Updates of China Activities on HPC

Zhong Jin¹, Xue-Bin Chi¹ and Yutong Lu²

¹Supercomputing Center, Computer Network Information Center, Chinese Academy of Sciences
²National University of Defense Technology
04/12/2012
Outline

• China’s Current Status
• Funding Agencies of HPC in China
• Research Plans of HPC in China
  □ NSFC
  □ MOST
• SCCAS
  □ CAS SCDI
  □ Applications
  □ SCE
  □ Co-Design in CAS
  □ Future plan
• NUDT
China’s Current Status
China’s Current Status

• Significant improvements in HPC and Grid
• Still far behind
  ➢ Kernel technologies
  ➢ Applications
  ➢ Multi-disciplinary research
  ➢ Professionals
• Sustainable development - crucial

* Refer to Professor Depei Qian’s report
Funding Agencies of HPC in China
Funding Agencies of HPC in China

- MOST – 863 Program, 973 Program (HW, SW & Apps)
- CAS – Informization Project (HW, SW & Apps)
- NSFC – General projects (Apps)
- Ministry’s funding (SW)
- Funding from local governments (HW)
Research Plans of HPC in China
NSFC

• Basic Algorithm and Computational Modeling for High Performance Scientific Computing
  ➢ Highly efficient algorithm for numerical calculation
  ➢ Computational modeling based on mechanism and data
  ➢ Evaluation on high performance computing and algorithm

• Duration: 2011～2015
• Budget: 40 Millions in RMB (2012)
• Projects: 25
NSFC (cont’)

- Research areas
  - Computing method for nonlinear eigenvalue problem of partial differential equation
  - Coupling model and algorithm for physical properties of materials
  - Computable modeling and algorithm of multi-media and multi-component fluid dynamics
  - New algorithm and verification of numerical simulation of transport
  - Reconstruction theory and algorithm of highly dimensional biological system based on small sample data and its application
  - Modeling and computing method of interactive dynamics between climate and vegetation
  - Modeling and basic algorithm of large scale complex optimizing design problem for aircraft
MOST – 863 Project

• High technology research and develop program (863 project, FY 2011~2015)
  ➢ Hardware
    ✓ two 100PF Level supercomputers by 2015
  ➢ Numerical Frame
    ✓ Structural mesh, non-structural mesh, non-mesh geometry and finite element method
    ✓ Scalable up to ~ 900,000 CPU/cores
    ✓ Parallel efficiency ~ 30%
    ✓ budget: 20 Million in RMB
Eight strategic applications

Software system will be developed and can be scaled up to 300,000 CPU/cores with the parallel efficiency of more than 30%.

Budget: ~80 Million in RMB

✓ Fusion
✓ Aircraft Design
✓ Aerocraft
✓ Drug Design
✓ Animation
✓ Mechanics of Giant Engineering Equipment
✓ Electromagnetic Environment Simulation
✓ New Type Material Design
MOST – 863 Project

- A key project on cloud computing
  - Key technologies and systems of cloud computing
    - Operating systems
    - Network search engines
    - Network based language translation

- Sustainable improvement - balanced development of high-productivity computers, application environment and HPC applications
MOST – 973 Project

• National Key Basic Research and Development Program (973 Project, FY2011~2015)

  ➢ New computing mode fit to petascale scientific computing
    ☐ Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences

  ☐ Goals
    ✓ Crucial common basic algorithm problem for petascale scientific computing
    ✓ Highly productive realizing method for parallel application software
    ✓ New computing mode for effectively using thousands and ten thousands CPU/cores
CAS SuperComputing Development Index, CAS SCDI

• Goal - Quantitatively evaluate the development of Supercomputing in CAS
• Six Components
  □ Individual Supercomputing Environmental Construction Index
  □ Individual Supercomputing Environmental Application Index
  □ Scientific Impact Index
  □ Individual Talents Training Index
  □ Individual Scientific Research Projects Support Index
  □ Individual Income Index
Applications

• Computational Material
• GPU-PEtot
• Eigenvalue Calculation on GPU
**Negative Index Meta-materials: Simulation and Shape Optimization**

Simulation - MoM + FGMRES for PMCHWT equations with Periodic FMM

Optimization - LM-BFGS, with Adjoint Variable Method

* Collaborating with Prof. Nishimura at Kyoto University, Japan
GPU-PEtot: DFT on GPU

**Testing systems:** 512 atoms GaAs bulk system with one As replaced by N.

13~22 times faster than CPU PEtot

<table>
<thead>
<tr>
<th>Number of Cores</th>
<th>16</th>
<th>32</th>
<th>64</th>
<th>128</th>
<th>256</th>
</tr>
</thead>
<tbody>
<tr>
<td>System</td>
<td>512-GaAs</td>
<td>512-GaAs</td>
<td>512-GaAs</td>
<td>512-GaAs</td>
<td>512-GaAs</td>
</tr>
<tr>
<td>PEtot (CPU)</td>
<td>735</td>
<td>396</td>
<td>221</td>
<td>128</td>
<td>91</td>
</tr>
<tr>
<td>PEtot GPU (GPU)</td>
<td>34.06</td>
<td>19.48</td>
<td>11.83</td>
<td>7.21</td>
<td>6.79</td>
</tr>
<tr>
<td>Speed-up (with PEtot CPU)</td>
<td>x22.11</td>
<td>x20.36</td>
<td>x18.69</td>
<td>x17.79</td>
<td>x13.52</td>
</tr>
<tr>
<td>Total flops (Tflops)</td>
<td>1.51</td>
<td>2.94</td>
<td>4.47</td>
<td>7.15</td>
<td>7.59</td>
</tr>
<tr>
<td>Efficiency</td>
<td>17.14%</td>
<td>16.69%</td>
<td>12.69%</td>
<td>10.15%</td>
<td>5.39%</td>
</tr>
</tbody>
</table>

The Scalability of CPU/GPU PEtot, AB-CG parts scalability

* Collaborating with Dr. Lin-Wang Wang, LBNL and Prof. Xingao Gong, Fudan Univ.*
**Eigenvalue Calculation on GPU**

- **Size of Matrix:** 20000

<table>
<thead>
<tr>
<th>GPU</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time/s</td>
<td>824.2</td>
<td>480.4</td>
<td>290.9</td>
<td>210.4</td>
<td>119.8</td>
</tr>
<tr>
<td>Speedup</td>
<td>1</td>
<td>1.72</td>
<td>2.83</td>
<td>3.9</td>
<td>6.9</td>
</tr>
</tbody>
</table>

- **Number of GPUs used:** 16

<table>
<thead>
<tr>
<th>Size of Matrix</th>
<th>20000</th>
<th>30000</th>
<th>50000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time/s</td>
<td>135.8</td>
<td>433.44</td>
<td>1388.33</td>
</tr>
<tr>
<td>Ratio/Gflops</td>
<td>274</td>
<td>290</td>
<td>419</td>
</tr>
</tbody>
</table>

*Dense matrix calculation*
SCE

- Overview
- Nodes
- Applications
- Users
- Jobs
Overview

• During the 11\textsuperscript{th} 5-year plan

• Extension of traditional computing grid
  \begin{itemize}
  \item multi-tree structure
  \item like a pyramid matrix
  \end{itemize}

• Grid nodes are not equal in functions
  \begin{itemize}
  \item root or master node dominate the whole system
  \item easy for operation and management in a special organization like CAS
  \end{itemize}
**SCE - Nodes**

- **Root:** 150 Tflops  
  - Deepcomp 7000
- **Middle:** 80 Tflops  
  - 8 nodes
- **Bottom:** 70 Tflops  
  - 17 institutes from CAS

- **GPU:** 3000 Tflops  
  - 11 institutes from CAS
Windows / Linux Clients

Users

Administrator

Web Portal

SCE Middleware

HPC, Cluster, Workstation, Storage
SCE– 83 Applications
Users

• Untill Mar. 2012
  – More then 200 grid users submitted jobs
Jobs

- Untill Mar. 2012
  - Number of Jobs > 120K
  - Walltime > 28M (CPU Hr.)
Co-Design in CAS

• Goal
  - Develop more efficient application software which is able to take advantage of the computing capability of faster supercomputers

• Candidate Applications
  - Electronic Structure Calculation
  - Molecular Dynamics
  - Climate
  - Fluid Dynamics
  - Bioinformatics
  - More
Co-Design in CAS (cont’)

• Key Algorithms
  - Adaptive mesh refinement
  - Sparse and dense linear algebra
  - PDEs: implicit
  - PDEs: explicit
  - FMM
  - FFT
  - ODE integrators
Co-Design in CAS (cont’)

• Co-Design Strategy

- Hardware Evaluation
- Performance Analysis
- Programming Model
- Mathematics
Co-Design in CAS (cont’)

• Co-Design Process

1. Application Community Identifies Needs
2. Identify Gap
3. Programming
4. Integration, Deployment

Feedback and Refining Design
• International Workshop on CO-DESIGN
  ➢ 2011.10.25-26, Beijing
  ➢ 60 participants, 24 invited talks
Future Plan

• Informization Project on HPC (12\textsuperscript{th} Five-year plan)
  ➢ A several Petaflops supercomputer
  ➢ Chinese Scientific Computing Environment
  ➢ Budget: \(~200\) million in RMB

• Application Software Development Center
  ➢ Goal - to improve computational efficiency in scientific computing and develop software systems
  ➢ Disciplines
    • Mathematics, Chemistry, Material Science, Climate, Fluid Dynamics, Bioinformatics, Drug Design, Geophysics and Astrophysics
Sunway Bluelight

- National Supercomputing Center in Jinan, China
- Ranked 14th on TOP500 (November, 2011)
  - 1PF peak
  - Power: 1074.00 kW
  - Cores: 137200
  - Memory: 139264 GB
  - Very compact system
    - 128TF/Rack
  - Implemented with domestic 16-core processors
  - Infiniband QDR 40Gbps
  - Exploring possible architectures and key technologies for 10-Petascale computers
NUDT’s Activities

• By Professor Yutong Lu