DoD High Performance Computing
Science and Engineering Applications

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Overview

- DoD High Performance Computing Modernization Program (HPCMP)
- DoD science and engineering applications
  - Use of modeling and simulation for aircraft certification
- HPCMP benchmarking for acquisitions
  - Overall acquisition process
  - Validated vendor benchmarking results
  - Uncertainty analysis in performance and price/performance scoring of offered systems
HPC Modernization Program

Mission
Accelerate development and transition of advanced defense technologies into superior warfighting capabilities by exploiting and strengthening US leadership in supercomputing, communications, and computational modeling.

Vision
A pervasive culture existing among DoD’s scientists and engineers where they routinely use advanced computational environments to solve the most demanding problems.

Tools for Discovery
HPC Modernization Program Goals

- Acquire, deploy, operate and maintain best-value supercomputers
- Acquire, develop, deploy and support software applications and computational work environments that enable critical DoD research, development and test challenges to be analyzed and solved
- Acquire, deploy, operate and maintain a communications network that enables effective access to supercomputers and to distributed S&T/T&I computing environments
- Continuously educate the RDT&E workforce with the knowledge needed to employ computational modeling effectively and efficiently
- Promote collaborative relationships among the DoD computational science community, the national computational science community and minority serving institutes
DoD HPC Modernization Program

HPC Centers

- Supercomputers
- High-Speed Networks
- Mass Storage
- Data Exploration
- Customer Assistance

Army HPCMP Resources
- ARL & ERDC MSRCs
- AHPCRC & SMDC ADCs
- 1,141 Users/25 Locations/87 Projects
- 52 DREN Sites
- 12 Challenge Projects/2 DHPIs
- 3 Institutes/1 Portfolio

Navy HPCMP Resources
- NAVO MSRC
- 1,040 Users/25 Locations/205 Projects
- 32 DREN Sites
- 13 Challenge Projects/4 DHPIs
- 1 Institute/2 Portfolios

Air Force HPCMP Resources
- ASC MSRC
- MHPCC ADC
- 1,199 Users/36 Locations/189 Projects
- 20 DREN Sites
- 16 Challenge Projects/1 DHPI
- 2 Institutes/1 Portfolio

Software Applications Support

- HSALs/Portfolios
- Education & Outreach

Resource Management

- Requirements & Allocations

Networking

Defense Research & Engineering Network

- DARPA, DTRA, JNIP, JFCOM, MDA, & OTE
- 401 Users/4 Locations/12 Projects
- 34 DREN Sites
- 2 Challenge Projects/2 DHPIs

Defense Agencies

Other

- ARSC ADC
- 1 DHPI

1/10/2007
HPCMP Serves a Large, Diverse DoD User Community

- 577 projects and 4,234 users at approximately 130 sites
- Requirements categorized in 10 Computational Technology Areas (CTA)
- FY2007 non-real-time requirements of 678.5 Habu-equivalents*

*One habu-equivalent year (Habu-yr) is the amount of computational power represented by a one habu system computing for one year. A one habu system has a capability, as defined by the program’s set of application benchmarks, of a 1,024 375 Mhz processor IBM SP P3.

Forces Modeling & Simulation – 235 Users
Integrated Modeling & Test Environments – 152 Users

Environmental Quality Modeling & Simulation – 128 Users
Computational Structural Mechanics – 440 Users
Computational Electromagnetics & Acoustics – 310 Users
Computational Fluid Dynamics – 1,664 Users
Computational Chemistry, Biology & Materials Science – 387 Users
Climate/Weather/Ocean Modeling & Simulation – 266 Users
Electronics, Networking, and Systems/C4I – 115 Users
Signal/Image Processing – 377 Users

160 users are self characterized as “Other”

Source: Portal to the Information Environment - April 9, 2007
**DoD HPCMP Application Software Requirements for FY 2007**

<table>
<thead>
<tr>
<th>Application</th>
<th>Type</th>
<th>Type</th>
<th>Total CPU Hours</th>
<th>Percentage of Total Requirement</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTH</td>
<td>Shock Physics</td>
<td>CSM</td>
<td>93,840,501</td>
<td>12.8%</td>
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<tr>
<td>HYCOM</td>
<td>Ocean Modeling</td>
<td>CWO</td>
<td>89,005,100</td>
<td>12.1%</td>
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<td>GAUSSIAN</td>
<td>Quantum Chemistry</td>
<td>CCM</td>
<td>49,455,900</td>
<td>6.7%</td>
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<tr>
<td>ALLEGRA</td>
<td>Shock Physics</td>
<td>CSM</td>
<td>32,815,000</td>
<td>4.5%</td>
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<tr>
<td>ICEPIC</td>
<td>Particle-in-Cell Simulation</td>
<td>CEA</td>
<td>26,500,000</td>
<td>3.6%</td>
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<tr>
<td>XPATCH</td>
<td>Radar Cross-section Simulation</td>
<td>CEA</td>
<td>23,469,500</td>
<td>3.2%</td>
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<tr>
<td>CAML</td>
<td>Fluid Dynamics</td>
<td>CFD</td>
<td>21,000,000</td>
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<tr>
<td>MOM</td>
<td>Electromagnetics</td>
<td>CEA</td>
<td>18,540,000</td>
<td>2.5%</td>
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<tr>
<td>VASP</td>
<td>Materials Simulation</td>
<td>CCM</td>
<td>18,435,000</td>
<td>2.5%</td>
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<tr>
<td>ANSYS</td>
<td>Structural Mechanics</td>
<td>CSM</td>
<td>17,923,580</td>
<td>2.4%</td>
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</tbody>
</table>
CREATE: Computational Research and Engineering
Acquisition Tools and Environments

- CREATE Goal: Enable acquisition programs to rapidly develop more fully optimized and integrated designs with fewer flaws and better performance.

- CREATE will develop and deploy three computational engineering tool sets for acquisition program engineers to exploit the exponential growth in supercomputer power:
  - Aircraft tools (Aerodynamics & Structures)
  - Ship tools (Hydrodynamics & Structures)
  - Antenna Integration tools (Electromagnetics)

- Quadrennial Defense Review and Congress call for an agile and effective acquisition process with reduced costs and schedule

- CREATE will:
  - Enable rapid assessment of design options to improve acquisition flexibility and agility and reduce schedules
  - Enable engineers to identify design defects and fix them early before major funding and schedule commitments
  - Enable early integration of major subsystems further reducing schedule, costs and risks

- CREATE is a 12 year program, (~ $35M/year including matching contributions of ~ 30% from the Services), that is endorsed by DoD S&T, T&E and acquisition programs and by DoD contractors
DoD Challenge Projects

The HPCMP recognizes and supports high priority computational work conducted within the DoD that may be done at its shared resource centers through its implementation of Challenge Projects. These projects represent the DoD’s highest-priority, highest-impact, computational work, both from technical and mission-relevance standpoints. The modeling and simulations conducted in these projects account for 30–35% of the allocation of resources at the HPC centers.

- Projects will lay the groundwork within the science and technology program for future weapons systems.
- Projects are headed by senior scientists and engineers within DoD science and technology and test and evaluation organizations, universities, and industry research partners.
- Projects use multiple hardware platforms and, in many cases, multiple HPC centers.
Increase the accuracy of fatigue life predictions across the DoD fixed wing fleet by developing new stress intensity factor solutions (K). New solutions are transitioned to the user via the USAF’s crack growth code, AFGROW.

Areas of Interest:
- Fatigue Critical Locations: CW 1, CW 5C, CW 7B, CW 9, CW 14, CW 17
- Corrosion Indications: SAIC beam cap corrosion inspections
- Crack Indications: SAIC FWD lower beam cap and all rainbow fitting inspections for cracks
Design of Energetic Ionic Liquids

Benefits to the warfighter include cost-effective and reliable access to space, control and exploitation of space by development of more robust propulsion technologies, and mitigation of environmental and biological hazards.

J. Boatz, AFRL/PR, Edwards AFB, CA; M. Gordon, Iowa State University, Iowa City, IA; S. Hammes-Schiffer, Penn State University, University Park, PA, OH; R. Pachter, AFRL/ML, WPAFB, OH; and G. Voth, University of Utah, Salt Lake City, UT; Sponsor: Air Force
This research will provide both a qualitative and quantitative understanding of complex, three-dimensional interactional aerodynamic problems and facilitate more timely and cost-effective modification and development of current and future combat systems.

Wake visualization of HART II rotor with blade-vortex interaction. Predicted ground plane acoustic sound pressure levels.

UH-60A rotor-hub-fuselage interaction. CFD/CSD coupled solution.

M. Potsdam and J. Lim, AMRDEC, Moffett Field, CA
Sponsor: Army

An FY 2007 DoD Challenge Project

1/11/2007
High fidelity signature modeling capability in all the relevant RF bands will provide the Army with the ability to trial through simulation proposed vehicle designs and modify those designs appropriately to degrade enemy detection and terminal targeting.

A. Sullivan, W. Coburn, C. Kenyon, and C. Lee, ARL, Adelphi, MD; Sponsor: Army
Explosive Structure Interaction Effects in Urban Terrain

Provide the DoD community with an improved methodology predicting in-structure airblast and the external airblast propagated in the urban terrain while operating weapons or performing demolition operations in the complex urban terrain.

J. Baylot, J. Windham, T. Bevins, J. O’Daniel, B. Armstrong, D. Rickman, S. Akers, and D. Cargile, ERDC, Vicksburg, MS; P. Papados, ERDC, Alexandria, VA; Y. Sohn and S. Lee, DTRA, Alexandria, VA; D. Littlefield, University of Texas, Austin, TX; R. Weed, Mississippi State University, Vicksburg, MS; G. Bessette, Sandia National Laboratory, Albuquerque, NM; and M. Schmidt, AFRL, Eglin AFB, FL; Sponsor: Army

Blast environment from embedded detonation

Pressure

MAX

MIN

Reinforced Concrete Slab

Interior surfaces of reaction structure & reaction mass

Time = 0.00150
This research will allow the US Navy to routinely produce timely, probabilistic forecasts of the atmosphere-ocean environment, and to provide insight into the predictability of high-impact phenomena in the battlespace environment.


Ensemble track forecasts of Hurricane Charley from 10 August 2004, color, and observed track, black with hurricane symbols. The ensemble that included stochastic perturbations representing model error (right) captured the possibility of the observed recurvature onto the Florida peninsula (right). The control ensemble based on perturbations to the initial state only (left) did not contain this scenario.
This project increases combat capability for the current fleet of tactical and strategic aircraft with associated weapon systems, providing time-critical support for engineering analyses used to optimize the application of ground and flight testing, and reducing risk and lowering cost of fielding new weapons.
Air Force SEEK EAGLE

- **USAF Aircraft-Store Certification Program**
  - Store loading procedures
  - Carriage loads*
  - Store separation*
  - Flutter
  - Ballistic accuracy
  - Stability & control*
  - Safe escape

- **Stores Include**
  - Munitions, fuel tanks
  - Suspension equipment
  - Pods for navigating, sensing, targeting

- **CFD Supports * Items Above Plus**
  - Miscellaneous aerodynamic analysis, flow visualization
  - Supplements wind tunnel (not physically constrained), test analogy assumptions, reduce flight test
AFSEO CFD Challenges

- Large number of grid points – 15-60 million
  - Full or symmetric aircraft
  - Pylons, launchers, etc. – level of detail
  - Store grid

- Complicated flow physics – transonic, high $\alpha$ cases
  - Compressibility, interference, shear/boundary layer effects
  - Viscous, flow separation, choked flow, shock waves
  - Multi-body motion, autopilot control, parachutes

- Rapid response – typically 2-6 weeks
  - Time-critical support of flight test
  - Quick turn-around for external customers (warfighter)
AFSEO CFD Project Summary

FY01
- F-16/MA-31
- F-16/Mk-82 fin crack
- F-15/GBU-27
- F-16/JASSM

FY02
- F-111/SSB
- F-16/CBU89/JSOW
- F-16/PPB
- B-52G/JASSM
- F-15E/SLV
- JDAM FZU Sim

FY03
- F-15E/JDAM
- F-15E/SATIRS
- F-16/SNIPER
- F-15E/SNIPER
- F-15E/LITENING
- F-16/BRU/CBU89
- B-52H/X-37
- F-15E WT Support
- GBU Aero Data
- F-16/ARGUS
- F-16/MALD
- F-15E/WCMD

FY04
- B-52H/Mailbox
- Predator/GBU-12
- Predator unsteady flow
- SDB-FTS (GBU-39B)
- B-52H/JASSM validation
- BQM-167 rocket plume
- FZU-55 on MQ-9/GBU-38
- MALD design studies
- B-1B/Mk-82/GBU-38
- F-15E S&C w/CBU-104
- B-52H/GBU-31
- F-16 w/active control surfaces
- F-16/600-gal tank
- F-16/WCMD-ER
- F-16/ECIPS/MA-31
- F/A-18C/GBU-12
- C-130/Store deployment
- Condensation predictions
- B-1B/SNIPER/GBU-38
- F-15E/GBU-28B/B
- F-15E/SNIPER/GBU-38
- F-15E/BRU61/GBU-39/B (SDB)
- B-52/GBU-12 Sabot
- B-2A/GBU-27
- JSF-CTOL/AIM-9X
- JSF-CV/AIM-9X
- F-16/MALD

FY05
- B-1B/Mk-82/GBU-38
- B-1B/IHAAA - turbulence study
- BQM-167A rocket plume
- BQM-167A RATO separation
- MALD design studies
- B-52H/MALD
- F-15E S&C w/CBU-104
- F-15E/GBU-31
- B-1B/SNIPER/GBU-38
- F-16/600-gal tank
- F-16/WCMD-ER
- F-16/ECIPS/MA-31
- F/A-18C/GBU-12
- C-130/Store deployment
- Condensation predictions
- B-1B/SNIPER/GBU-38
- F-15E/GBU-28B/B
- F-15E/SNIPER/GBU-38
- F-15E/BRU61/GBU-39/B (SDB)
- B-52/GBU-12 Sabot
- B-2A/GBU-27
- JSF-CTOL/AIM-9X
- JSF-CV/AIM-9X
- F-16/MALD

Captured JASSM jettison!

Realistic fin deployment!

Autopilot/flow interaction!

Complex grid fins!
AFSEO CFD Project Summary

FY06

**F-16/WCMD-ER**
- GBU-38 WT
- F-15E/GBU-38 Condensation
- F-16/AIM9X-9L Flutter
- B-52/GBU-38

**B-52/GBU-12B**
- F-18/GBU-12B
- JSF-CTOL/Aim-9X
- BQM-167/AFSAT

**F-15E/SDB**
- MK-82 WT
- F-15E/AGM-158
- B-1 Cavity study
- F-16/JSOW

**F-15E/GBU-38**
- YMQ-9A/GBU-12B
- F-15E/GBU-31 Condensation
- F-16/Tanks S&C
- B-2/GBU-28
- F-15E/GBU-28C/B
- F-16/MALD
- JSF Bay Study
- B-52/MALD
- F-15E/SNIPER/GBU38
- F-16/MA-31
- B-1/GBU38-MK82
- F-15C/AIM-54C
- F-16/GBU-39
# CFD Project Summary

## Computer Usage

<table>
<thead>
<tr>
<th>Year</th>
<th>Total Solutions</th>
<th>Avg # CPUs</th>
<th>Total Hrs</th>
<th>Avg Points (mil)</th>
<th>Avg RAM (GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY 01</td>
<td>112</td>
<td>20</td>
<td>215,000</td>
<td>3.9</td>
<td>5.0</td>
</tr>
<tr>
<td>FY 02</td>
<td>226</td>
<td>24</td>
<td>511,400</td>
<td>5.4</td>
<td>6.1</td>
</tr>
<tr>
<td>FY 03</td>
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<td>24</td>
<td>741,000</td>
<td>7.5</td>
<td>8.0</td>
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<td>FY 04</td>
<td>540</td>
<td>30</td>
<td>1,453,000</td>
<td>15.0</td>
<td>12.0</td>
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<tr>
<td>FY 05</td>
<td>845</td>
<td>30</td>
<td>1,870,000</td>
<td>23.2</td>
<td>14.7</td>
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<td>FY 06</td>
<td>4607</td>
<td>42</td>
<td>3,450,000</td>
<td>34.7</td>
<td>46.0</td>
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Technology Insertion Process

- Executed annually to acquire new HPC systems for major shared resource centers (MSRCs)
  - Two of the four MSRCs acquire new systems each year

- Two major evaluation criteria
  - Usability
  - Performance and Price/Performance

- Performance based on synthetic and application benchmark times-to-solution compared to a DoD standard system

- Price/performance determined both as a weighted average and optimized by sharing workload on a set of systems
Overview of TI-XX Acquisition Process

1. **Determination of Requirements, Usage, and Allocations**
   - Choose application benchmarks, test cases, and weights

2. **Vendors provide measured and projected times on offered systems**
   - Measure benchmark times on DoD standard system
   - Measure benchmark times on existing DoD systems
   - Determine performance for each offered system on each application test case
   - Determine performance for each existing system on each application test case

3. **Usability/past performance information on offered systems**
   - Use optimizer to determine price/performance for each offered system and combination of systems

4. **Collective Acquisition Decision**
   - Center facility requirements
   - Life-cycle costs for offered systems
   - Vendor pricing

Life-cycle costs for offered systems
TI-08 Synthetics Benchmark Suite

- CPUBench – Single processor tests
- IC Bench - Interconnect bandwidth and latency tests
- LANBench - External network interface/connection tests
- MultiMAPS - Memory bandwidth and latency tests
- OSBench – Operating system noise tests
- SPIOBench - Streaming parallel I/O tests
TI-08 Application Benchmark Codes

- **AMR** – Gas dynamics code
  - (C++/FORTRAN, MPI, 40,000 SLOC)
- **AVUS (Cobalt-60)** – Turbulent flow CFD code
  - (Fortran, MPI, 19,000 SLOC)
- **CTH** – Shock physics code
  - (~43% Fortran/~57% C, MPI, 436,000 SLOC)
- **GAMESS** – Quantum chemistry code
  - (Fortran, MPI, 330,000 SLOC)
- **HYCOM** – Ocean circulation modeling code
  - (Fortran, MPI, 31,000 SLOC)
- **ICEPIC** – Particle-in-cell magnetohydrodynamics code
  - (C, MPI, 60,000 SLOC)
- **LAMMPS** – Molecular dynamics code
  - (C++, MPI, 45,400 SLOC)
- **OOCore** – Out-of-core solver; surrogate for electromagnetics code
  - (Fortran, MPI, 39,000 SLOC)
- **Overflow2** – CFD code originally developed by NASA
  - (Fortran, MPI, 83,600 SLOC)
- **WRF** – Multi-Agency mesoscale atmospheric modeling code
  - (Fortran and C, MPI, 100,000 SLOC)
### Application Scores

**Total app score is workload sensitive**

### Synthetic Scores

**Total synth score is workload insensitive**

#### Prices

<table>
<thead>
<tr>
<th>System</th>
<th>Price</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$</td>
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<tr>
<td></td>
<td>$</td>
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<tr>
<td></td>
<td>$</td>
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#### Systems Test Cases

<table>
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<tr>
<th>System</th>
<th>Test Cases</th>
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<tbody>
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</tbody>
</table>

#### Workload Distribution Matrix

- **Application Test Cases**
  - **Best set of systems to buy**
  - **Best allocation of work for best set of systems**

#### Budget Limits

- **HI**:
  - $200
- **LO**:
  - $100

#### Acquisition & Life-cycle

- **Applied to total acquisition cost**

#### Tolerance

- **Target distribution of work**
  - **Tolerance = +/-10%**
Validation of Vendor Benchmarking Results

- Each application test case result must be validated via a specific validation check of output results within stated tolerances
  - Simple inspection of output values
  - Complex script that autochecks output values

- Specific validation check and tolerances are determined by discussions with the developer and/or key users
The figures of merit for determining accuracy of your GAMESS benchmark are the FINAL R-B3LYP ENERGY and RMS GRADIENT for the standard test case, and the FINAL RHS ENERGY, E(MP2), and RMS GRADIENT for the large test case. Complete standard out/error files have been provided for reference for several runs. Any discrepancy in the number of iterations performed is not significant.

For the standard test case, check for the presence of the following lines:

- FINAL R-B3LYP ENERGY IS -8880.4747875977 AFTER 19 ITERATIONS
- RMS GRADIENT = .014171968

In the standard test case, your value of FINAL R-B3LYP ENERGY should match the above value to within 1.0E-07, and your value of RMS GRADIENT should match the above value to within 1.0E-04.

All of the standard out output files must contain a statement similar to the following time-stamped message:

- EXECUTION OF GAMESS TERMINATED NORMALLY Sat Mar 18 08:23:18 2006
NOTE: The accuracy test is run in the batch job with the OVERFLOW 2 executable. This discussion is supplied in case you wish to re-run or examine the accuracy test. The accuracy test examines the batch output file. If your system heavily buffers the output of this file, you may need to re-run the accuracy test again after the batch job completes.

For both standard and large cases, a bash script ovrfl-acc-check is provided in the ref/subdirectories to check the accuracy of your results. First, if needed, you may edit the first line of the script to point to the correct bash shell location on your system. ***No other edits to the scripts may be made.*** Now, from the directory containing your batch output, issue the command

```bash
../ref/ovrfl-acc-check <batch output file> <standard | large> <num CPUs>
```

where `<batch output file>` is the simple file name of the batch output file from your OVERFLOW 2 run.
The script will check the batch output file to determine whether the requisite number of time steps were run, whether some required "bookkeeping" was completed at the end of the run, and whether the code exited smoothly. If all your output passes, the perl script will return

- OVERFLOW 2 output PASSES the accuracy test

Otherwise, it will return

- OVERFLOW 2 output FAILS the accuracy test

Together with the specific problems detected in the output.
Should We Do Uncertainty Analysis?
Assumption: Uncertainties in measured performance values can be treated as uncertainties in measurements of physical quantities.

For small, random uncertainties in measured values $x, y, z, \ldots$, the uncertainty in a calculated function $q(x, y, z \ldots)$ can be expressed as

$$
\delta q = \sqrt{\left( \frac{\partial q}{\partial x} \delta x \right)^2 + \cdots + \left( \frac{\partial q}{\partial z} \delta z \right)^2}
$$

Systematic errors need careful consideration since they cannot be calculated analytically.
**Benchmarking and Performance Prediction Uncertainty Analysis**

- **Overall goal:** Understand and accurately estimate uncertainties in benchmarking and performance prediction calculations.

- **Develop uncertainty equations from analytical expressions used to calculate performance and price/performance.**

- **Estimate uncertainties in quantities used for these calculations.**

- **Eventual goal:** Propagate uncertainties in performance predictions and benchmarking results to determine uncertainties in acquisition scoring.
Propagation of Uncertainties in Benchmarking and Performance Modeling

**Benchmark Times**
\[ \frac{1}{T} \]

**Amdahl Law**

**Benchmark Performance**
\[ \delta P \geq 3\% \]

**Least Squares Fit**

**Benchmark Scores**
\[ \sigma_S, \sigma_P \geq 3\% \]

**Optimizer**

**Average Performance for Each System**
\[ \sigma_j \leq 6\% - 20\% \]

**Benchmark Weights**

**Total Performance for Solution Set**
\[ \sigma_{TS} \leq 6\% - 20\% \]

**Life-Cycle Costs**

**Price/Performance for Solution Set**
\[ \sigma_{S/TS} \leq 6\% - 20\% \]

**Averaging over spans of Solution Sets**

**Rank Ordering and Histograms of Solution Sets**
\[ \sigma_\% \leq 10\% \]
Architecture % Selection by Processor Quantity (Example)
Summary

- DoD uses a wide variety of HPC applications in a diverse set of computational technology areas
- Modeling and simulation is having a real impact on the design and operation of DoD systems
- Verification and validation is an important component of new DoD application software developments and application benchmarking for acquisition purposes
- Uncertainty analysis is explicitly used in the determination of performance of HPC systems on DoD application benchmarks for acquisition decisions