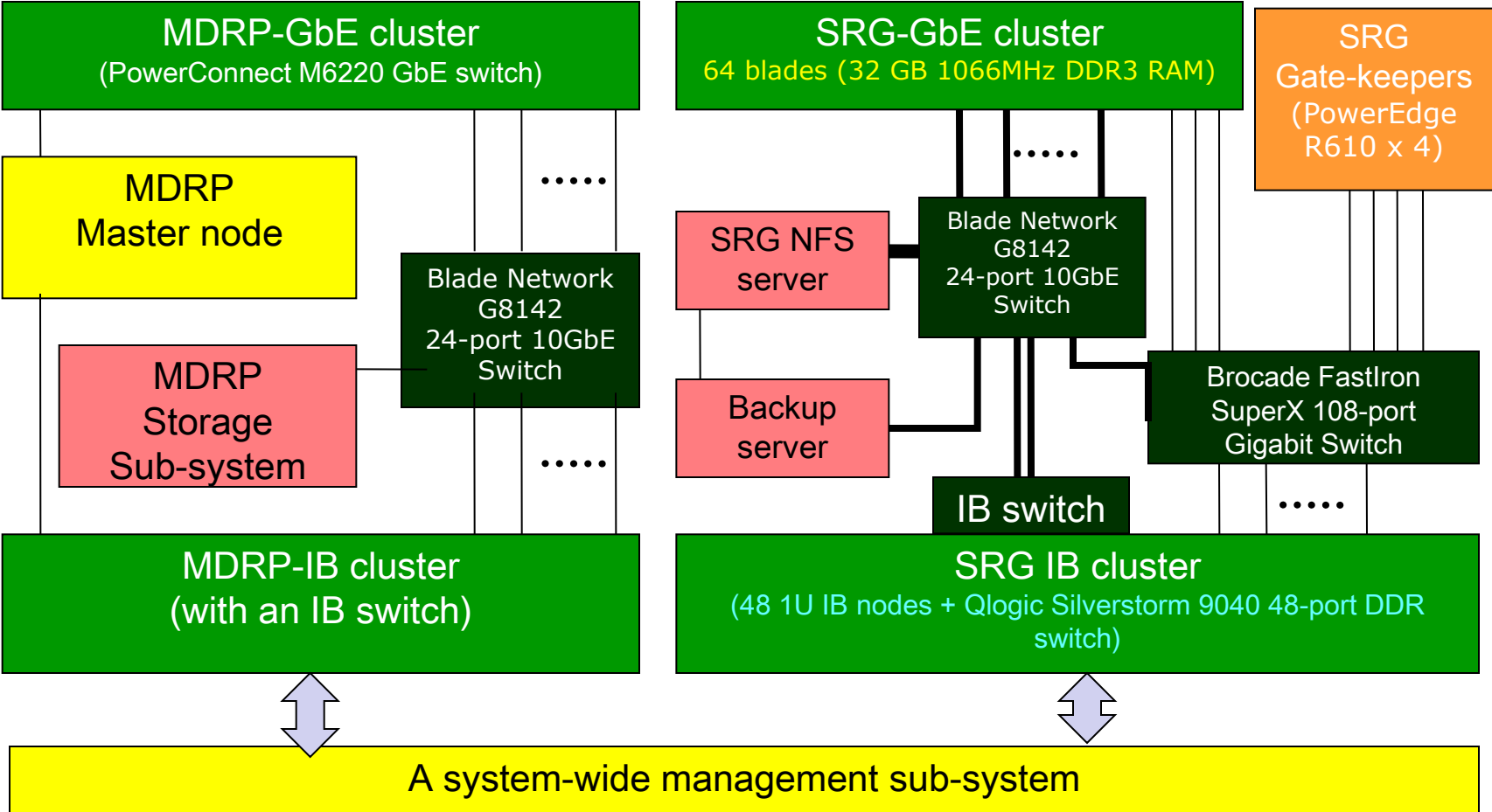
UK's Recommendations

1. Strengthen the <u>computational infrastructure</u> by:
    *   systematically deploying <u>leading-edge capability systems</u>, large-scale capacity computing, and resources deployed widely at universities
    *   supporting and developing a <u>state-of-the-art applications software infrastructure</u> encompassing algorithms, data management and analysis, visualization, and best-practices software engineering.
2. Develop <u>human resources</u> in HPC.
3. Bridge disciplines and build a <u>computational science community</u> by increasing interactions and fostering collaborations between disciplinary groups nationally and internationally.

HKU's New Infrastructure

**HKU Computer Center
(MDRP Cluster)**
(128 blades in 8 chassis)

**HKU Computer Science
(Gideon II Cluster)**

MDRP-GbE cluster
(PowerConnect M6220 GbE switch)

MDRP
Master node

MDRP
Storage
Sub-system

Blade Network
G8142
24-port 10GbE
Switch

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. . . . .

MDRP-IB cluster
(with an IB switch)

SRG-GbE cluster
64 blades (32 GB 1066MHz DDR3 RAM)

. . . . .

SRG NFS
server

Blade Network
G8142
24-port 10GbE
Switch

Backup
server

IB switch

SRG
Gate-keepers
(PowerEdge
R610 x 4)

Brocade FastIron
SuperX 108-port
Gigabit Switch

. . . . .

SRG IB cluster
(48 1U IB nodes + Qlogic Silverstorm 9040 48-port DDR
switch)

A system-wide management sub-system

HKU Grid Point Cluster: 2009-10

Performance Evaluation

• **Gideon-II 64-node GbE cluster (via Foundry Switch)**	**3.45Tflops / 5.181Tflops =** 66%
• **Gideon-II 64-node GbE cluster (via 10GbE switch)**	**3.115Tflops / 5.181Tflop =** 60%
• **Gideon-II 48-node IB-cluster**	**3.275Tflops / 3.886Tflops =** 84%
• **MDRP 32-node IB cluster**	**2.210Tflops / 2.590Tflops =** 85%
• **MDRP 96-node Gigabit Ethernet cluster**	**5.283Tflops / 7.772Tflops =** 67%

Grid Computing – Development & Collaborations

Local HPC clusters

Campus Grid

Regional Grid (HK Grid)

National Grid (CN Grid)

International Grid (EGEE, APGrid, PRAGMA)
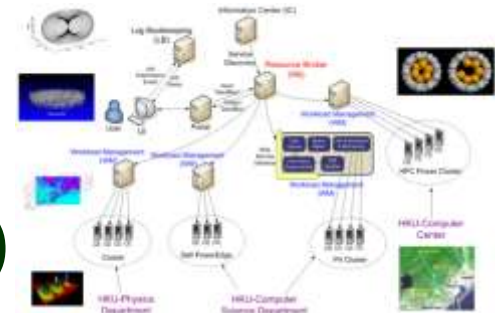
Central HPC/Grid Computing Facility Advancement

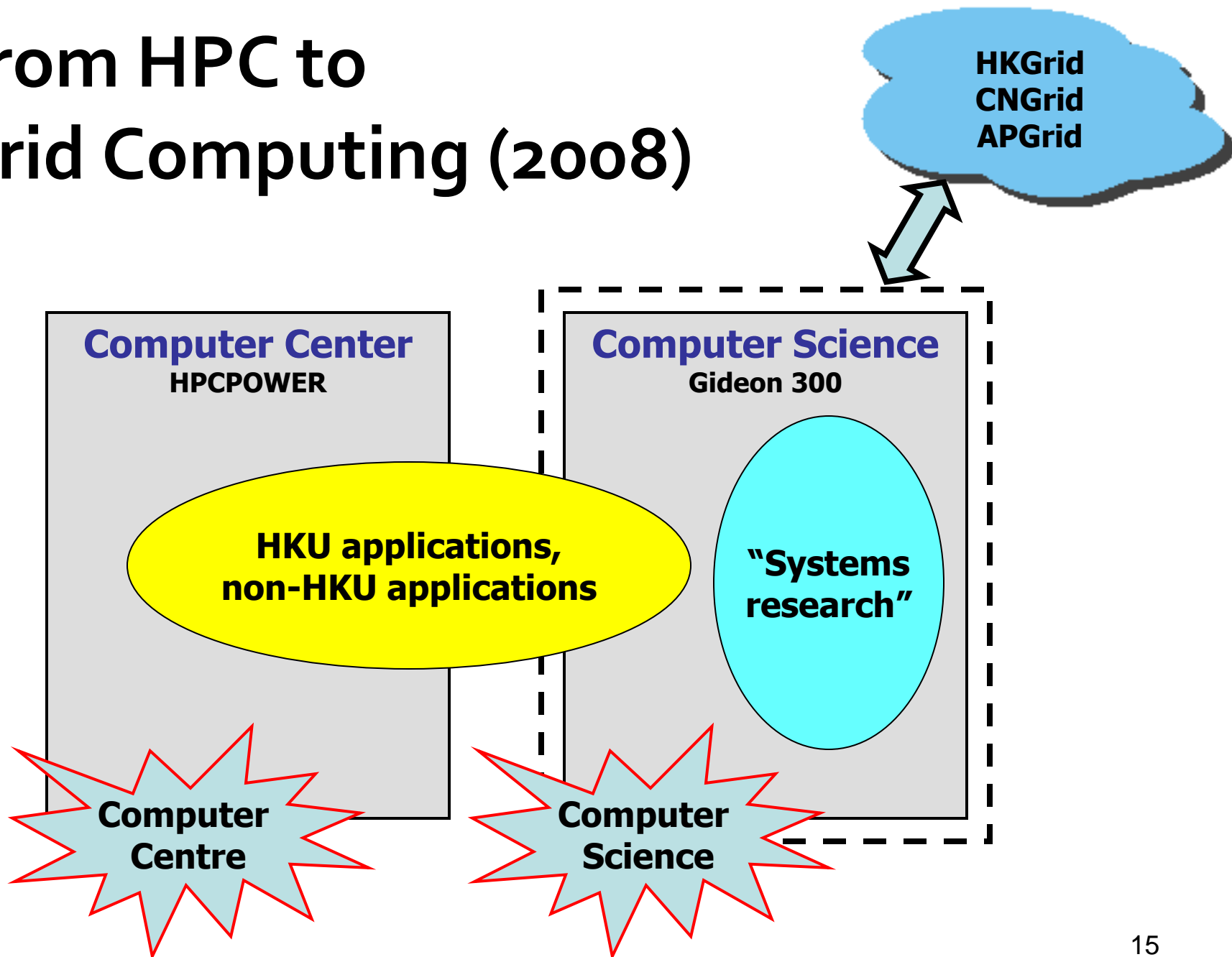| Year	Top500	System	Rmax(TF)	Rpeak(TF)
2011	---	HKU Grid Point System (Total)	---	27050.4
2010	---	HKU Grid Point System (1st phase)	14218	19430.4
2008	---	192-Cores + 356-CPU IBM Linux Cluster	2376.3	4337.6
2005	---	356-CPU IBM Linux Cluster	1086.19	2033.6
2003	240th	256-CPU IBM Linux Cluster	637.8	1433.6
2001	---	64-CPU HP Linux Cluster	---	64.0
2000	---	8-CPU Linux Cluster	---	12.8
1998	345th	48-CPU IBM SP2	22.2	30.7
1995	186th	32-CPU IBM SP2	6.6	8.5
1993	---	8-CPU IBM SP1	---	1.0

* → 2001

* Department of CS's Gideon cluster – 175th in Top500 (11/2002)

Research Projects using Central HPC/Grid Computing Service

Departments Hosting Research Project	No. of Major Projects		
	2010/09	2009/08	2008/07
Department of Chemistry	51	46	36
Department of Statistics and Actuarial Science	23	30	19
Department of Physics	26	24	22
Department of Mechanical Engineering	20	13	8
Department of Civil Engineering	7	8	5
Department of Electrical and Electronic Engineering	5	2	2
Other departments in the facilities of Engineering, Medicine, Sciences, Social Sciences and Dentistry	32	30	7
Total	164	153	99

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From HPC to Grid Computing (2008)

**HKGrid
CNGrid
APGrid**

Computer Center
HPCPOWER

Computer Science
Gideon 300

**HKU applications,
non-HKU applications**

"Systems research"

Computer Centre

Computer Science

HKU Grid Point UGC Project

Phases 1 & 2 (27.05 TF)

High-speed Network
to Campus & Grid partners

Master node &
Gatekeepers

10Gb Ethernet

Infiniband &
10Gb-Ethernet
switches

10Gb Ethernet

10Gb Ethernet

4X DDR (20Gbps)
InfiniBand

4X QDR (40Gbps)
InfiniBand

**Phase-2 Storage
(30TB)**

**Phase-1 equipments
(19.43TF & 21TB)**

**Phase-2 Infiniband-Based
Compute Nodes (7.62TF)**

China National Grid : Phase II

The China National Grid II (CNGrid II) (2006-2010)

Tsinghua University
清华大学

Computer Network Information Center,
Chinese Academy of Sciences
中国科学院计算机网络信息中心

Shandong University
山东大学

Institute of Applied Physics
and Computational Mathematics
北京应用物理与计算数学研究所

University of Science
and Technology of China
中国科学技术大学

Xian JiaoTong University
西安交通大学

Shanghai Supercomputer
Center
上海超级计算中心

National University of
Defense Technology
国防科学技术大学

Huazhong University of
Science and Technology
华中科技大学

ShenZhen Institute of Advanced Technology,
Chinese Academy of Sciences
中国科学院深圳先进技术研究院

The University of Hong Kong
香港大学

The only institution outside Mainland China

High speed Network Connections supporting HKU Grid Point

- **Research & Education Networks**
  - **Internet2, TEIN3 (Trans-Eurasia Information Network), CERNET, APAN , etc. through HARNET**

- **Grid Research connections established:**
  - **CNGrid over China Science and Technology Network (CSTnet)**
  - **KISTI (Korea Institution of Technology and Science Information)**
  - **ASGCC of Taiwan**

HKU e-Research Community Website

- **For enhancing e-Research collaboration http://community.grid.hku.hk/**

International Collaboration – with EGEE development

- **Pilot Set-up of EGEE (Enabling Grids for E-sciencE) in HKU in 2007**
  - **CE (Computing Element)**
  - **SE (Storage Element)**
  - **MON (Information System)**
  - **UI (User interface)**
- **Some HKU researchers already started deploying EGEE computational resources for their needs**

EGEE - Enabling Grids for E-sciencE

- **More than 90 partners**
- **32 countries**
- **12 federations**
- **27 countries through related projects:**
  - **BalticGrid**
  - **SEE-GRID**
  - **EUMedGrid**
  - **EUChinaGrid**
  - **EELA**

egee **EGEE – international e-infrastructure**
Enabling Grids for E-sciencE
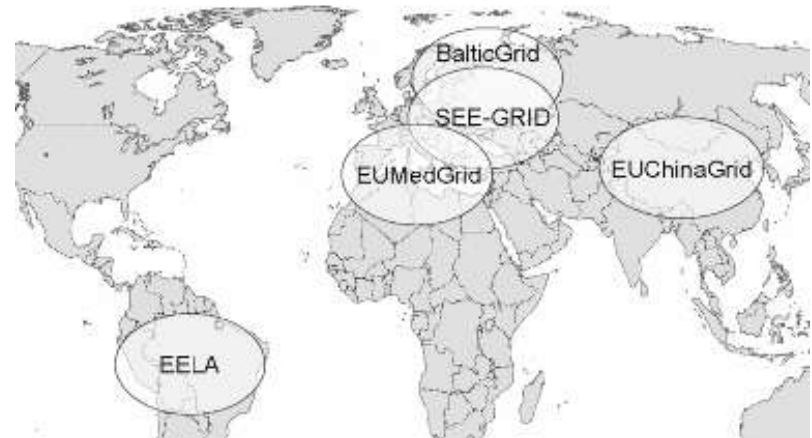
EGEE & Interoperation

- **Expanded consortium**
- **Emphasis on providing an infrastructure**
  - → increased support for applications
  - → interoperate with other infrastructures
  - more involvement from Industry
- **Relies on APGrid PMA, EUGrid PMA,**
  - **& Americas Grid PMA for CA Service**
- **HKU Joined APGrid PMA in 2008**
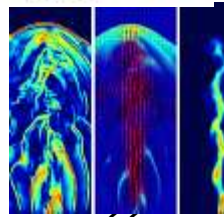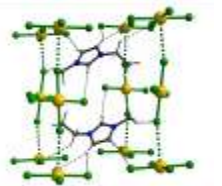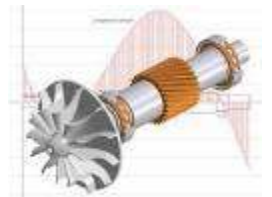
International Collaboration – with PRAGMA and APGrid PMA

- HKU Joined Asia Pacific Grid Policy Management Authority (APGrid PMA) in 2008

- Joined as full member of PRAGMA (Pacific Rim Application and Grid Middleware Assembly) that connects NCSA, SDSC, CNIC, AIST, etc. through PRAMGA Grid

PRAGMA 20

- **Everyone is welcome to join the PRAGMA 20 workshop cum HKU Centennial IT Conference on 2-4 March 2011 at the University of Hong Kong**

- **http://www.hku.hk/cc/HKU100/pragma20/**

HKU Grid Certificate Authority

- **HKU Grid Certificate Authority is accredited to be APGrid PMA (IGTF compliant) Certificate Authority in April 2009**
- **The HKU Grid CA system becomes the foundation for HKU to build trust and collaborations with other universities and research institutes on Grid Computing areas**

Software for HPC/Grid Computing

- **Biology: Simwalk, MrBayes, HYPHY, PhyML**
- **Chemistry: Gaussian 03, NWChem**
- **Geosciences: WRF, MM5, NCL**
- **Modeling/Simulation: Abaqus**
- **Physics: Siesta, VASP, CASINO**
- **Mathematics: VNI IMSL, Intel MKL, BLAS, LAPACK, Matlab Compiler**
- **Language compiler: Portland Group C & Fortran, Intel C & Fortran, Perl, Java, etc**
- **Parallel Computing: MPICH, MPI-LAM**
- **Grid Middleware: Globus, GOS, gLite**

JESSICA Distributed Java VM

Java
Enabled
Single
System
Image
Computing
Architecture

- **A cluster-wide JVM with**
  - **Dynamic thread mobility in JIT mode**
  - **Global Object Space (GOS)**
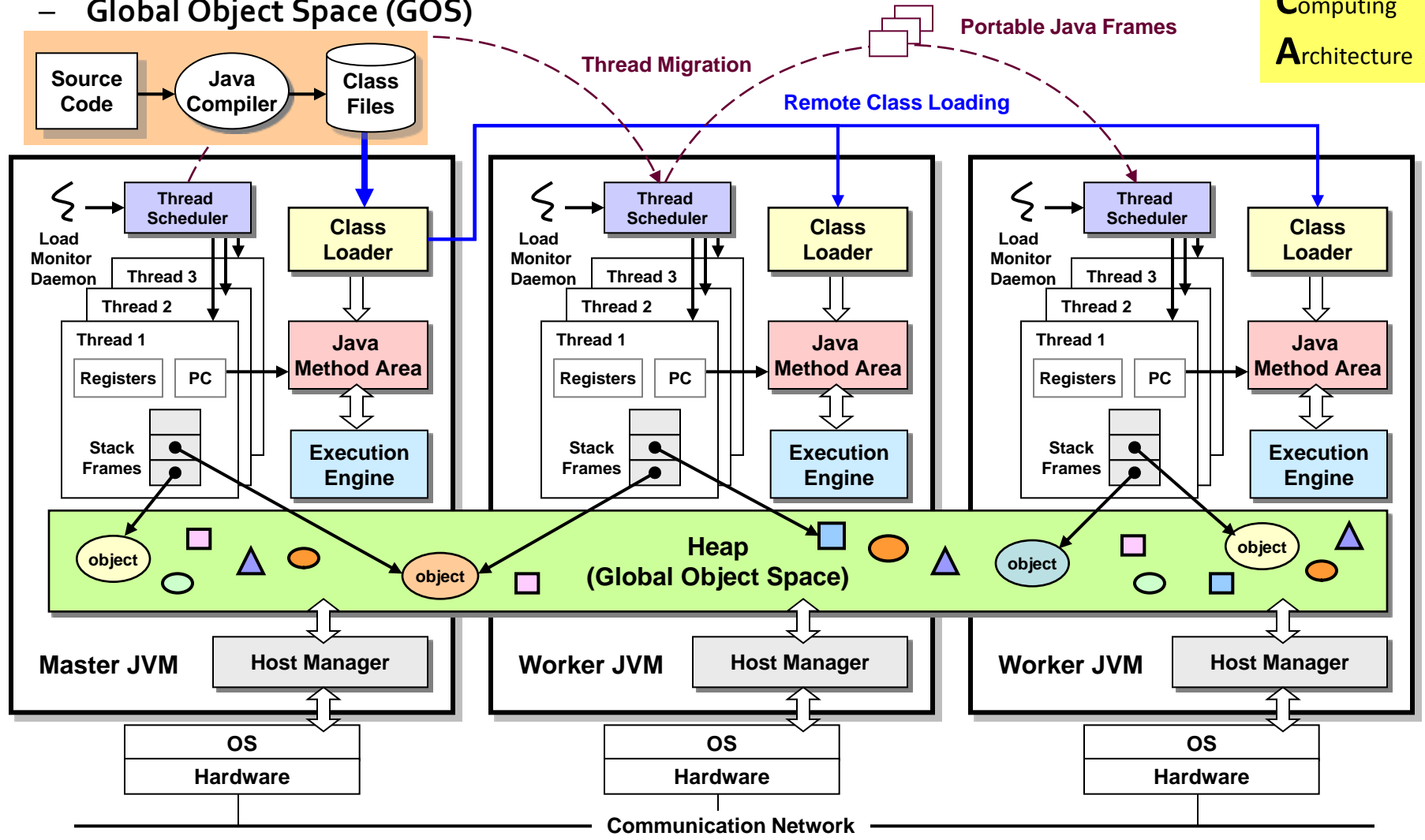
Conclusions

- **Leading-edge computational science is possible only when supported by long-term, balanced R&D <u>investments in software, hardware, data, networking, and human resources</u>.**

- **Universities must significantly change their organizational structures to <u>promote and reward collaborative research</u> that invigorates and advances multidisciplinary science.**

- **The computational science community must <u>confront the discipline's most intractable R&D challenges</u> in a sustained and serious manner.**