Updates of China Activities on HPC

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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 trasport
  - 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

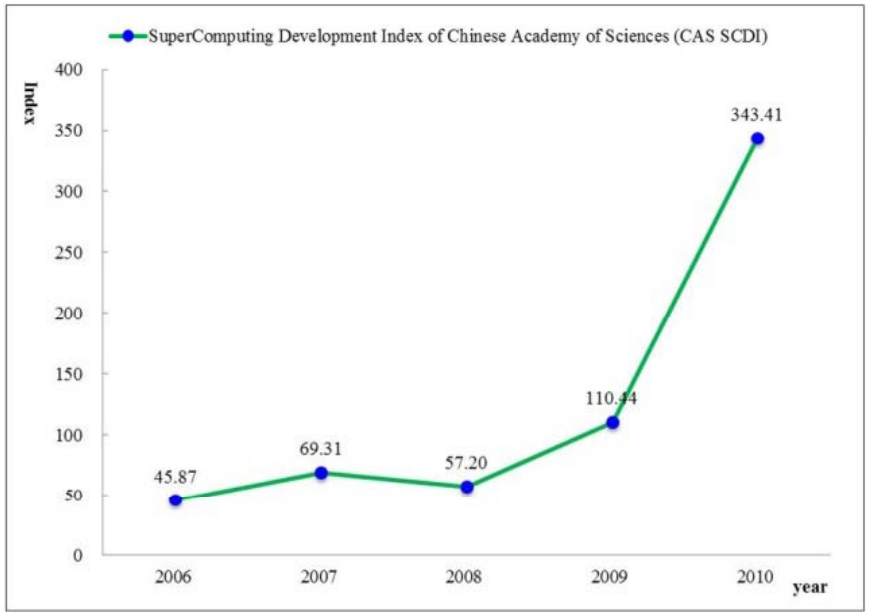
MOST – 973 Project

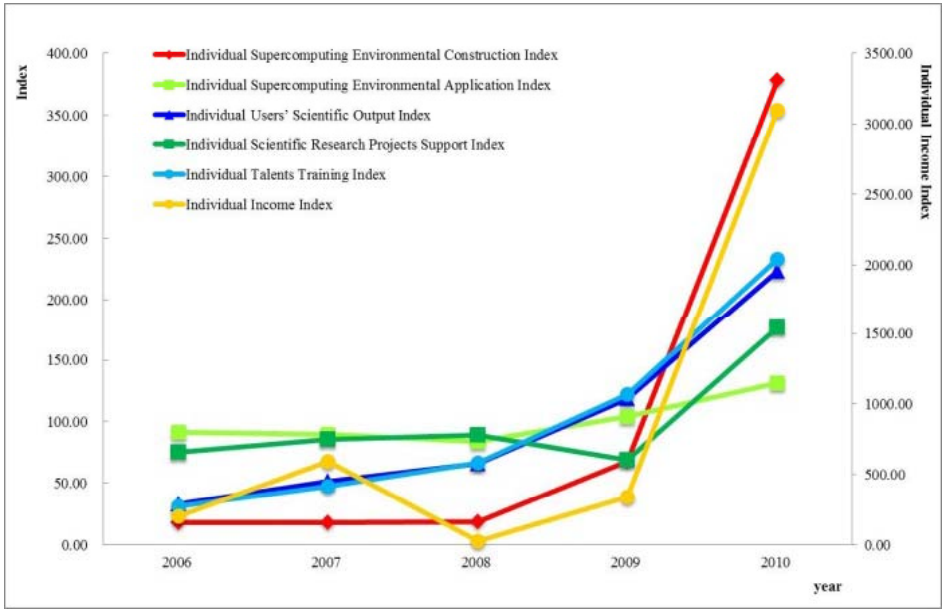
- National Key Basic Research and Development Program (973 Project, FY2011~2015)
  - New computing mode fit to petascale scientific computing
    - Institute of Computational Mathematics and Scientific /Engineering Computing, Chinese Academy of Sciences
    - Goals
      - ✓ Crucial common basic algorithm 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

SCCAS

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

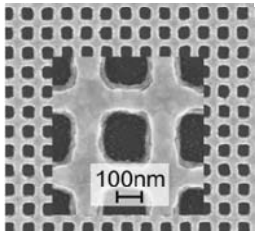




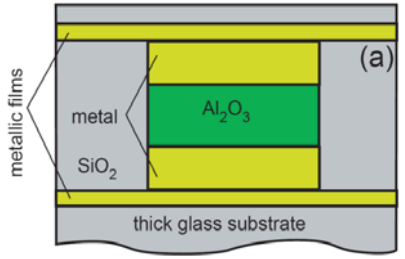
Applications

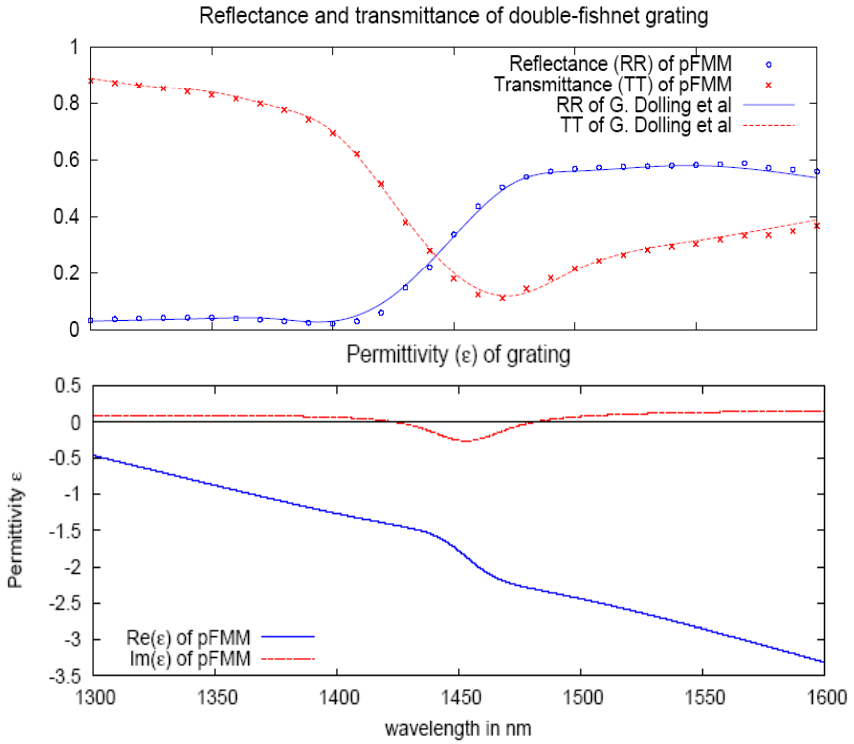
- Computational Material
- GPU-PEtot
- Eigenvalue Calculation on GPU

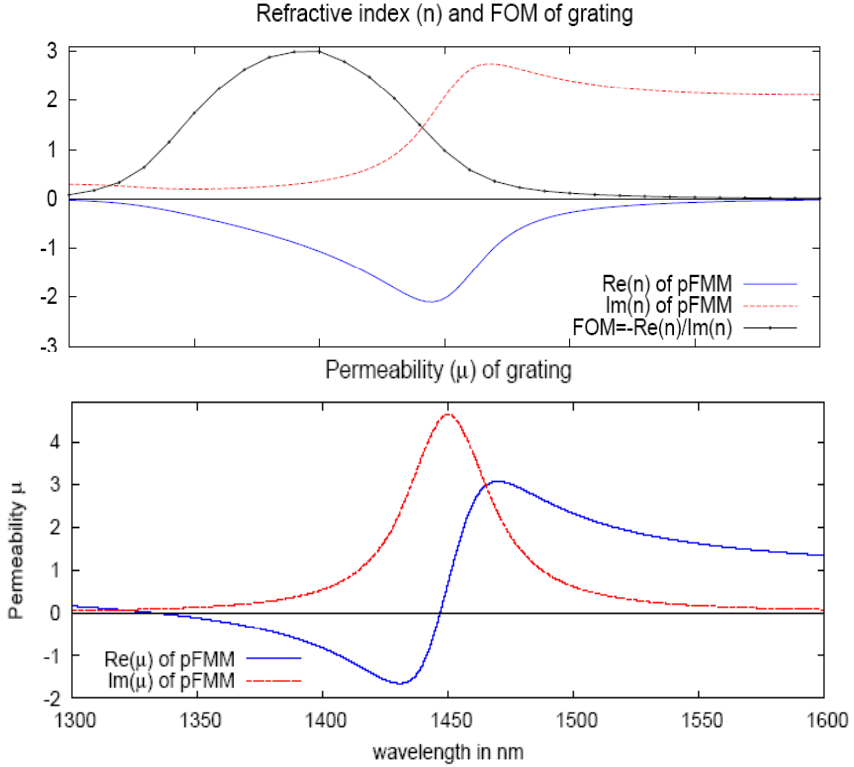
Negative Index Meta-materials: Simulation and Shape Optimization



Negative index material







Simulation - MoM + FGMRES for PMCHWT equations with Periodic FMM

Optimization - LM-BFGS,with Adjoint Variable Method

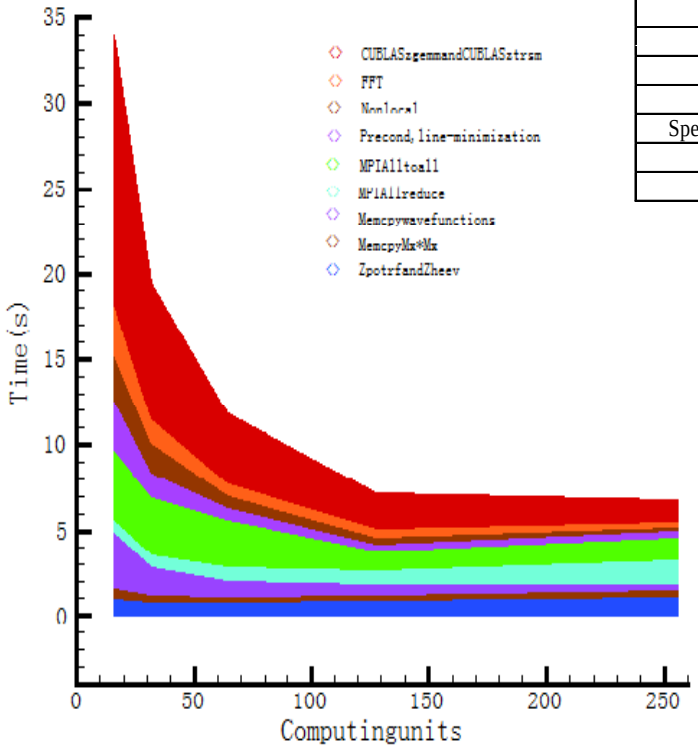
* Collaborating with Prof. Nishimura at Kyoto University, Japan

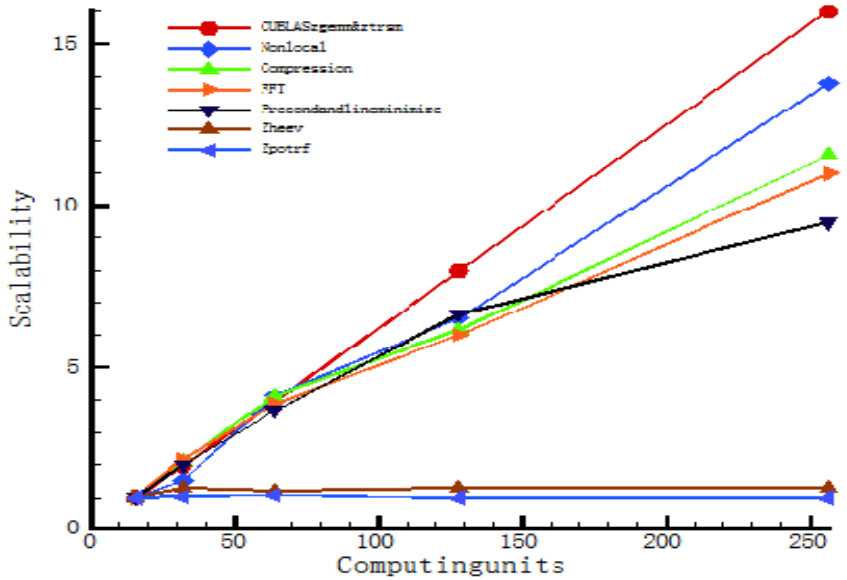
GPU-PEtot: DFT on GPU

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

13~22 times faster than CPU PEtot

Number of Cores	16	32	64	128	256
System	512-GaAs	512-GaAs	512-GaAs	512-GaAs	512-GaAs
PEtot (CPU)	735	396	221	128	91.8
PEtot_GPU0(GPU)	87.3	55.9	33.3	23.4	19.8
PEtot_GPU (GPU)	34.06	19.48	11.83	7.21	6.79
Speed-up (with PEtot CPU)	x22.11	x20.36	x18.69	x17.79	x13.52
Total flops (Tflops)	1.51	2.94	4.47	7.15	7.59
Efficiency	17.14%	16.69%	12.69%	10.15%	5.39%





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

GPU	1	2	4	8	16
Time/s	824.2	480.4	290.9	210.4	119.8
Speedup	1	1.72	2.83	3.9	6.9

- Number of GPUs used: 16

Size of Matrix	20000	30000	50000
Time/s	135.8	433.44	1388.33
Ratio/Gflops	274	290	419

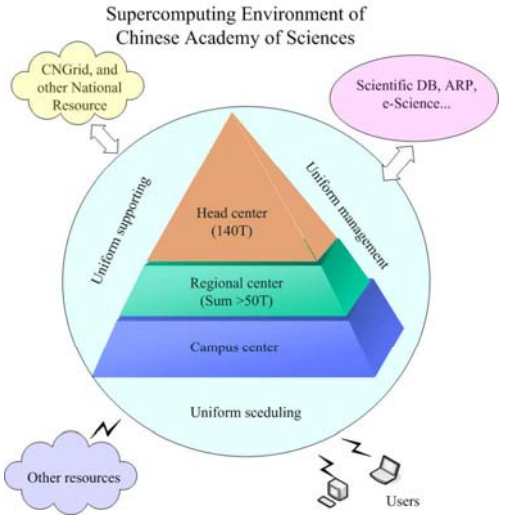
*Dense matrix calculation

SCE

- Overview
- Nodes
- Applications
- Users
- Jobs

Overview

- During the 11th 5-year plan

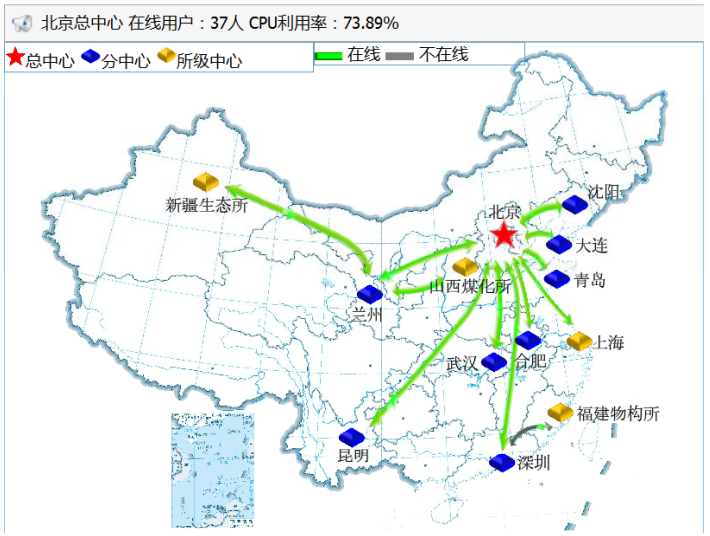


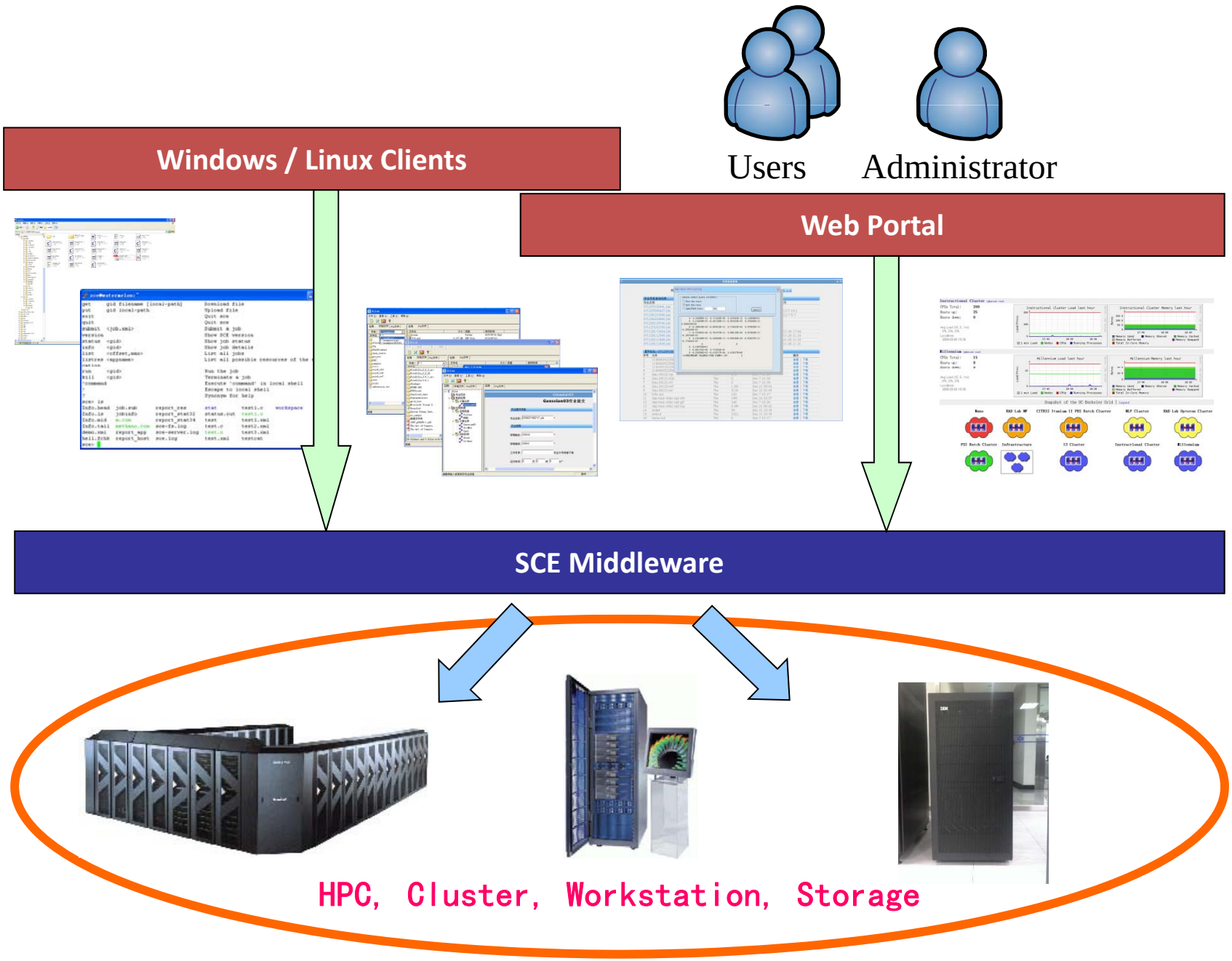
- Extension of traditional computing grid
  - ➢ multi-tree structure
  - ➢ like a pyramid matrix

- Grid nodes are not equal in functions
  - – root or master node dominate the whole system
  - – easy for operation and management in a special organization like CAS

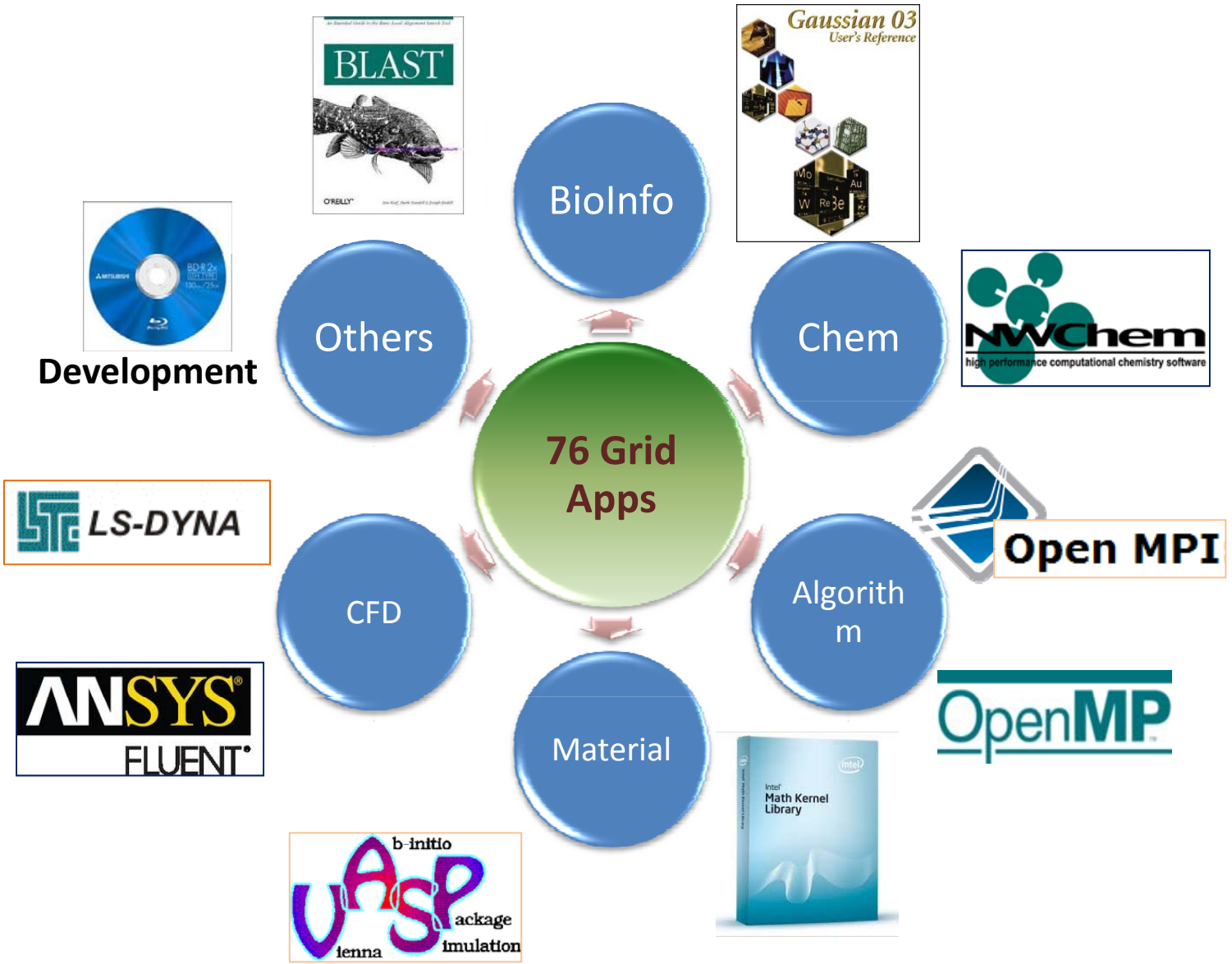
SCE –Nodes

- Root: 150Tflops
  - Deepcomp 7000
- Middle: 80Tflops
  - 8 nodes
- Bottom: 70Tflops
  - 17 institutes from CAS
- GPU: 3000 Tflops
  - 11 institutes from CAS



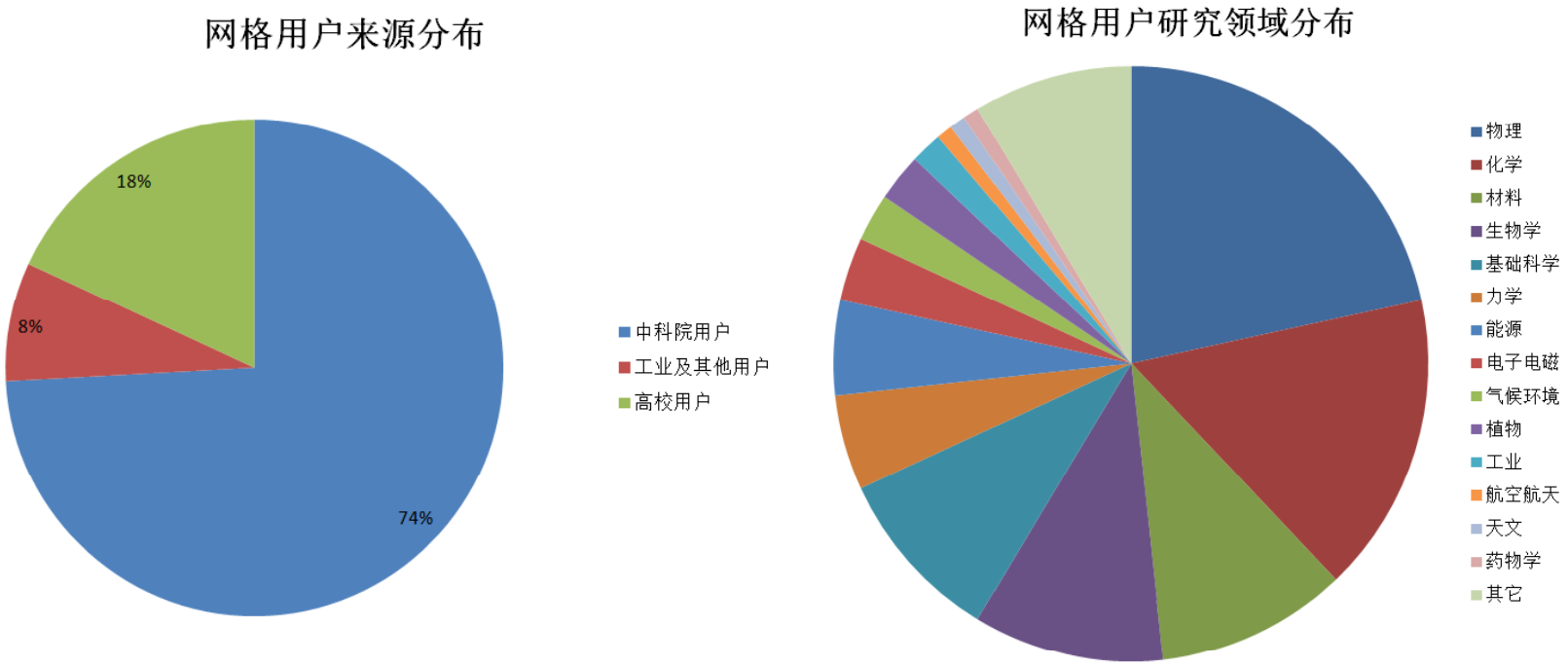

Windows / Linux Clients
Users
Administrator
Web Portal
SCE Middleware
HPC, Cluster, Workstation, Storage

SCE– 83 Applications



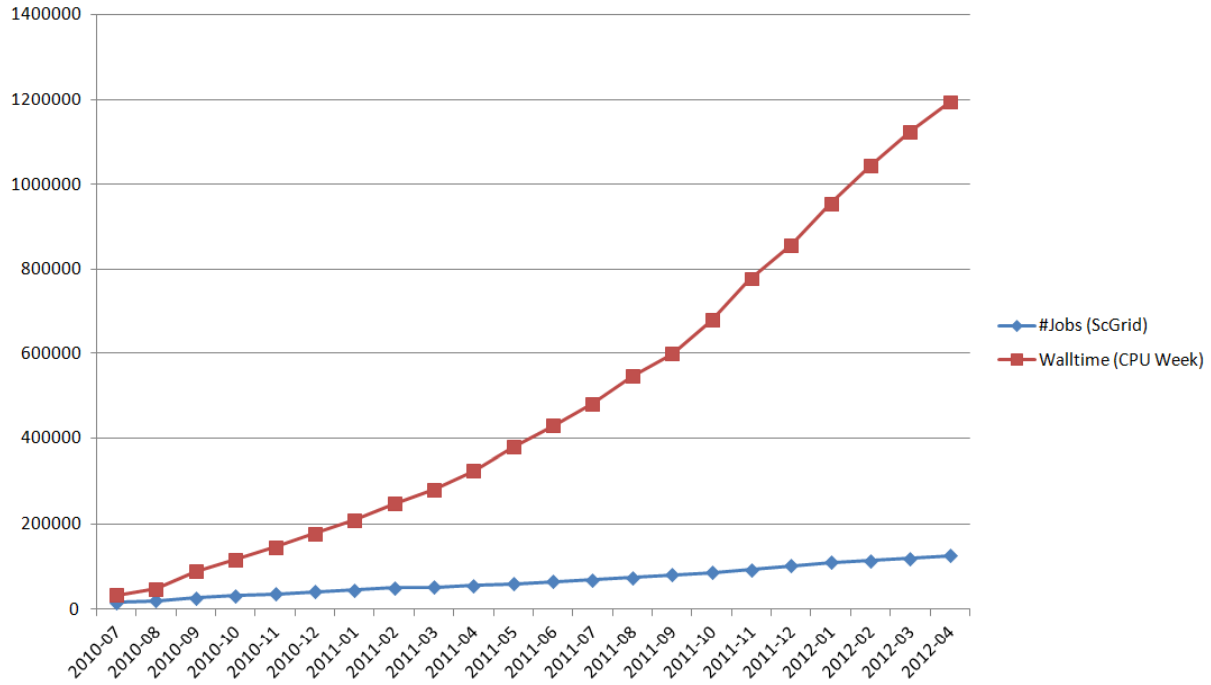
Users

- 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

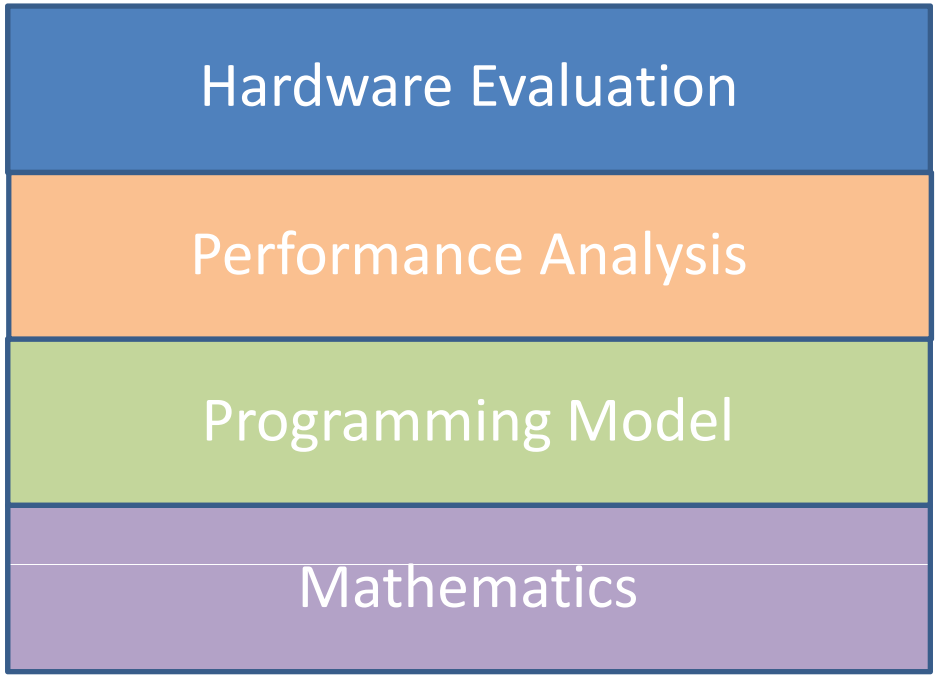
- Goal
  - Develop more efficient application software which is able to take advantage of the computing capability of faster supercomputers
- Candidate Applications
  - Electronic Structure Calculation
  - Molecular Dynamics
  - Climate
  - Fluid Dynamics
  - Bioinformatics
  - More

Co-Design in CAS (cont')

- Key Algorihms
  - Adaptive mesh refinement
  - Sparse and dense linear algebra
  - PDEs: implicit
  - PDEs: explicit
  - FMM
  - FFT
  - ODE integrators

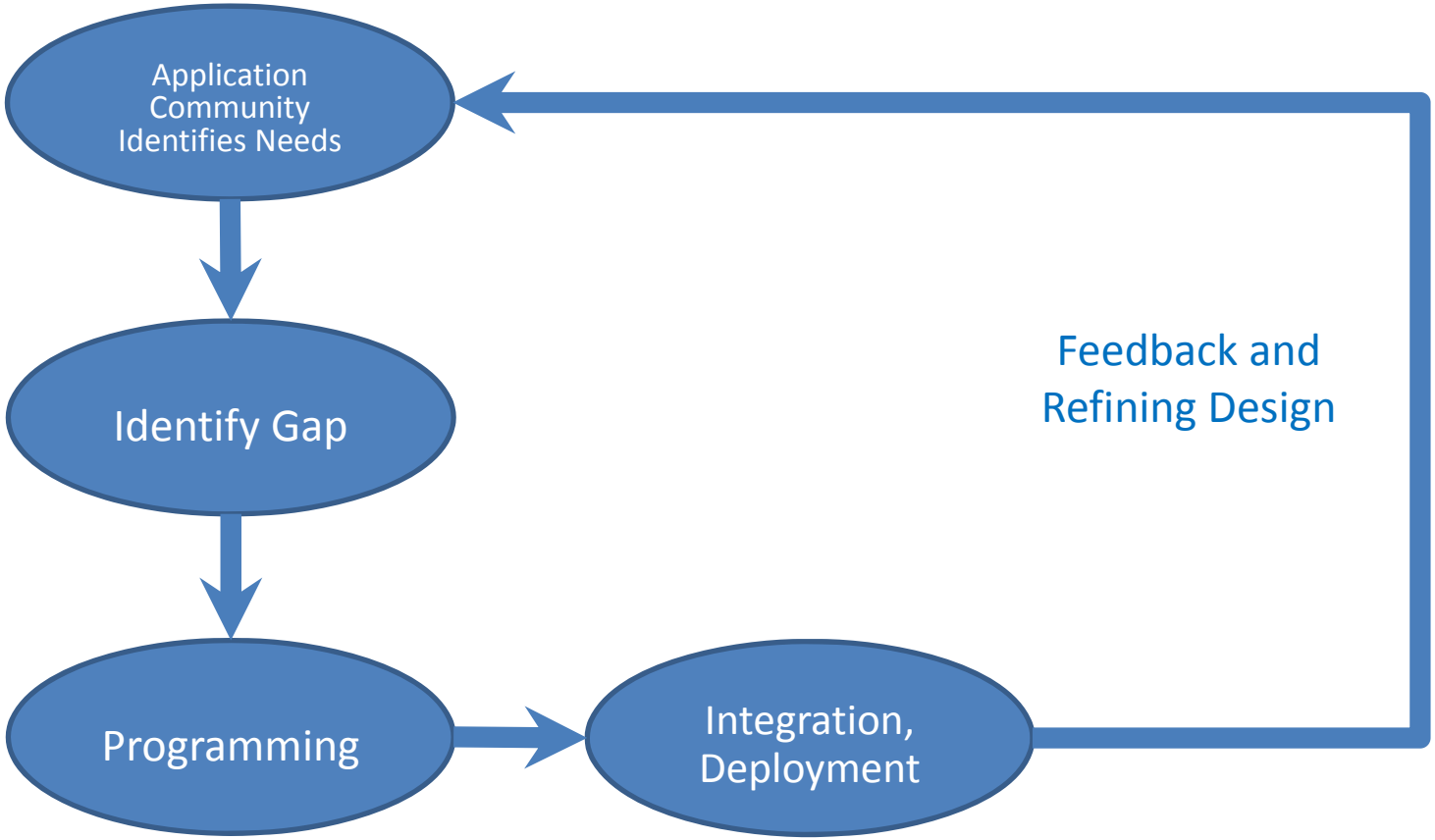
Co-Design in CAS (cont')

- Co-Design Strategy



Co-Design in CAS (cont')

- Co-Design Process



- International Workshopp on CO-DESIGN
  - 2011.10.25-26, Beijing
  - 60 participants, 24 invited talks

International Workshop on CO-DESIGN

CO-DESIGN:
COllaborative **DE**velopment of **SI**mulation
software of next **Ge**N**e**ration

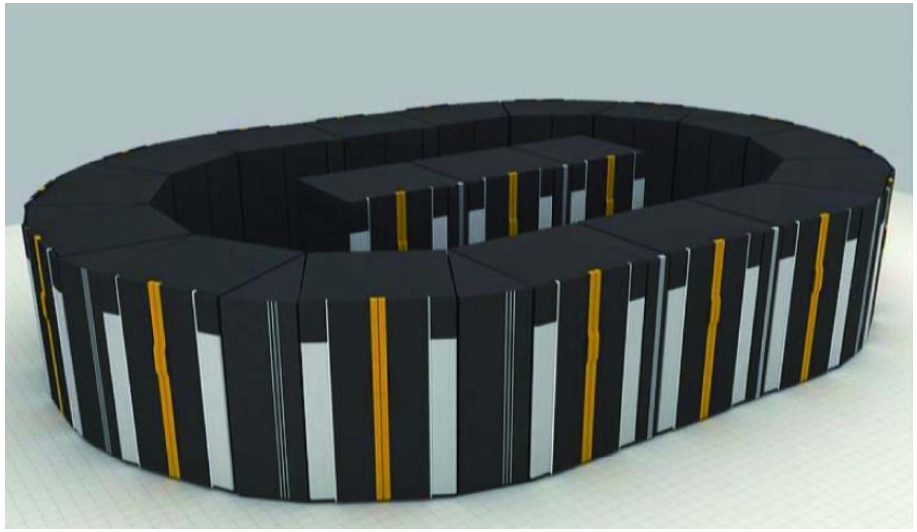
October 25-26, 2011
Institute of Computing Technology,
Chinese Academy of Sciences,Beijin

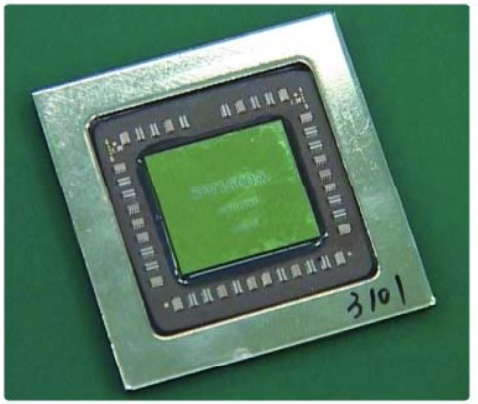
Future Plan

- Informization Project on HPC (12th 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**





国产 “申威”16核CPU

NUDT's Activities

- By Professor Yutong Lu