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Computer Network Information Center,
Chinese Academy of Sciences

Computing Environment in Chinese Academy of Sciences

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Supercomputing Center
Computer Network Information Center
Chinese Academy of Sciences
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Outline

- Glance at Supercomputing Center
- Computing Facilities
- Parallel Software
- User Environment
- Application Areas
- Main Node of China National Grid
- Conclusions

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Supercomputing Center

- 4 divisions: System maintenance, Parallel computing research, Application software development and Grid technology application
- Focus on parallel computing, parallel libraries, and provide solutions for complicated large scale applications in science and engineering
- Objective: Provide computing and storage facilities and service for CAS

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Computing Facilities

- ICT Dawning 2000

Peak: 111 Gflops
Memory: 46GB
Storage: 628GB
Total number of processors: 164
Total number of nodes: 82
CPU: double 333Mhz Power PC 604e (Thin/thick nodes); double 200Mhz Power3 (High performance nodes, Main server nodes)

OS: AIX

Installation: May, 2000

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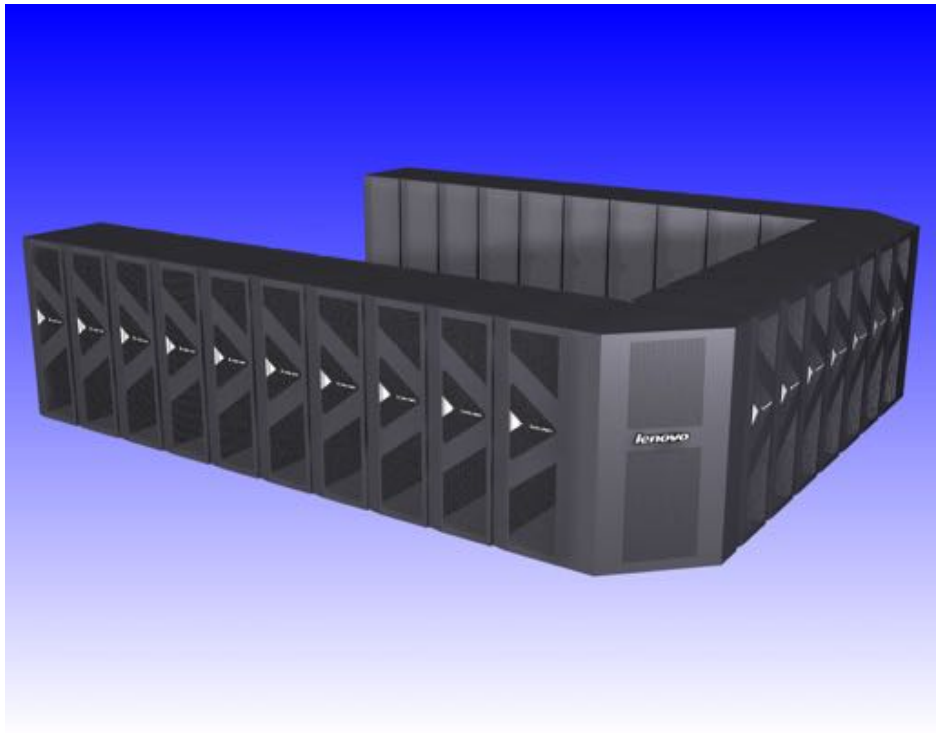
Computing Facilities (con.)

- Lenovo DeepComp 6800

Peak: 5.3TeraFLOPS
HPL: 4.2 TeraFLOPS
Rank in TOP500: 14 (2003)
Number of nodes: 265
Number of processors: 1060
Processor: Itanium 2, 1.3 GHz
Memory: 2.6 TBytes
Storage: 80 TBytes
Network: Quadrics QSnet
OS: Red hat AS 2.1

Installation :December, 2003



Computing Facilities (con.)

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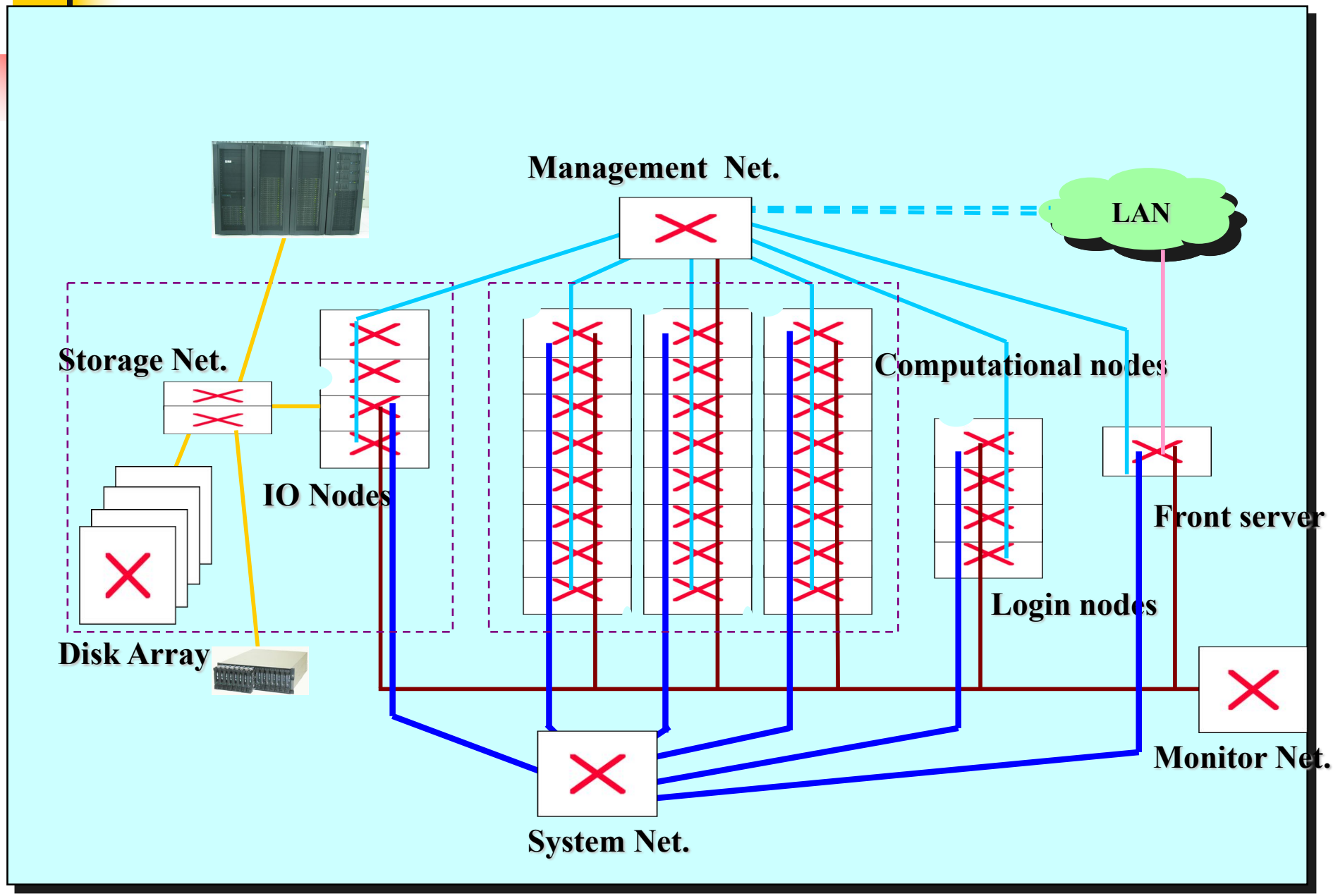

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Computing Facilities (con.)

- SGI Onyx 350

Peak: 38GFLOPS
HPL: 22 GFLOPS
Number of processors: 32
Processor: r16000, 600MHz
Memory: 32 GBytes
Storage: 500 GBytes
OS: IRIX 6.5

Installation (March, 2004)

Parallel Software

- Commercial Software
  - Gaussian 2003
  - ADF
  - Ansys LS-Dyna (ABAQUS)
  - Platform LSF
  - Totalview
  - Parawise

Parallel Software (con.)

- Free Software
  - LAPACK, ScaLAPACK
  - PETSc, FFTW
  - Paraview, VTK, Vis5D, Pymol, Rasmol, VMD, GMT
  - GAMESS, CPMD, DOCK
  - BLAST, Clustalw, Blat, Predpharp, etc
  - ……

Parallel Software (con.)

- Development of Application Software
  - MPI_AltSplice, MPI_SiClone
  - Auto-Program Generator of FEM
  - BDF
  - Material Science
  - Fluid Dynamics
  - ……

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User Environment

- ScGrid Portal
  - User Module: Login & logout, User configuration, Job submission (batch and interactive), Job viewing, resource querying, file manager, file transfer, etc.
  - Accounting Module
  - Admin Module: Portal Administrator and CA manager
- ssh, ftp

User Environment (con.)

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User Environment (con.)

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Application Areas

- Computational Chemistry
- Computational Physics
- Computational Mechanics
- Bioinformatics
- Geophysics
- Atmospheric Physics
- Astrophysics
- Material Sciences
- ……

Application Areas（ con.）

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A successful earthquake prediction on the Yangjiang region in Guangdong Province broke out in Sep. 2004

- using Load/Unload Response Ratio (LURR);
- Using Deepcom 6800, SGI Power Onyx350.

On the first of September this year, we conducted the LURR spatial scan of the Chinese Mainland on the DeepComp 6800 supercomputer, with radii of the scan space window of 100, 200, 300, and 400km respectively and the scan step of just 0.125°. After finishing the computation on the Deepcom 6800, SGI Power Onyx350 was used for visualization. Of all the abnormal areas in the results, the Yangjiang region in Guangdong Province was the most remarkable (see the Fig. 1). The results had been submitted to the Department of Monitor and Prediction and the Center for Analysis and Prediction of China Seismological Bureau，and were reported on the user conference of the Deepcom 6800 held on September 11 this year. Just six days later the Yangjiang region was hit by an earthquake. This emphasizes the need for timely results and ratifies the use of supercomputers.

Application Areas（ con.）

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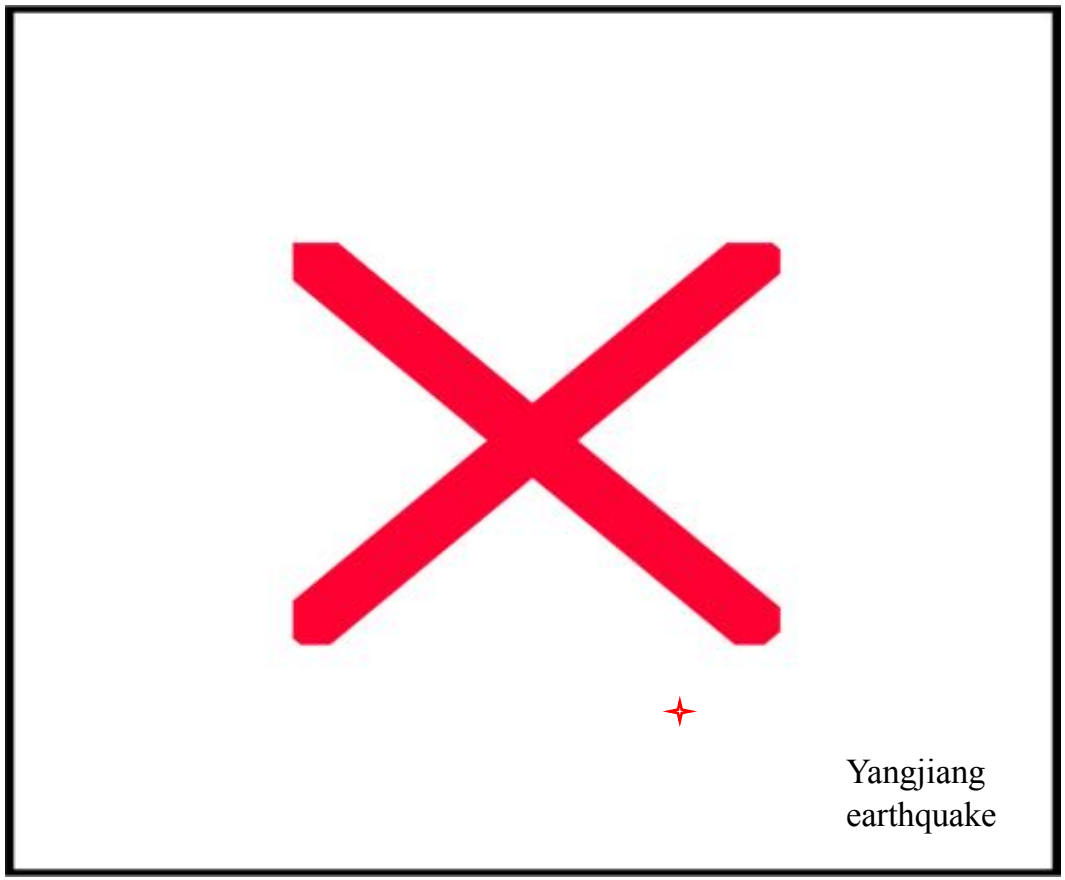

Fig.1 LURR special scan of the Chinese Mainland and the location of Yangjiang earthquake

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Will be a node of ACES_iSERVO Grid

ACES grew from discussion commencing in 1995 between scientists of USA,China,Japan and Australia.

ACES___APEC cooperation for Earthquake Simulation

APEC__the Asia Pacific Economic Cooperation,

iSERVO___international Solid Earth Research Virtual Observatory Institute

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- Be a main node of China National Grid
- Be the operation and support center of China National Grid

China National Grid

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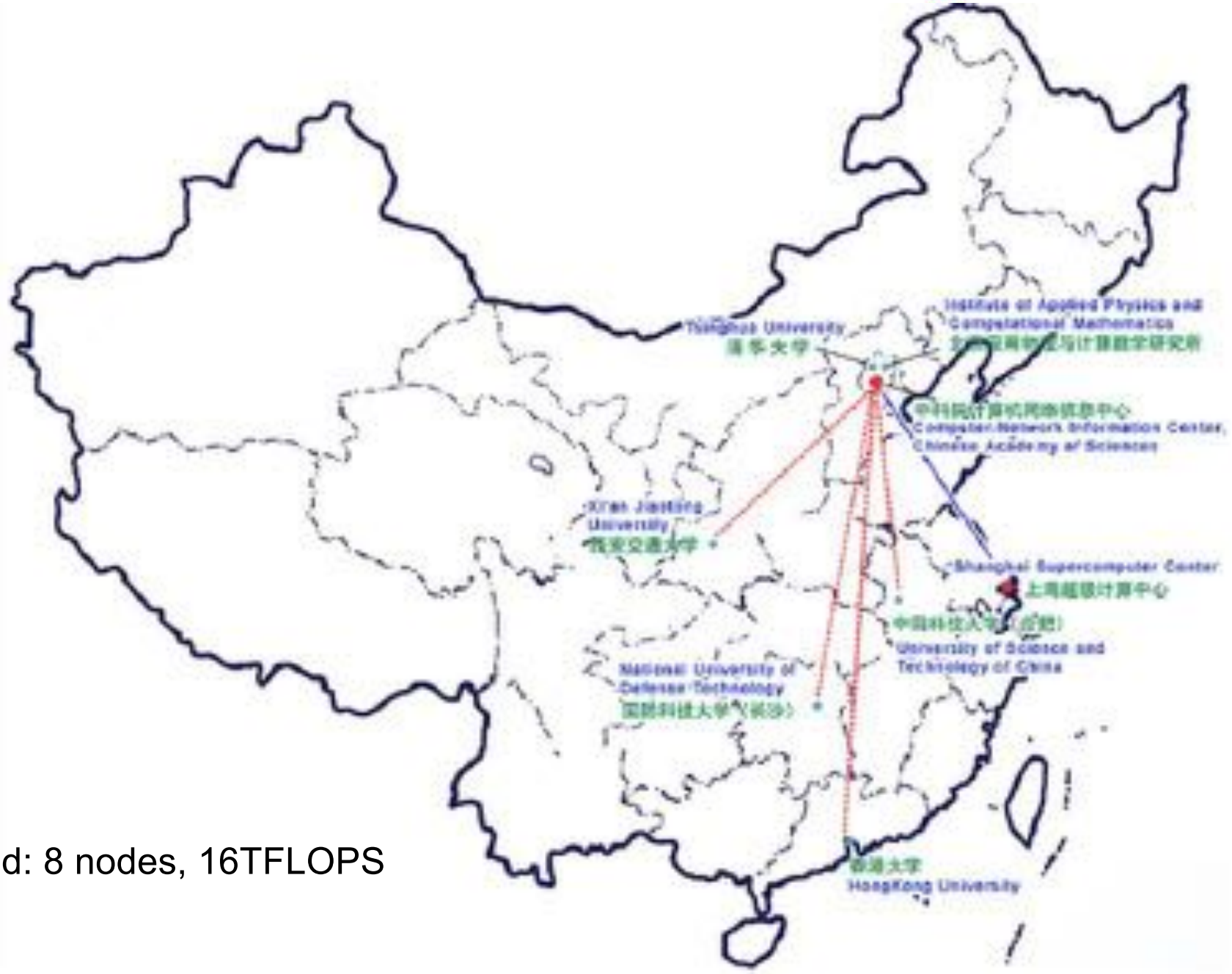

CNGrid: 8 nodes, 16TFLOPS

Conclusions

- World class supercomputer
- Various applications

- User friendly interface
- Grid computing service
- Research on seamless computing
- Computational science alliance

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Welcome you to visit our center and do cooperative research work

Thank you very much for your attention