U.S. Department of Energy's
Office of Science

Program Area Presentation

Computer Science

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Computer Science Research

- Challenge – HPC for Science is (*still after fifteen years!*)
  - Hard to use
  - Inefficient
  - Fragile
  - An unimportant vendor market
- Vision
  - A comprehensive, integrated software environment which enables the effective application of high performance systems to critical DOE problems
- Goal– Radical Improvement in
  - Application Performance
  - Ease of Use
  - Time to Solution

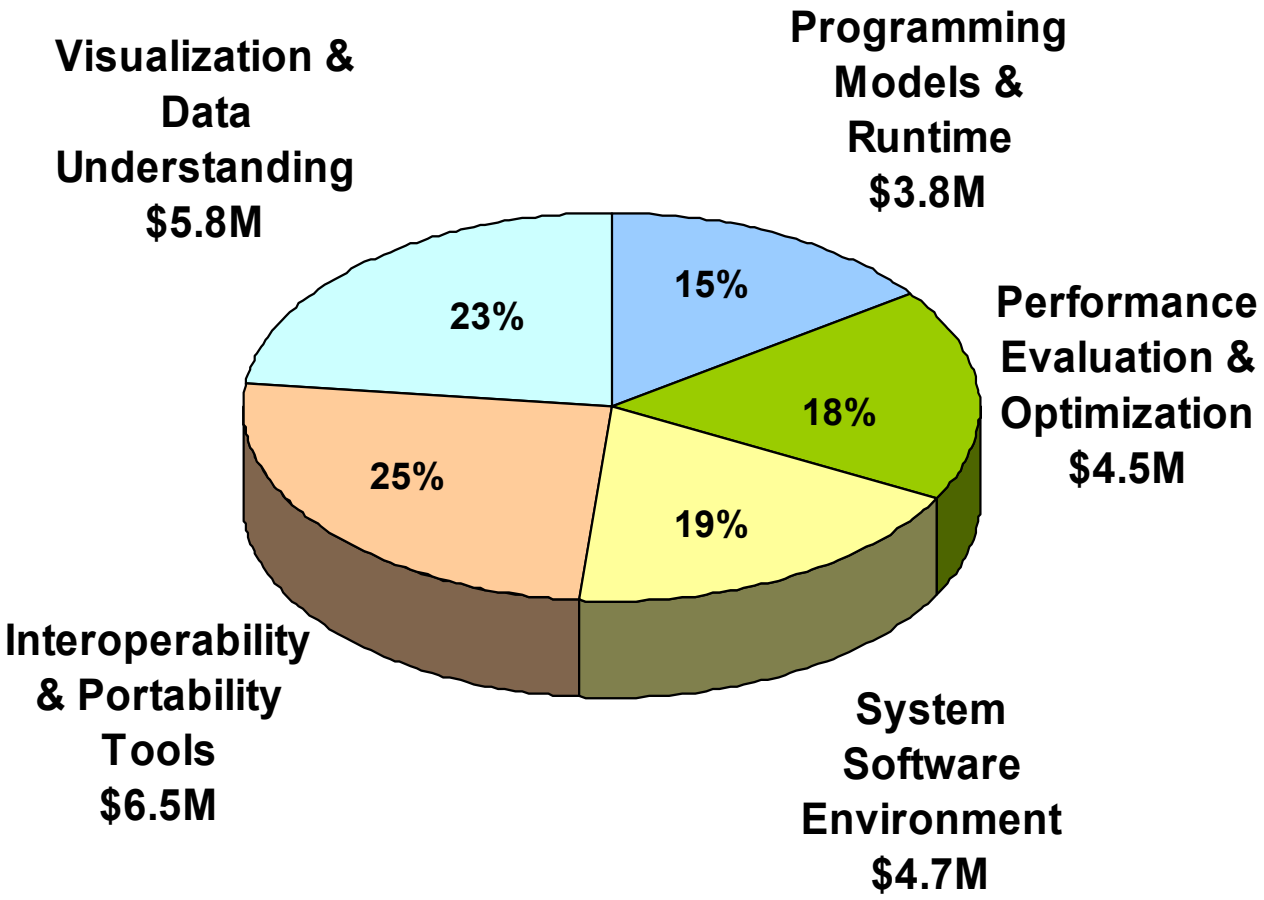
System Admin	Software Development	Scientific Applications
Res. Mgt	Framewrks	PSEs
Scheduler	Compilers	Viz/Data
Chkpt/Rstrt	Debuggers	Math Libs
File Sys	Perf Tools	Runtme
User Space Runtime Support		
OS Kernel		OS Bypass
Node and System Hardware Arch		

HPC System Elements

Program Components

- **Base Program**
  - Evolutionary and revolutionary software methodologies for future generations of HPC architectures
- **SciDAC Integrated Software Infrastructure Centers**
  - Enable effective application of current terascale architectures to SciDAC applications through focused research and partnerships

Computer Science Technical Elements



Some Major Accomplishments

- PVM – the first widely successful model for parallel computing
- MPI – the lingua franca of today's parallel computing
- MPICH – the open source version of MPI that is the basis for all vendor adaptations
- Global Arrays – the distributed shared memory programming model that is at the core of NWChem, the motivating application for SciDAC
- CTSS – the first interactive operating system for high performance computers
- SUNMOS/Puma/Cougar – the most successful high performance parallel operating system
- OSCAR – a partnership with industry, the most widely used open source toolkit for management of Linux clusters

Computer Science

Contribution of Program Element to Overall ASCR Strategic Goal

- **Research, Development, Testing, Evaluation of high performance software infrastructure to support the effective use of HPC systems for scientific applications**

Program Element Name

Planning horizon for Program Element

- **SciDAC ISIC's – 5 years**
- **Base Program – 5 – 10 years ++**

Program Element Name

Areas of research Program Element currently invests in

- **Total Program: $28M, About 20% each in:**
- **Interoperability/Portability Tools**
  - **Parallel component technology**
  - **CCA ISIC**
- **Performance Evaluation and Optimization**
  - **PERC ISIC**
  - **Benchmarking, performance modeling and prediction**
- **Systems Software Environment**
  - **Scalable Systems Software ISIC**
  - **Cougar LWK**
  - **Science Appliance SSI cluster**
  - **OS research framework (FY04)**
- **Programming Models/Runtime**
  - **Programming Models Center -- CoArray Fortran, common runtime (UPC, Global Arrays, MPI, …)**
- **Visualization/Data Understanding**

Program Element Name

How does Program Element transfer knowledge or provide services to application scientists?

- **Base program:**
  - Publications, PI meetings, laboratory staff interactions, conferences, publications, invited talks, program reviews, workshops, ACTS/NERSC user training and support

ISIC's:

Joint application/CS SciDAC PI meetings

Poster Sessions

Active outreach to applications

Program management emphasis on application progress as metric

Program Element Name

Program Element Strengths

- **Particular leadership in:**
  - Performance modeling, evaluation and optimization
  - Parallel programming models, esp MPI and Global Arrays
  - Parallel operating system environments
  - High Performance component architecture
- **Unique Capabilities**
  - Large, coordinated research activities
  - Software testbed
  - Comprehensive character of research, with HPC focus
  - Strength of laboratory and academic participants
- **Ongoing Partnerships**
  - DARPA – HPCS review team
  - DOD – Performance tools
  - NNSA – Open source support, reviews, planning
  - NSA – UPC, benchmark, programming model projects
  - HECRTF

Program Element Name

Program Area Weaknesses/Challenges

- Testbeds
- Community building (no SIAM for high-end CS)
- Application community interest
- Technology transfer to application community
- Technology development timeframe

Program Element Name

Program Element Opportunities

- Petaflop parallel OS
- Intelligent Development Environments
- Parallel Languages/compiler/runtime
- Application specific problem solving environments

From the HECRTF Report

- Operating systems (OSs)
- Languages, compilers, and libraries
- Software tools and development environments
- Algorithms
- Programming Models

Program Element Name

Program Element Threats

- Complexity
- Architecture diversity
  - Memory wall, end of Moore's law
- Long-term software evolution and support
- Intellectual Property/Open Source
- Loss of Focus/user trust

Program Element Name

Program Element Gap Analysis

- Petascale systems by 2010 (100,000 + processors)
- Serious architecture diversity – X1, Red Storm, BG/L, DARPA HPC systems
- Reliability/fault management