



Researching computing support in HKU Information Technology Services (ITS) and the fostering of International research collaboration



PRAGMA33 and eRESEARCH Australasia 2017

W.K. Kwan
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Personal Information

- Asst. IT Director in ITS, HKU
- 1976 B.Sc. Mech. Engin. in HKU
- 1976/11 Postgrad. in Mech. Engin. Studying flow distribution within a plate distillation column. After building the testing model, huge data collected using hotwire and LDA devices, with computed theoretical results compared, hoping to develop a math. Model using traditional CFD theory
- 1980 on a rare chance switched from a user to work in HKU Computer Centre
- 1994 designated to work on the establishment of the HPC and research computing support team, till now



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The University of Hong Kong

- Founded in **1912** (2011 the 100th anniversary)
- Ranked **28th** in "THES-QS World University Rankings 2018"
- Ranked **2nd** in "QS.com Asian University Rankings 2016"
- Ranked **40th** in "Times Higher Education (THE) World University Rankings 2018"
- Ranked **3rd** in "THE World's Most International Universities 2017"
- **28,744** students (in 2016-2017)
 - **16,809** undergraduates, **11,935** postgraduates
- A comprehensive University - **10** faculties
 - Architecture, Arts, Business and Economics,
Dentistry, Education, Engineering,
Law, Medicine, Science, Social Sciences



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Our Services: Teaching

– Undergraduate studies

- Course work requirement
- Final year project

– Taught Postgraduate Studies

- M. Sc. (normally 2 years, course project requirement)

– Research Postgraduate Studies (M.Phil., PhD)

- High quality of intake, Normally 4 years for a PhD
- More than ½ from Mainland China on Sc./Tech. areas
- > 250 our HPC users graduated with earning of PhDs in last 20 years
- Collaboration established thereafter
 - China
 - Overseas
 - HK



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Our Services: Research

- In the old days: “Publish or Perish”!
 - Essential for tenure substantiation or promotion
- Now:
 - One of the three research universities in HK
 - University UGC/RGC projects
 - HKSAR ITF (Innovation and Technology Funds)
 - International collaboration projects
 - China 973 or 863 projects
 - Shenzhen (HKU-SIRI), Zhejiang (HKU-ZIRI) or other local Municipal government projects



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HKU main Research Focus

Strategic Research at The University of Hong Kong

- More global research collaborations on
 - technology development
 - knowledge discovery
 - Inventions/solutions for quality life and sustainable environment
- In 2008, HKU identified 5 strategic research areas comprising 16 strategic research themes and 5 emerging themes (<http://www.hku.hk/strategic-research/>)
- HKU is a comprehensive university, whereas CUHK and HKUST both miss some disciplines





Our Mission in Research



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Computing Support

- Maximize institutional resources, enhance research capabilities, effectiveness and remain competitive.
 - Support researchers from diverse disciplines whose work required intensive computation with the use of advance hardware infrastructure, software, tools and programming techniques
 - Enable HKU researchers to be equipped with the **latest HPC technologies** in doing their **cutting-edge researches** effectively so that HKU’s leading status as the top research university in Hong Kong and Asia can be maintained





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Role of ITS in Research Computing Support



Computing facilities
provider



Information exchange



Solution consultant (hardware, network, software advice,
self-developed program optimization, parallelization)



International Research
Collaboration contact



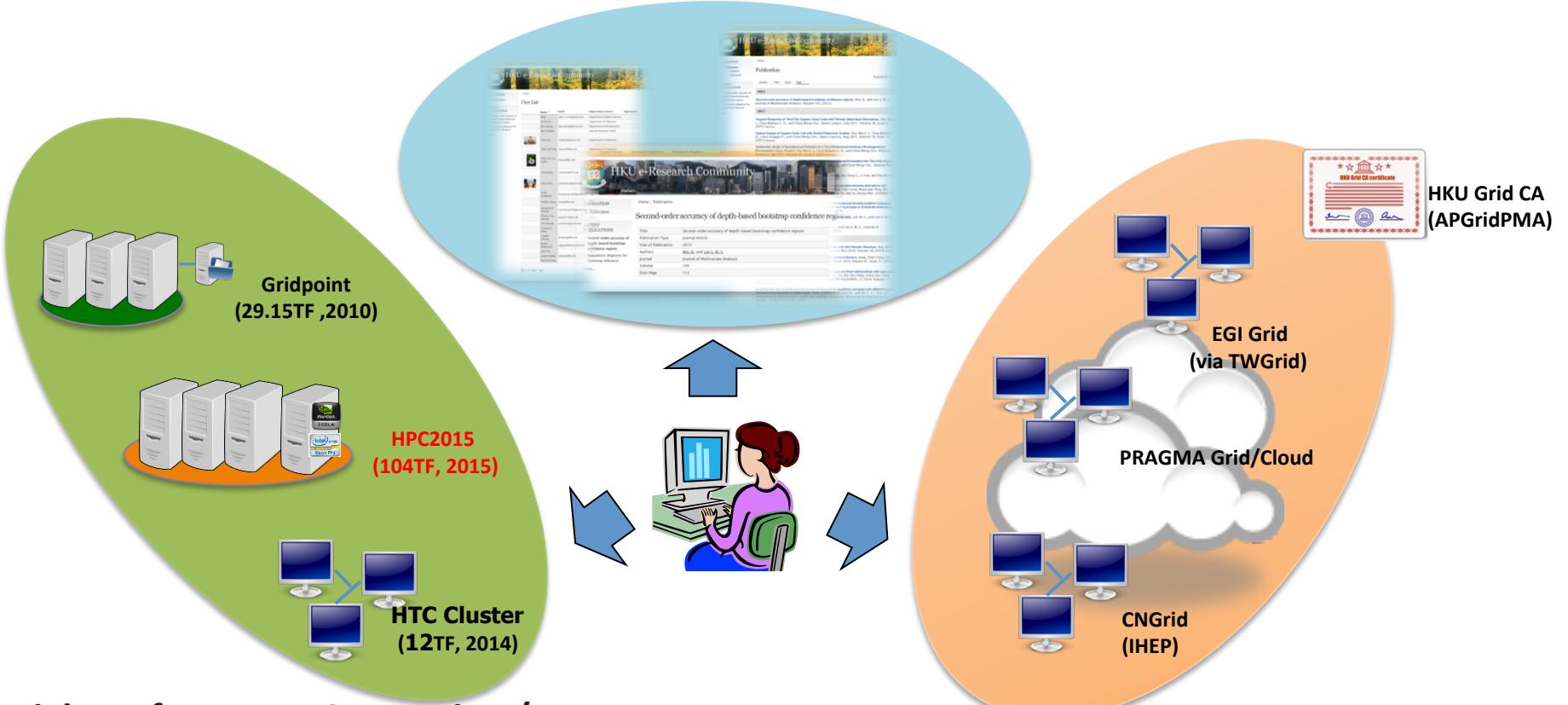
Grid Certificate publisher
(HKU Grid CA)



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HPC Services and Support

HKU Scientific Research Community



High Performance Computing /
High Throughput Computing

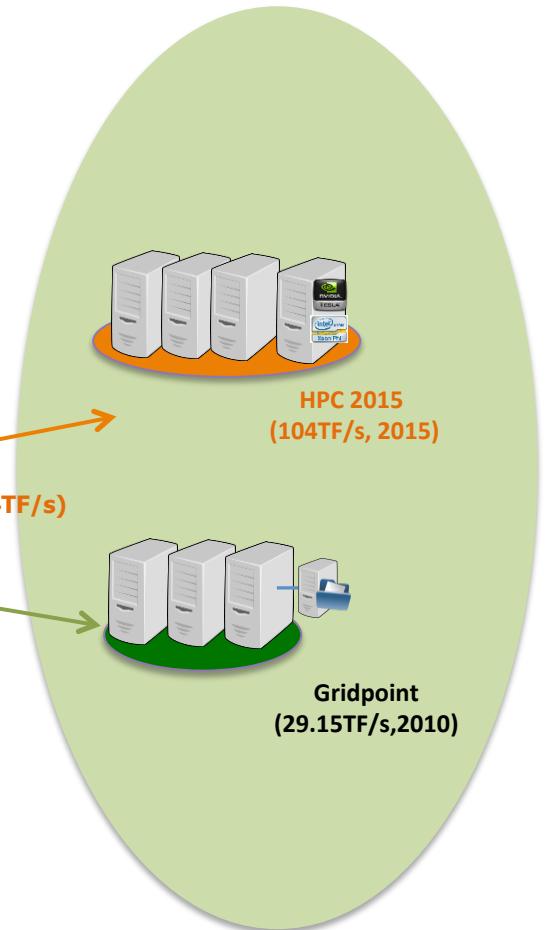
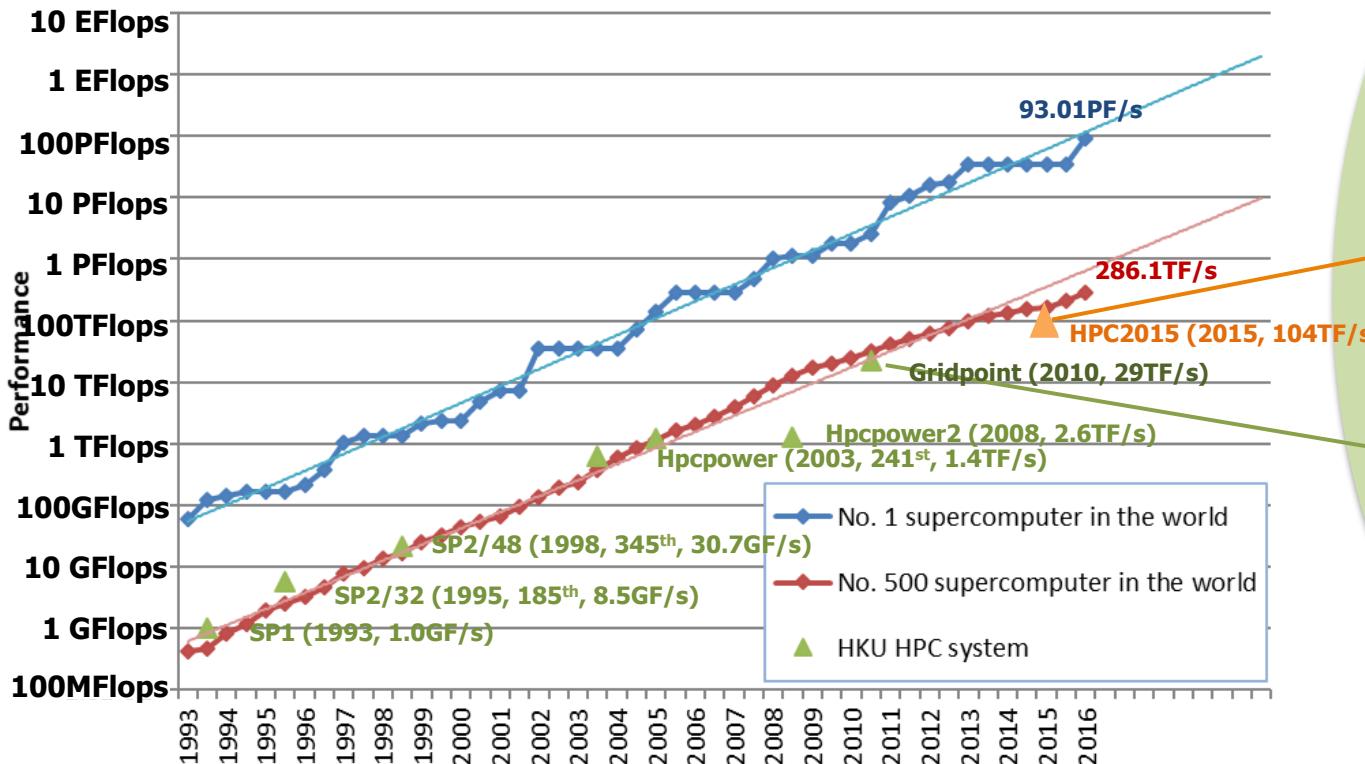
Grid Computing



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HPC Facilities at HKU

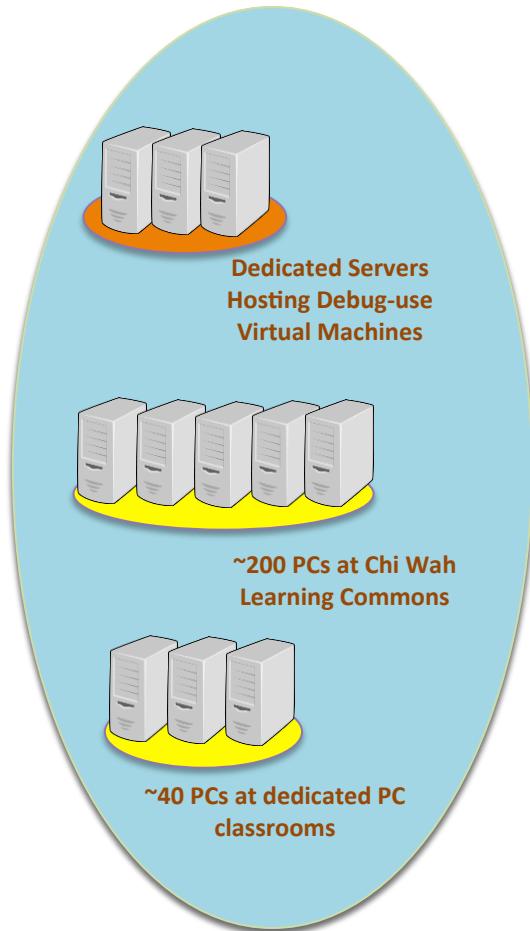
Performance of Supercomputer in the world





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HTC Facilities at HKU



- Recent re-establishment of HTC services in HKU
- A demonstration of the University's commitment in environment protection and "Green Computing"
- HTCondor: Utilizing ITS Windows PCs at night for research
 - Provide computing time for researchers
 - Better use of the machines in their useful life



Some milestones in HKU HPC development (1)



| Year | Activity |
|---------------|---|
| (Pre-history) | (ICL1902/04, IBM3031, Sperry UNIVAC, PDP 117/70, VAX750...) |
| 1993 | IBM 8-nodes SP1 |
| 1995 | IBM 32-nodes SP2 |
| 1998 | IBM 48-nodes SP2 |
| | |
| 2000 | Home-brewing LINUX system, 8 PCs |
| 2001 | HKUHPCC, 32-nodes Compaq 1G Xeon3 |
| | |
| 2003 | HPCPOWER, 128-nodes IBM 2.8G Xeon4 |
| 2004 | WINHPC, Dell hardware |
| | 1 st attending CNGRID in Beijing |

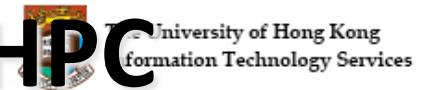


Some milestones in HKU HPC development (2)

| Year | Activity |
|------|---|
| 2006 | Joining 2 nd phase of CNGRID (for 5 years) |
| 2007 | Setup of HCPOWER2 (1 st 64-bit experimental LINUX cluster < 1 mil. HK\$) Setup of 1GBit direct link to CNIC BJ via CSTNET after joining CNGRID 1 st attending ASGC in Taiwan, joining TWGRID, enabling EGI access |
| 2008 | Installation of GRIDPOINT, 132 * 8 cores Xeon5, inauguration ceremony |
| 2009 | Setup of HKUGridCA (accredited by APGrid PMA) Serving as a evaluation committee for SIAT “小超算” Joining PRAGMA as an Institutional member |
| 2011 | Hosting PRAGMA20 in HKU, in conjunction with the centennial celebration KWK became a steering committee member |



Some milestones in HKU HPC development (3)



| Year | Activity |
|------|--|
| 2012 | Mini-PRAGMA conducted in HK and organized by HKU |
| | 3 invited speeches in “2012 Symposium on Economics Laboratory” , Wang Yanan Institute for Studies in Economics (WISE), Xiamen University, 2012 March |
| 2013 | KWK invited to be a judge panel member of the annual ASC competition |
| 2014 | HPC2015 system awarded |
| | Attending the 1 st meeting of 超级计算创新联盟 |
| 2015 | HPC2015 installation completed |
| 2016 | Visits between HKU and NSCC-GZ (TianHe II) |
| 2017 | AI & DNN seminars, specially arranged with the Medical faculty |



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Salient Features of the New HPC System

| HPC System | # CPU node | System Configuration | Total CPU cores | Theoretical CPU Power |
|--------------------------------|------------|--------------------------|-----------------|-----------------------|
| HPCPOWER (2003) | 128 | 2 x CPU, 2GB RAM | 256 cores | 1.4 Tera-FLOPS |
| HPCPOWER2 (2008) | 24 | 2 x 4-core CPU, 8GB RAM | 192 cores | 2.6 Tera-FLOPS |
| GRIDPOINT (2010) (ITS-MDRP) | 128 | 2 x 4-core CPU, 36GB RAM | 1216 cores | 12.1 Tera-FLOPS |
| | 16 | 2 x 6-core CPU, 48GB RAM | | |

HPC2015 Cluster System (Launched at 2015)

| System component | Qty | Configuration Highlights | Total Sys. Size | Theoretical CPU Power | |
|------------------|-----|--|-----------------------------------|-----------------------|------------------|
| General Nodes | 104 | 2x Haswell 10-core CPU, 96GB RAM | CPU: 2080 cores | 84.5 Tera-FLOPS | |
| GPU Nodes | 4 | 2x 10-core CPU, 2x Tesla K20X GPU accelerator | CPU: 80 cores GPU: 21504 cores | 12.0 Tera-FLOPS | 104.1 Tera-FLOPS |
| MIC Nodes | 2 | 2x 10-core CPU, 2x Xeon Phi coprocessor 7120P | CPU: 40 cores MIC: 244 cores | 5.5 Tera-FLOPS | |
| Huge Mem. Nodes | 3 | 4x Intel 10-core CPU, 512GB RAM | CPU: 120 cores | 2.06 Tera-FLOPS | |
| File Storage | | Lustre Parallel File System | 150TB usable capacity | | |
| Interconnect | | FDR10 40Gb/s InfiniBand | Latency: 200ns; Throughput: 4Tb/s | | |

Theoretic Peak Performance ~104 Tera-FLOPS



State-of-the-art Technology



Intel latest core (Haswell) processor

- Multiple(up to 18) cores optimized for sequential serial processing
- Compared to Ivy Bridge, faster in vector processing performance and single/multi-threaded performance
- Support for DDR4 memory



GPGPU (General Purpose computing on Graphical Processing Unit)

- Thousands of smaller cores in single chip for handling multiple task simultaneously.
- Need CUDA/OpenCL programming
- Wide range of applications are GPU-accelerated (e.g GROMACS, NAMD, LAMMPS, QCHEM, VASP, PyMol, MATLAB, ABAQUS, WRF, etc)



Intel MIC (Many Integrated Core)

- First product launched at late 2012
- ~60 Pentium-graded cores in single chip for multiple task parallelization
- Not requiring new programming model. Using MPI/OpenMP/OpenCL with standard programming languages, such as C, C++, FORTRAN

CUDA: Compute Unified Device Architecture, a parallel computing platform and programming model created by NVIDIA



Software for HPC Support (*partial list*)

- **Biology:** Simwalk, MrBayes, HYPHY, PhyML, MEME, BLAST
- **Chemistry:** Gaussian, ADF, Gamess, NAMD, Gromacs, CPMD, ORCA, Firefly
- **Geosciences:** WRF, MM5, NCL
- **Modeling/Simulation:** Abaqus, LAMMPS
- **Physics:** Siesta, VASP, CASINO, Quantum Espresso
- **Mathematics:** IMSL, Intel MKL, BLAS, LAPACK, MATLAB, NAG, R
- **Language compiler:** Portland Group C & Fortran, Intel C & Fortran, Perl, Java, Python etc
- **Parallel Libraries:** MPICH, Open MPI, Intel MPI
- GPU/MIC related utilities and GPU/MIC enabled s/w





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Remarks

- ✿ HKU is **not rich** in hardware facilities
(can never compare with a national computer centre)
- ✿ We are always lagging behind modern HPC technologies
(We only have budget for hardware upgrade per 4-5 years)
- ✿ Experienced in HPC applications in different areas
- ✿ Experienced in using facilities **EFFICIENTLY** and **EFFECTIVELY** (yearly utilization > 90%)
- ✿ > (survey in 2013) 500 high impact papers published based on results obtained from our HPC facilities during last 5 years



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International Research Collaboration

Contact

- HKU is a comprehensive University with much research activity in different disciplines
- Links with many international research consortiums
- Unique institutional memberships to:
 - CNGrid
 - TWGRID->EGI Grid
 - PRAGMA



China National Grid : Phase II

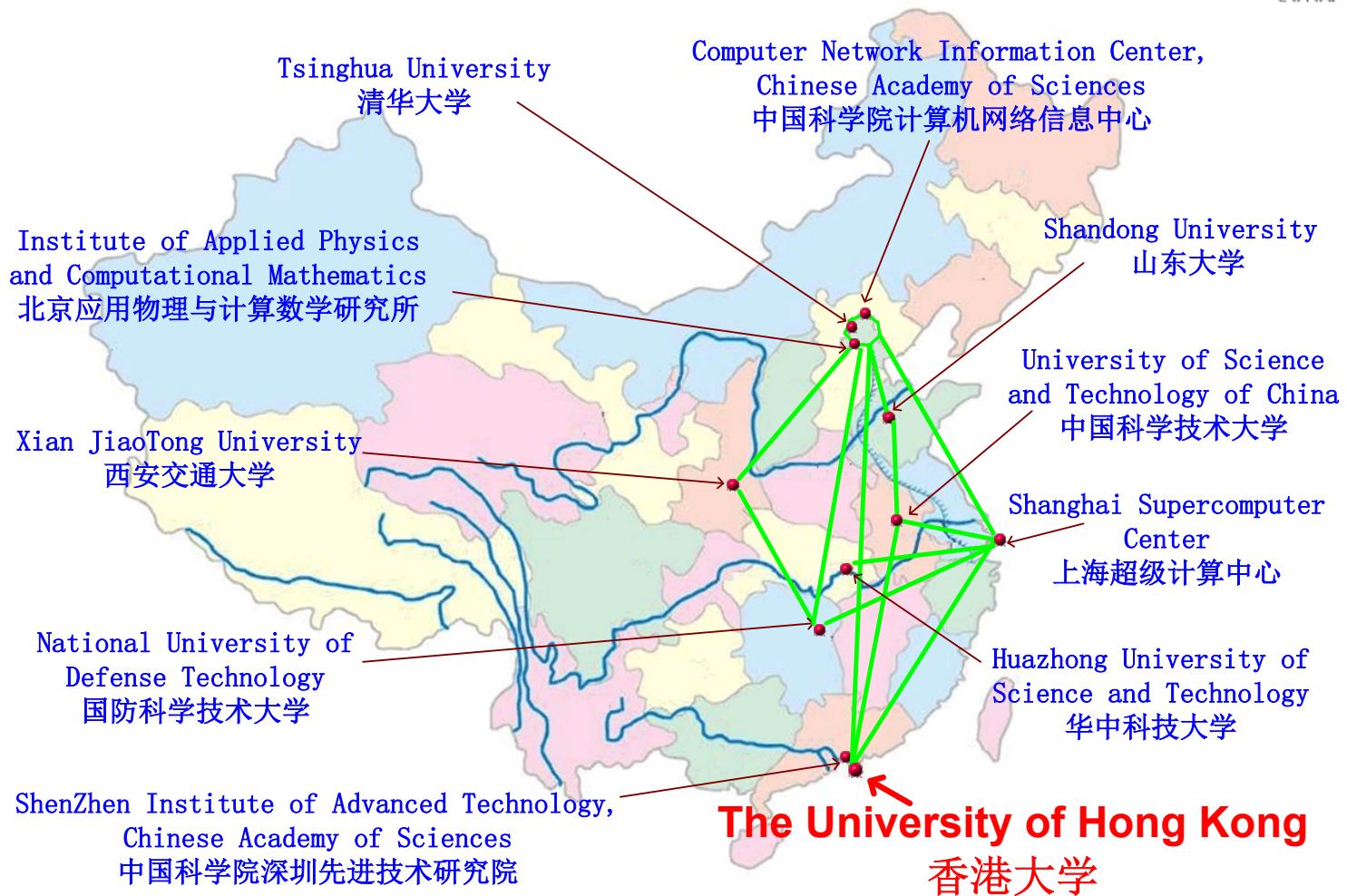
The China National Grid II (CNGrid II) (2006-2010)



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国家863计划



The only institution outside Mainland China



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EGI – European Grid Infrastructure

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



EGEE – international e-infrastructure

Enabling Grids for E-sciencE



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PRAGMA – Pacific Rim Application and Grid Middleware Assembly

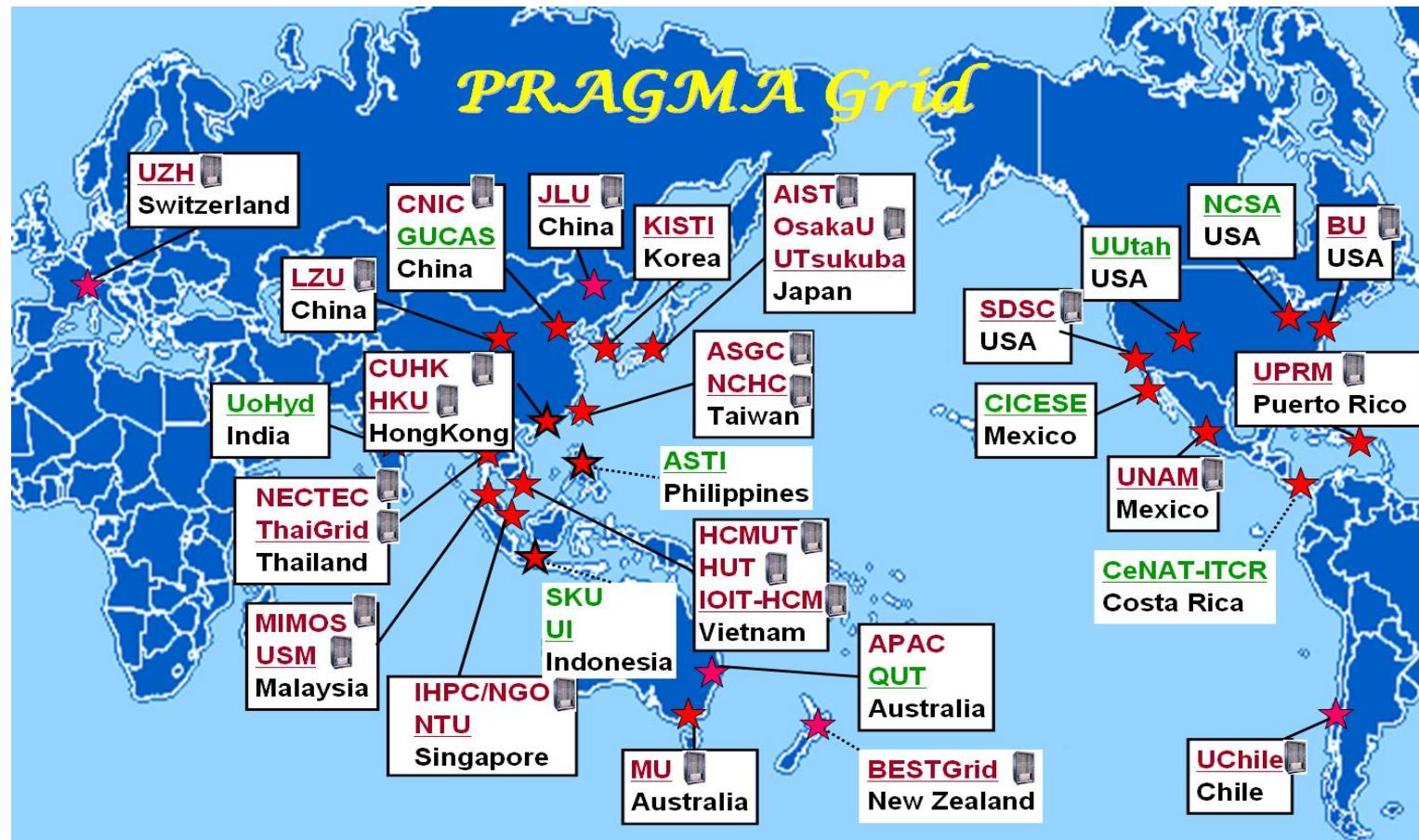
- Formed in 2002 for advancing the use of grid technologies in applications among investigators in leading institutions around the Pacific Rim
- Regular workshop meeting twice a year
- Aim to provide an “assembly” to allow researchers for academic knowledge exchange and research collaboration
- HKU joined PRAGMA in 2009 as an Institutional Member. Hosting PRAGMA workshop in 2011.





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PRAGMA



29 institutions in 15 countries/regions, 25 compute sites (+ 10 in preparation)

Last update: 2/23/2009





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2011 March PRAGMA 20 in HKU

<http://pragma20.pragma-grid.net>





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HKU Grid Certificate Authority

- HKU Grid Certificate Authority is accredited to be APGrid PMA (IGTF Compliant) Certificate Authority in April 2009
- Certificate issued by HKU Grid CA accepted by the 3 earlier mentioned international consortia
- 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.





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HKU GRID Connections



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



- Grid Research Connections:
 - CNGrid over China Science and Technology Network (CSTnet)
 - KISTI (Korea Institution of Technology and Science Information)
 - ASGC of Taiwan





HKU as Research Hub in South China region



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HKU Researchers

- Many research connections locally with other HK tertiary institutes
- Many researchers in other HK tertiary institutes are actually graduates of HKU
- Many researchers already have research collaborations in China
- Many China Post-docs. Return to China after working several years in HKU



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Shenzhen

- A SEZ (Special Economic Zone)
- Fast growing economic and industrial town
- The back-up hinterland of HKSAR
- 1.5 hr. travel from HKU
- One of the “One Belt, One Road” pivots
- Guangdong-Hong Kong-Macao Big Bay Area (GHMBBA) 粵港澳大灣區



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Research Inst. In Shenzhen

- SIAT (Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, local HQ of several CAS inst. In SZ)
- BGI (華大基因)
- NSCC-SZ (National Supercomputing Center in Shenzhen)
- ISCAS (Institute of Software Application Technology, another branch from CAS)
- Many many international renowned Big-corps: Huawei (華為), BYD (比亞迪), ZTE (中興), Da-Jiang Innovations (大疆無人機) ...



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MINI-PRAGMA (2012/07/17)

To facilitate global research and academics collaborations and for prosperous development to the region and to the world, ITS and PRAGMA co-organized the Workshop on Building Collaborations in Clouds, HPC, and Application Areas (first of this kind in PRAGMA history).

About 30 participants from HKU, local and South-China research organizations and international PRAGMA institutes shared their cutting-edges research projects and initiated potential collaborations in the workshop.





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Categories of HPC applications

- User written programs (Fortran, C, Python, R, Matlab, CUDA...)
- Scientific packages (Gaussian, VASP, LAMMPS...) May or may not be GPU-enabled.
- Big data applications (Transport, Environment, Bioinfo...)
- AI DNN frameworks (Caffe, TensorFlow, Theano)



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Macroscopic view

- Asia is the region with fastest economic growth in the world
- US uses HPC technology to maintain its competitive edge over the world especially in the areas requiring high-tech (car, aircrafts, financing engineering, drug...)
- How Asian countries can boost up their industries through using HPC
- We have to chase, and we have to leap



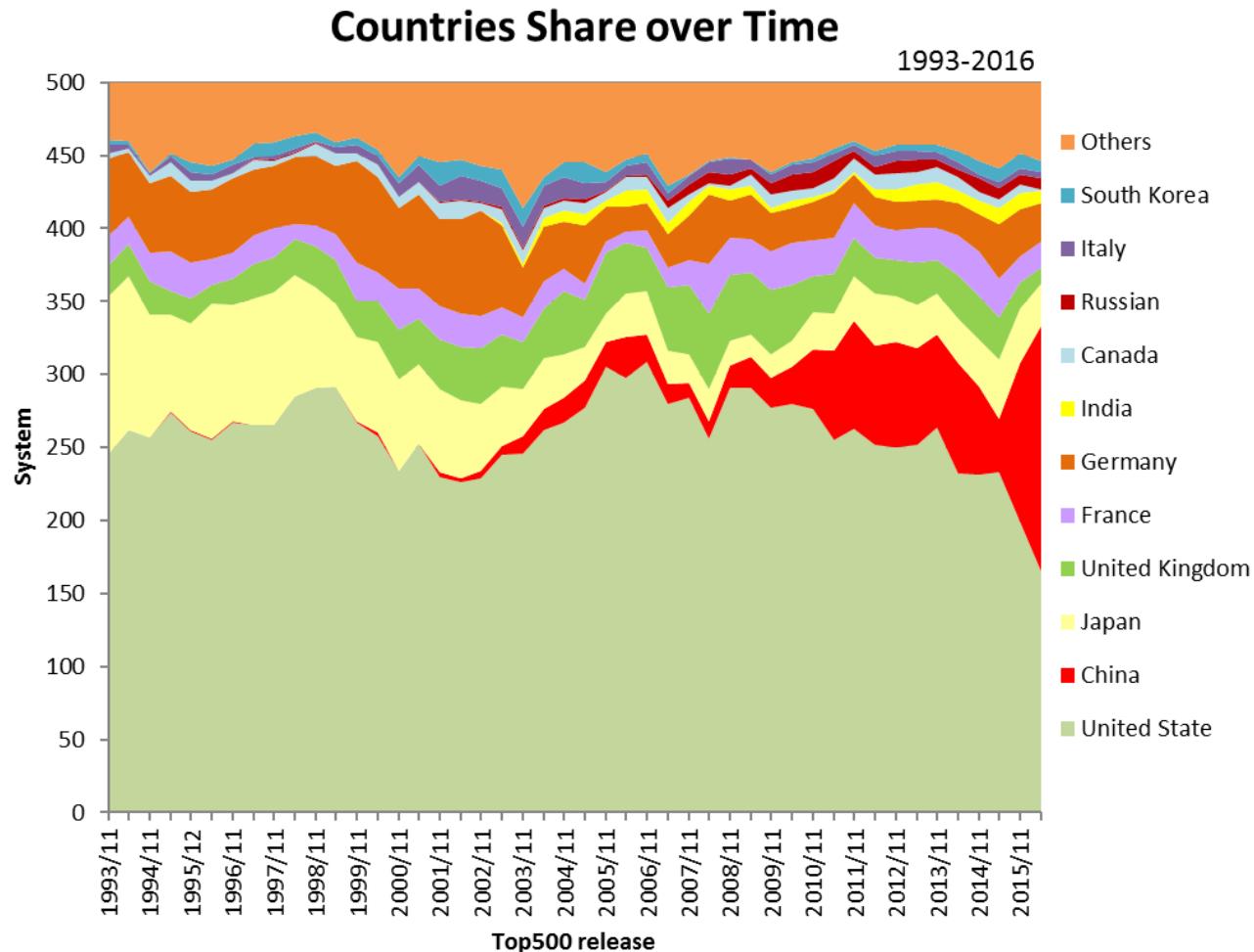
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Out-sourcing for HPC resources from China national supercomputing centres, through research collaboration



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TOP500 trend in the world



Top500 supercomputer site <http://www.top500.org>



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Top10 supercomputer (June 2016)

| Rank | System | Country | Rmax (Petaflop/s) |
|------|-------------------|---------------|-------------------|
| 1 | Sunway TaihuLight | China | 93.0146 |
| 2 | Tianhe-2 | China | 33.8627 |
| 3 | Titan | United States | 17.59 |
| 4 | Sequoia | United States | 17.1732 |
| 5 | K Computer | Japan | 10.51 |
| 6 | Mira | United States | 8.5866 |
| 7 | Trinity | United States | 8.1009 |
| 8 | Piz Daint | Switzerland | 6.27 |
| 9 | Hazel Hen | Germany | 5.642 |
| 10 | Shaheen II | Saudi Arabia | 5.537 |

Top500 supercomputer site <http://www.top500.org>



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Comparison in Power

| | Implement . year | No. of cores | Theoretical rating (Tflops) | Relative power | Remark |
|---------------|------------------|--------------|-----------------------------|----------------|--------------------------------|
| HKU Gridpoint | 2010 | 2,256 | 29.15 | 1 | Only 12 NVIDIA GPUs (in CS) |
| NSCC-SZ | 2009 | 120,640 | 2,984.3 | 102 | GPUs |
| NSCC-GZ | 2013 | 3,120,000 | 54,902.4 | 1883 | MICs (now with GPUs and DGX-1) |
| HKU HPC2015 | 2015 | 24,064 | 103.4 | 3.55 | CPUs +GPUs +MICs |



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HKU Researchers

- Many research connections locally with other HK tertiary institutes
- Many researchers in other HK tertiary institutes are actually graduates of HKU
- Many researchers already have research collaborations in China
- Many China Post-docs. Return to China after working several years in HKU (esp. to the several univs. In SZ and GZ)



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NSCC-SZ

- Established in 2009
- Systems owned by the Shenzhen Municipal Government
- Rich in commercial software
- Not associated with any R&D institutions



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NSCC-GZ

- Established in 2013
- System original funding: 1/3 GZ, 1/3 Guangdong, 1/3 Central, Sun Yat-sen Univ. just provided the system housing
- Admin. restructuring in 2016 March/April:
Data and Computer Science School established (Prof. QIAN Depei)
NSCC-GZ admin. under D&C Sc. School (Prof. LU Yutong)



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NSCC-GZ (2)

- Most software is of open source
- “Full Quota” 150 supporting staff position granted, with many post-doc. in different R&D areas.
- Welcome research collaboration either through their NSCC-GZ or via SYSU different academic departments
- Low charging rate (standard)



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Project migration (HKU to TianHe-II)

- Similar hardware
- Similar software (compilers, libraries, app. s/w)
- Normally the user' program should already be well-tuned in term of single-node multicore parallelization.
- Need more attention to multi-node parallelization (instead of 8-16 nodes, you are facing 100 nodes)
- Execution queue setting, data I/O ...



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Meeting with Prof. Lu Yu-tong





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Some of our users and their research projects