Department of Defense

High Performance Computing Modernization Program

DoD High Performance Computing Science and Engineering Applications

Larry Davis

25 April 2007

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

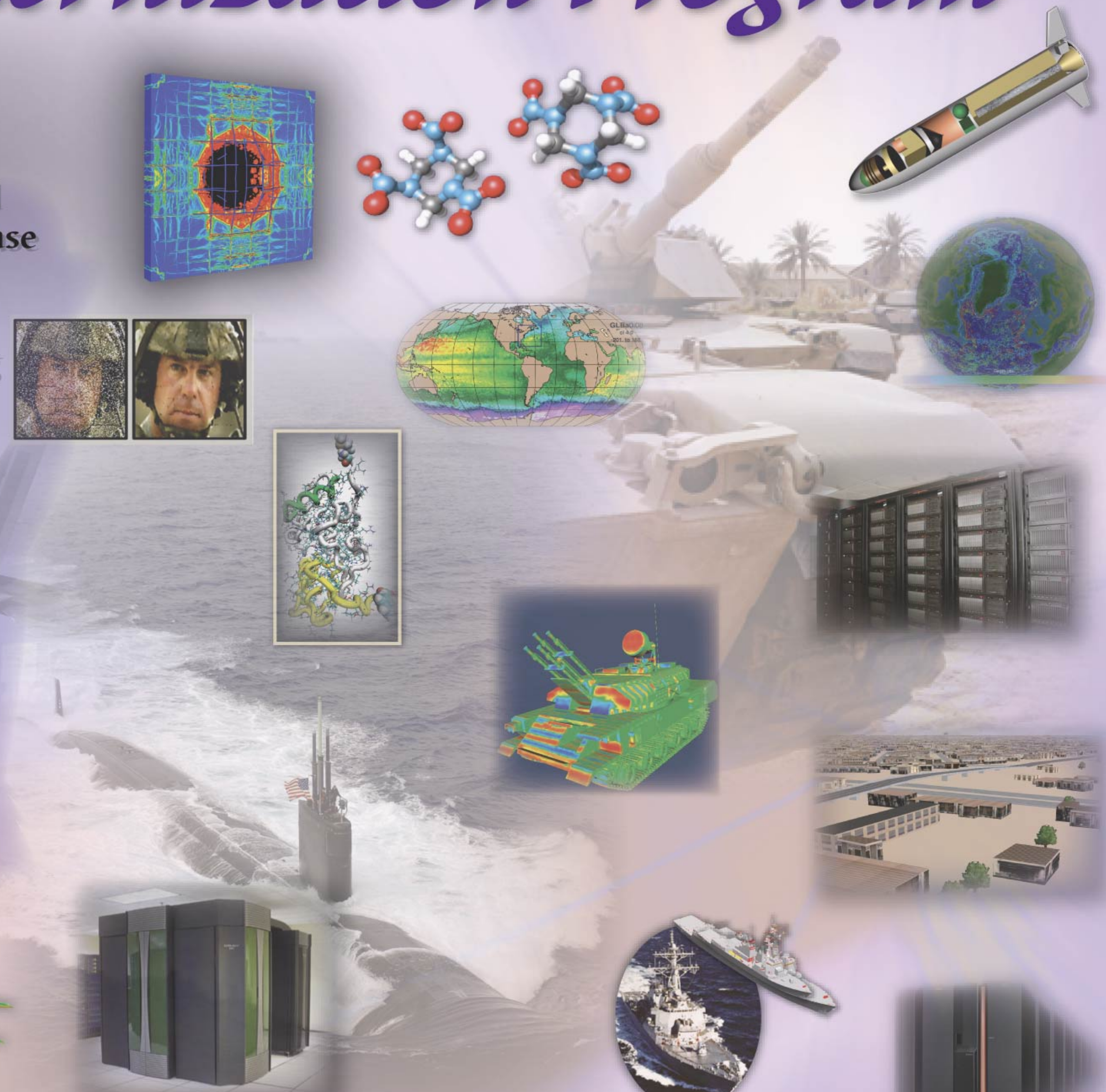
HPC Modernization Program

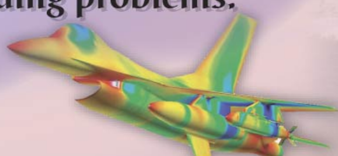
Mission

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&E 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

Networking

Defense Research & Engineering Network

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

Defense Agencies

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

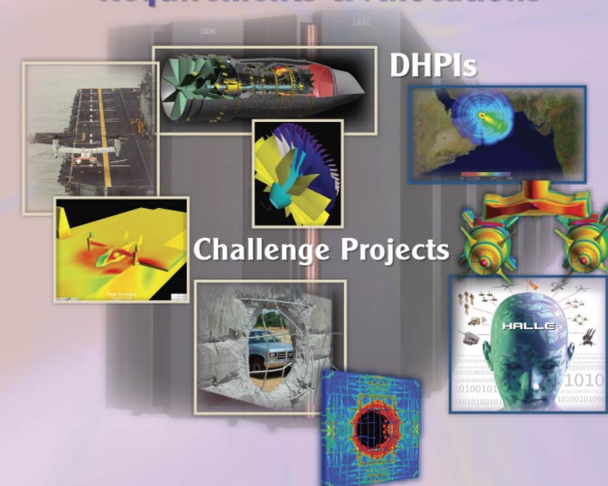
Other

ARSC ADC
1 DHPI

Software Applications Support

Resource Management

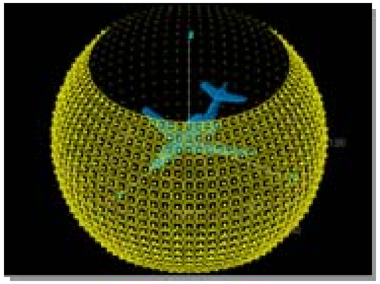
Requirements & Allocations



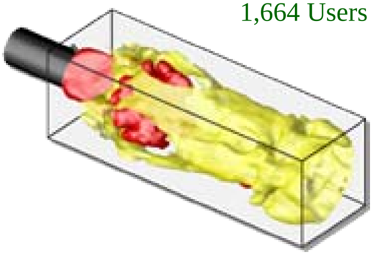
HPCMP Serves a Large, Diverse DoD User Community

- **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***

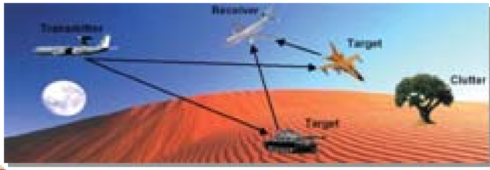
Computational Electromagnetics & Acoustics – 310 Users



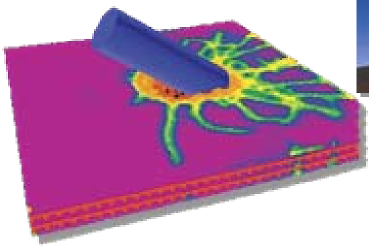
Computational Fluid Dynamics – 1,664 Users



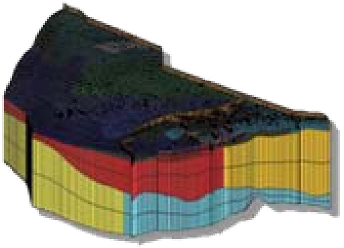
Electronics, Networking, and Systems/C4I – 115 Users



Computational Structural Mechanics – 440 Users

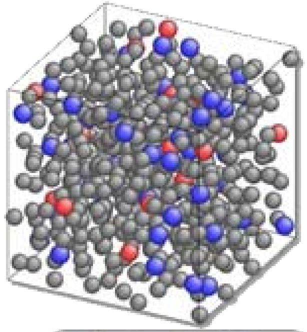


Environmental Quality Modeling & Simulation – 128 Users

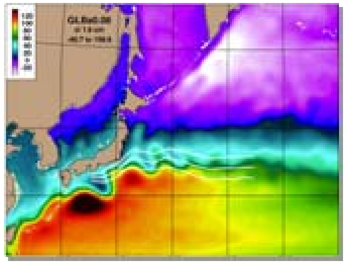


Forces Modeling & Simulation – 235 Users

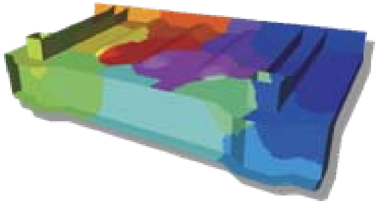
Computational Chemistry, Biology & Materials Science – 387 Users



Climate/Weather/Ocean Modeling & Simulation – 266 Users



Integrated Modeling & Test Environments – 152 Users



Signal/Image Processing – 377 Users

*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.

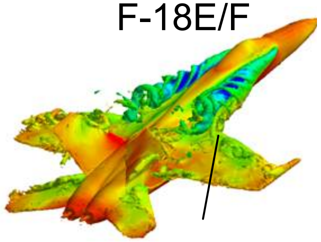
160 users are self characterized as "Other"

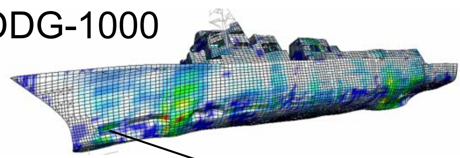
DoD HPCMP Application Software Requirements for FY 2007

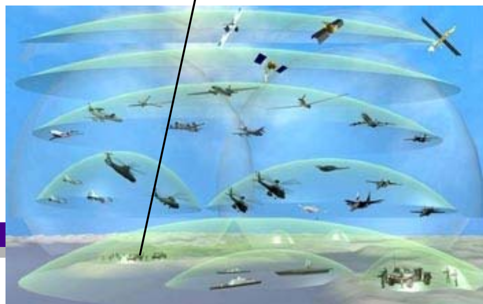
Application	Type	CTA	Total CPU Hours	Percentage of Total Requirement
CTH	Shock Physics	CSM	93,840,501	12.8%
HYCOM	Ocean Modeling	CWO	89,005,100	12.1%
GAUSSIAN	Quantum Chemistry	CCM	49,455,900	6.7%
ALLEGRA	Shock Physics	CSM	32,815,000	4.5%
ICEPIC	Particle-in-Cell Simulation	CEA	26,500,000	3.6%
XPATCH	Radar Cross-section Simulation	CEA	23,469,500	3.2%
CAML	Fluid Dynamics	CFD	21,000,000	2.9%
MOM	Electromagnetics	CEA	18,540,000	2.5%
VASP	Materials Simulation	CCM	18,435,000	2.5%
ANSYS	Structural Mechanics	CSM	17,923,580	2.4%

CREATE: Computational Research and Engineering Acquisition Tools and Environments

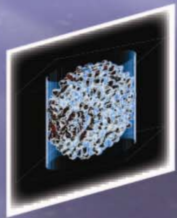
- **CREATE Goal: Enable acquisition programs to rapidly develop more fully optimized and integrated designs with fewer flaws and better performance.**
- **CREATE will develop and deploy three computational engineering tool sets for acquisition program engineers to exploit the exponential growth in supercomputer 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**

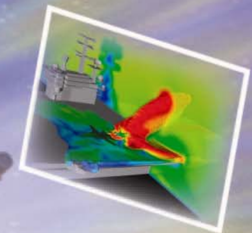




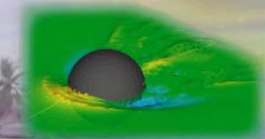


DoD Challenge Projects

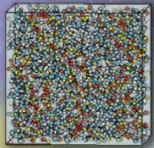


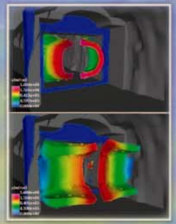


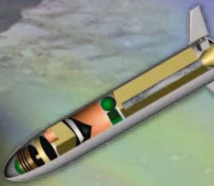
The HPCMP recognizes and supports high priority computational work conducted within the DoD that may be done at its shared resource centers through its implementation of Challenge Projects. These projects represent the DoD's highest-priority, highest-impact, computational work, both from technical and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

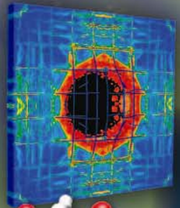


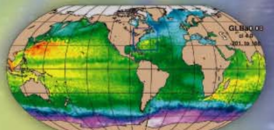
- Projects will lay the groundwork within the science and technology program for future weapons systems.
- Projects are headed by senior scientists and engineers within DoD science and technology and test and evaluation organizations, universities, and industry research partners.
- Projects use multiple hardware platforms and, in many cases, multiple HPC centers.

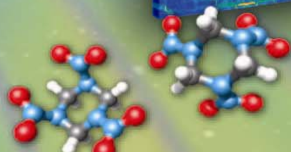


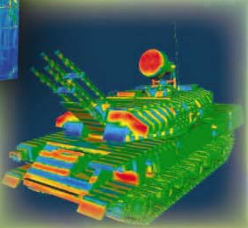








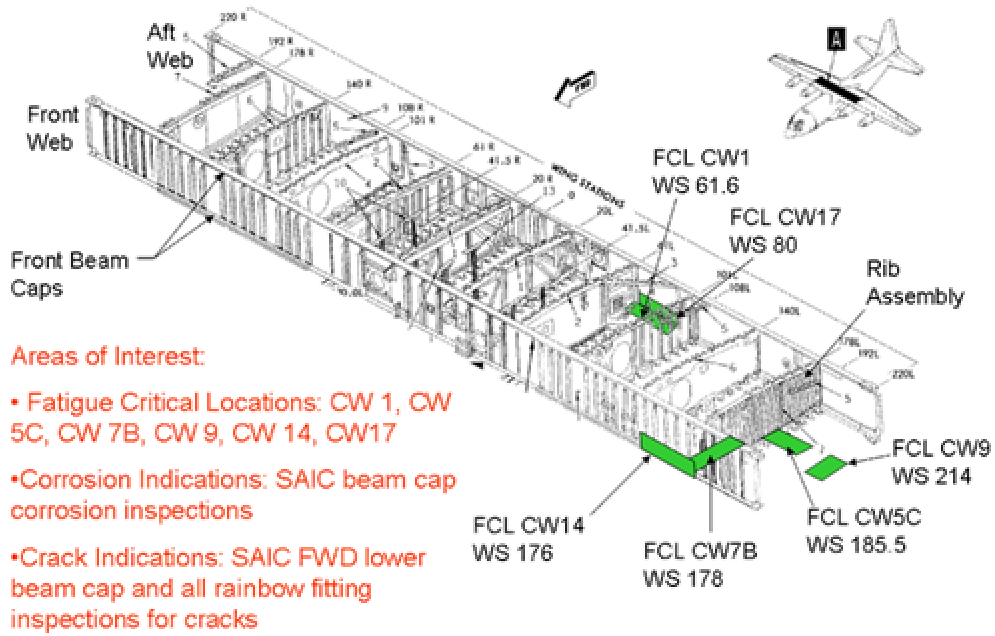




Statistical Fatigue and Residual Strength Analysis of New and Aging Aircraft Structure

S. Fawaz, USAFA, Colorado Springs, CO; and B. Andersson, The Swedish Defence Research Agency FOI; Sponsor: Air Force

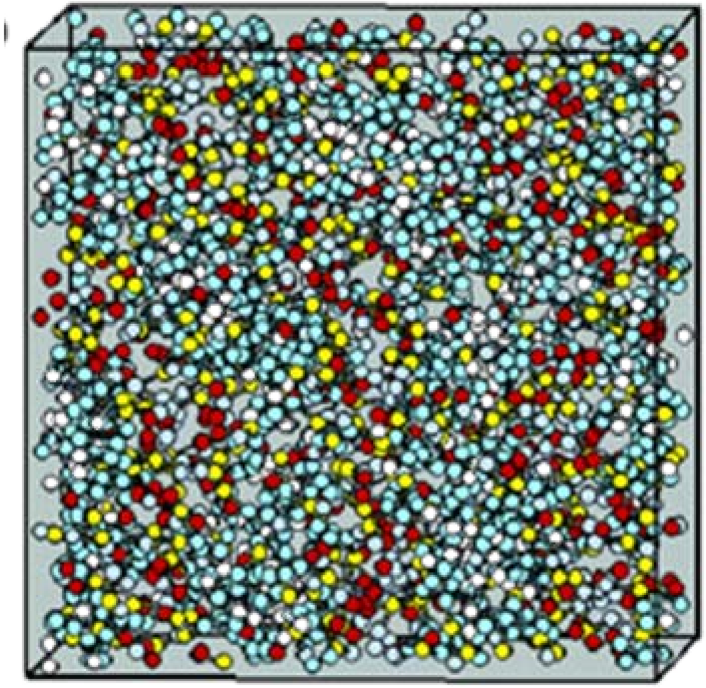
Increase the accuracy of fatigue life predictions across the DoD fixed wing fleet by developing new stress intensity factor solutions (K). New solutions are transitioned to the user via the USAF's crack growth code, AFGROW.



Design of Energetic Ionic Liquids

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

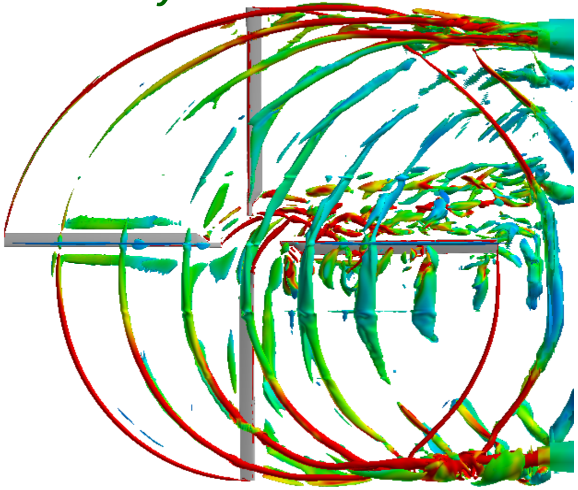
Benefits to the warfighter include cost-effective and reliable access to space, control and exploitation of space by development of more robust propulsion technologies, and mitigation of environmental and biological hazards.

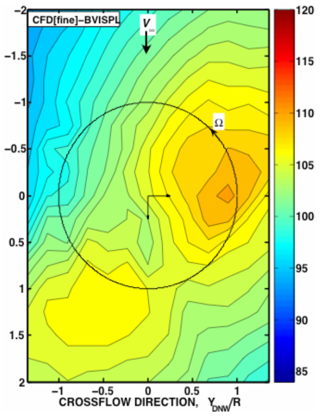


Unsteady, Multidisciplinary Rotorcraft Simulations for Interactional Aerodynamics

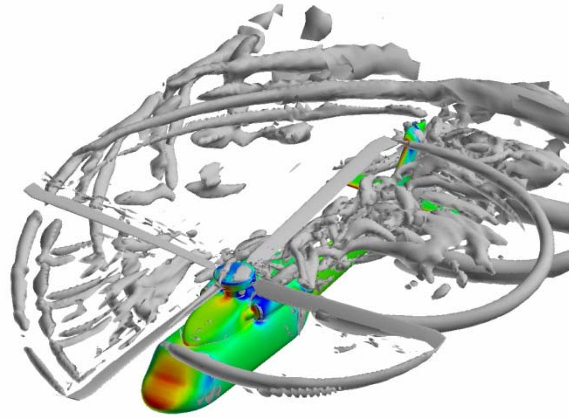
M. Potsdam and J. Lim, AMRDEC, Moffett Field, CA
Sponsor: Army

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.

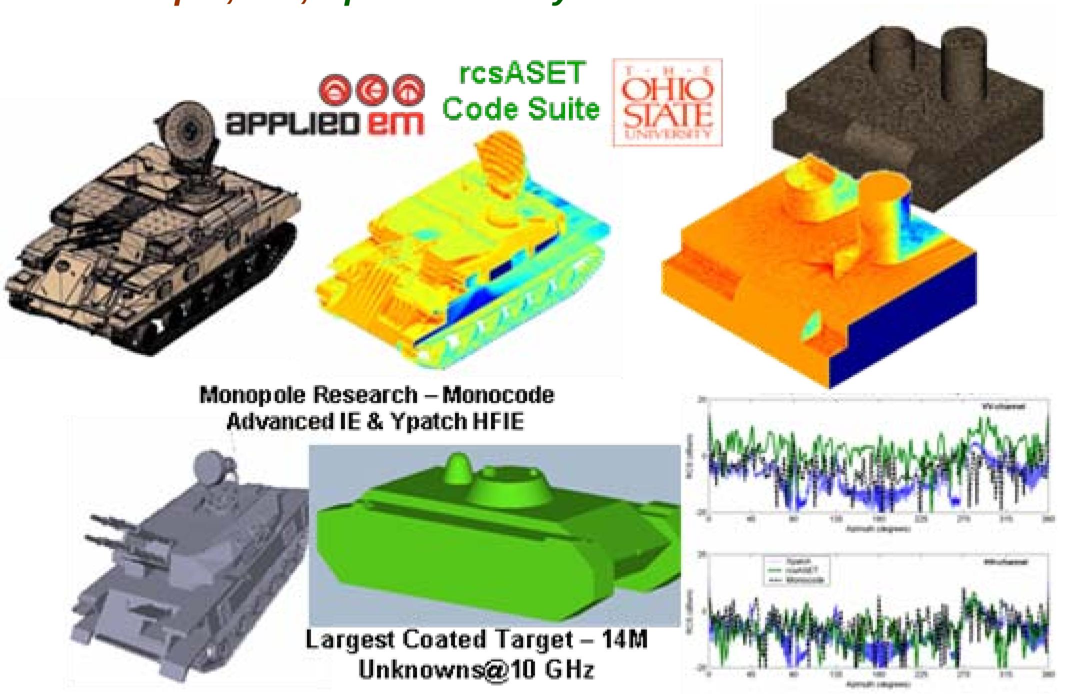


UH-60A rotor-hub-fuselage interaction. CFD/CSD coupled solution.

Millimeter-Wave Radar Signature Prediction Improvement for Ground Vehicles

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

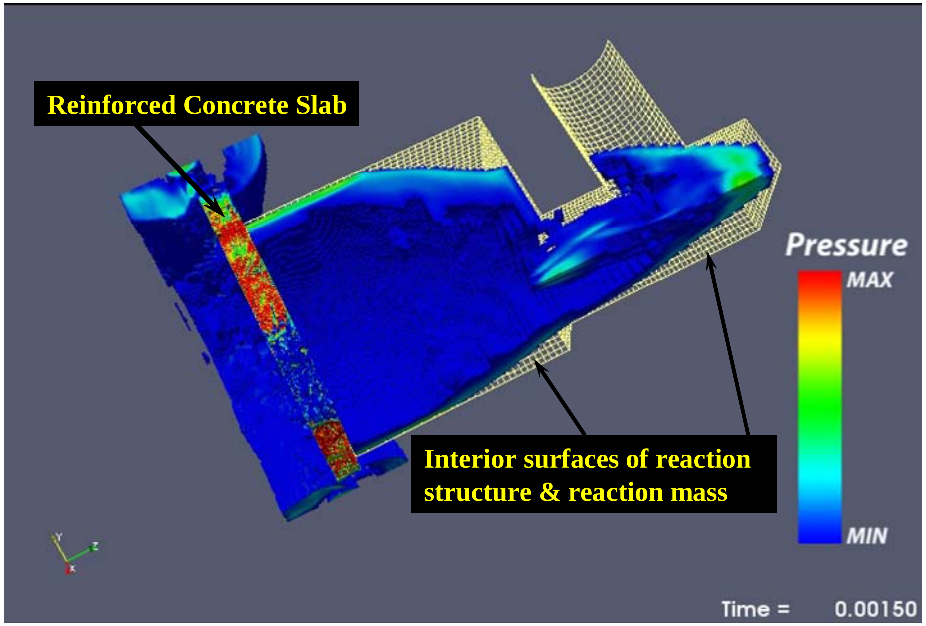


Explosive Structure Interaction Effects in Urban Terrain

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

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.

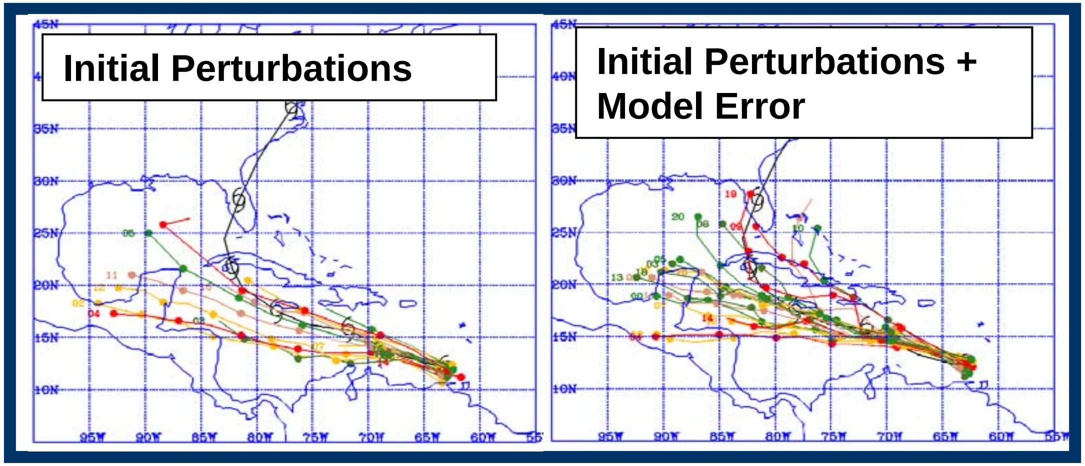
Blast environment from embedded detonation



Multi-Scale Predictability of High-Impact Weather in the Battlespace Environment

J. Doyle, C. Reynolds, C. Bishop, R. Hodur, R. Langland, M. Liu, J. Nachamkin, J. Pullen, and S. Wang, NRL-MRY, Monterey, CA;
Sponsor: Navy

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.



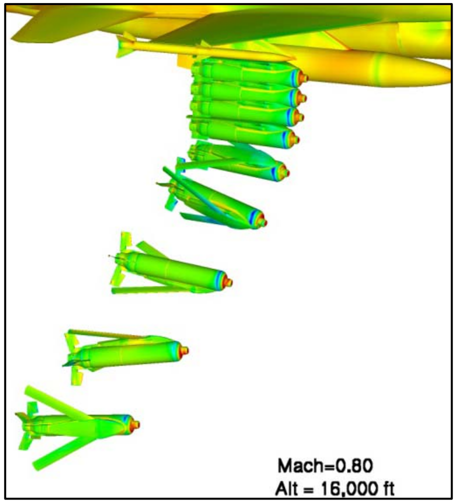
Ensemble track forecasts of Hurricane Charley from 10 August 2004, color, and observed track, black with hurricane symbols. The ensemble that included stochastic perturbations representing model error (right) captured the possibility of the observed recurvature onto the Florida peninsula (right). The control ensemble based on perturbations to the initial state only (left) did not contain this scenario.

Applied Computational Fluid Dynamics (CFD) in Support of Aircraft-Store Compatibility and Weapons Integration

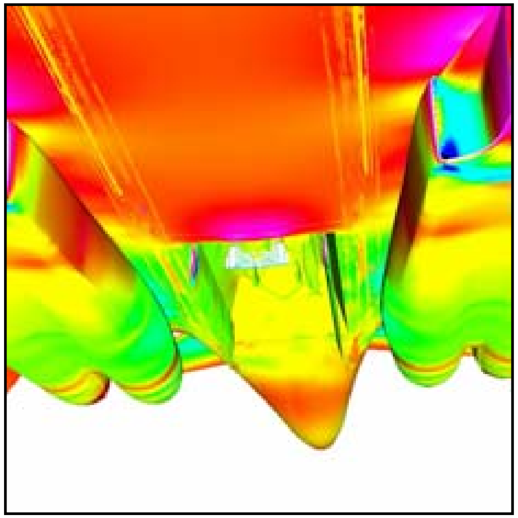
J. Keen, R. Moran, J. Dudley, J. Torres, Lt. J. Babcock, C. Cureton, and T. Eymann, AFSEO, Eglin AFB, FL; B. Jolly, J. Martel, M. Rizk, and J. Fay, Sverdrup Technology Inc., Eglin AFB, FL; M. Kannapel and R. Spinetti, Tybrin Corp., Eglin AFB, FL; and S. Kernazhitskiy, CACI/TEAS, Eglin AFB, FL;

Sponsor: Air Force

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.



CBU-115 separation from F-16



GBU-38 separation from B1B

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 α 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

Captured JASSM jettison!

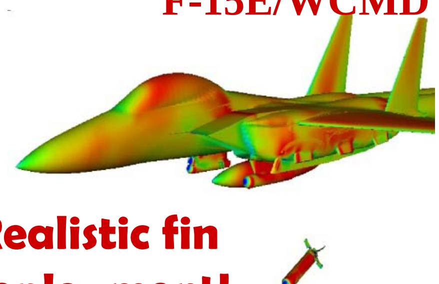
FY02

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



Realistic fin deployment!

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
F-16/600-gal tank
B-52H/MALD
F-16/MALD
F-15E/GBU-28
F-16/WCMD-ER

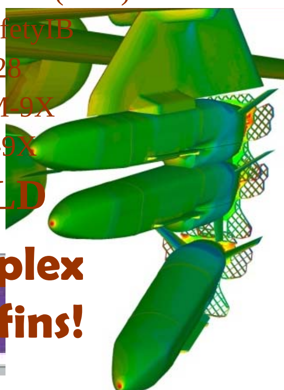
B-52H/X-37

Autopilot/flow interaction!

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
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 SafetyIB
B-2A/GBU-28
JSF-CTOL/AIM-9X
JSF-CV/AIM-9X

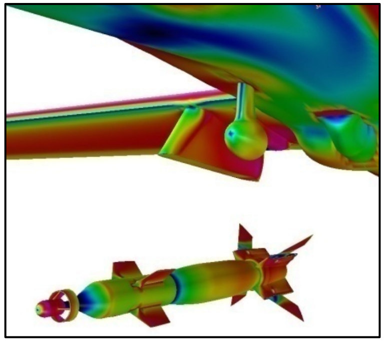
F-16/MALD



Complex grid fins!

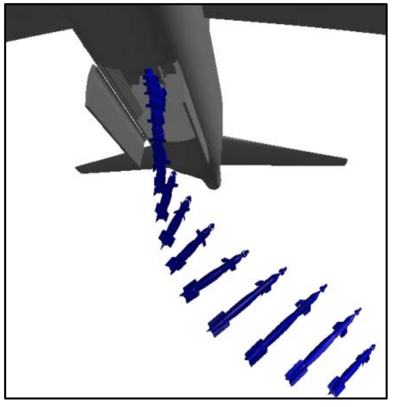
AFSEO CFD Project Summary

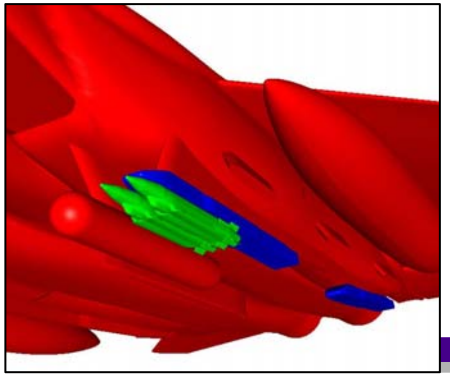
FY06

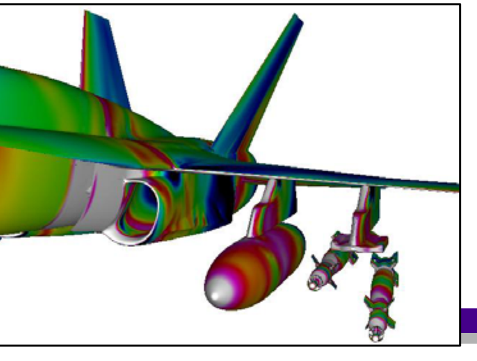


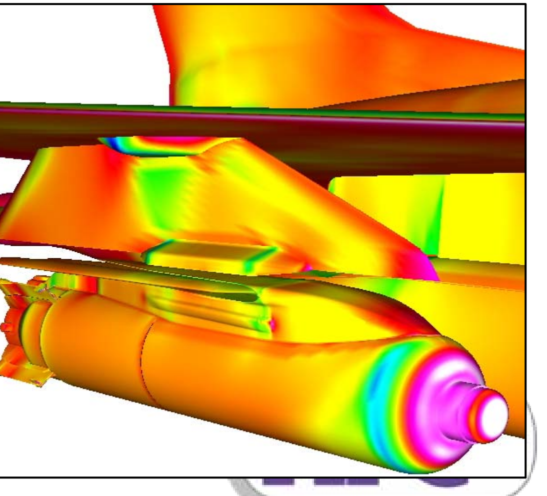
F-16/WCMD-ER
GBU-38 WT
F-15E/GBU-38 Condensation
F-16/AIM9X-9L Flutter
B-52/GBU-38
B-52/GBU-12B
F-18/GBU-12B
JSF-CTOL/Aim-9X
BQM-167/AFSAT
F-15E/SDB
MK-82 WT
F-15E/AGM-158
B-1 Cavity study
F-16/JSOW

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

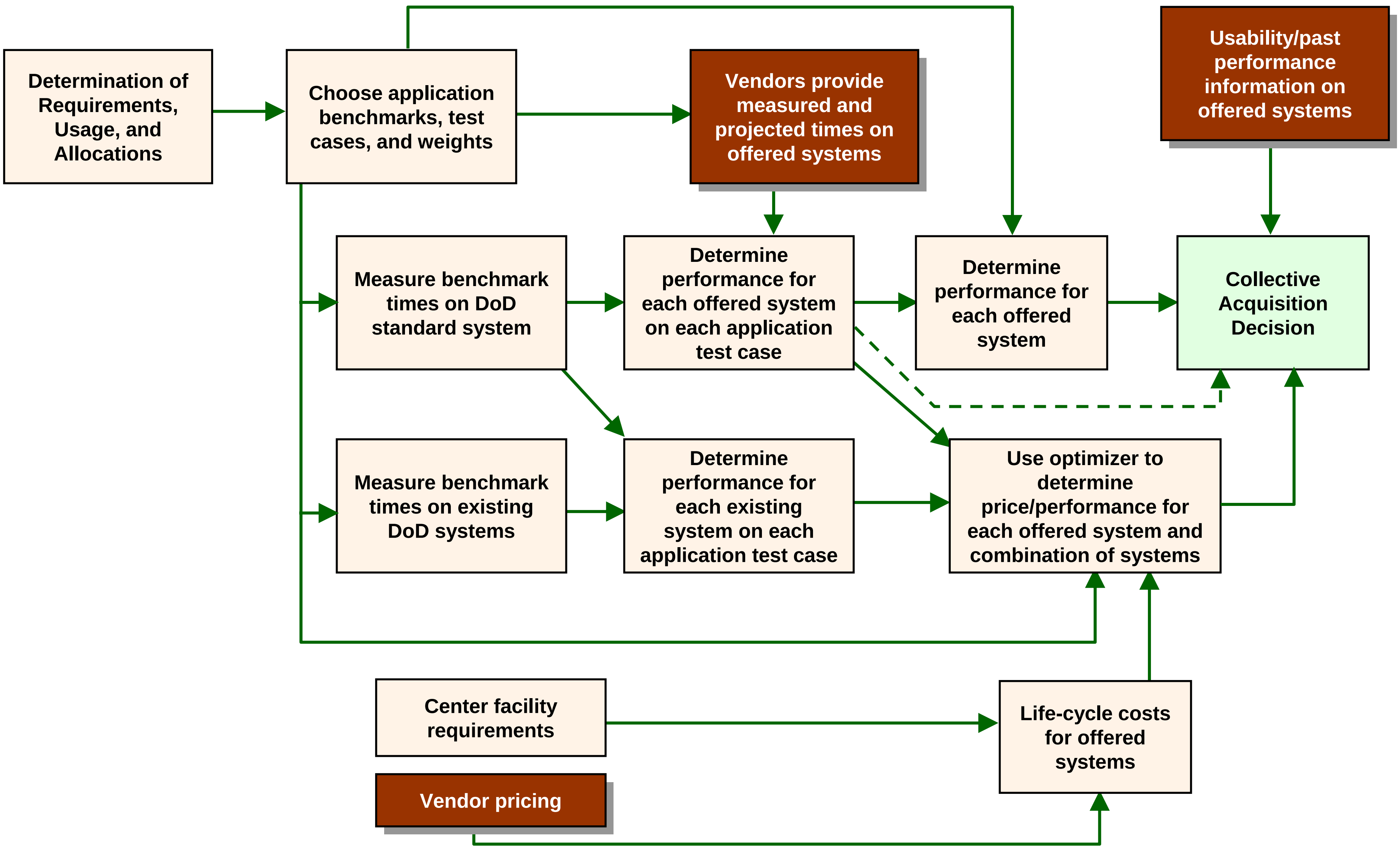
Computer Usage

	Total Solutions	Avg # CPUs	Total Hrs	Avg Points (mil)	Avg RAM (GB)
FY 01	112	20	215,000	3.9	5.0
FY 02	226	24	511,400	5.4	6.1
FY 03	337	24	741,000	7.5	8.0
FY 04	540	30	1,453,000	15.0	12.0
FY 05	845	30	1,870,000	23.2	14.7
FY 06	4607	42	3,450,000	34.7	46.0

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

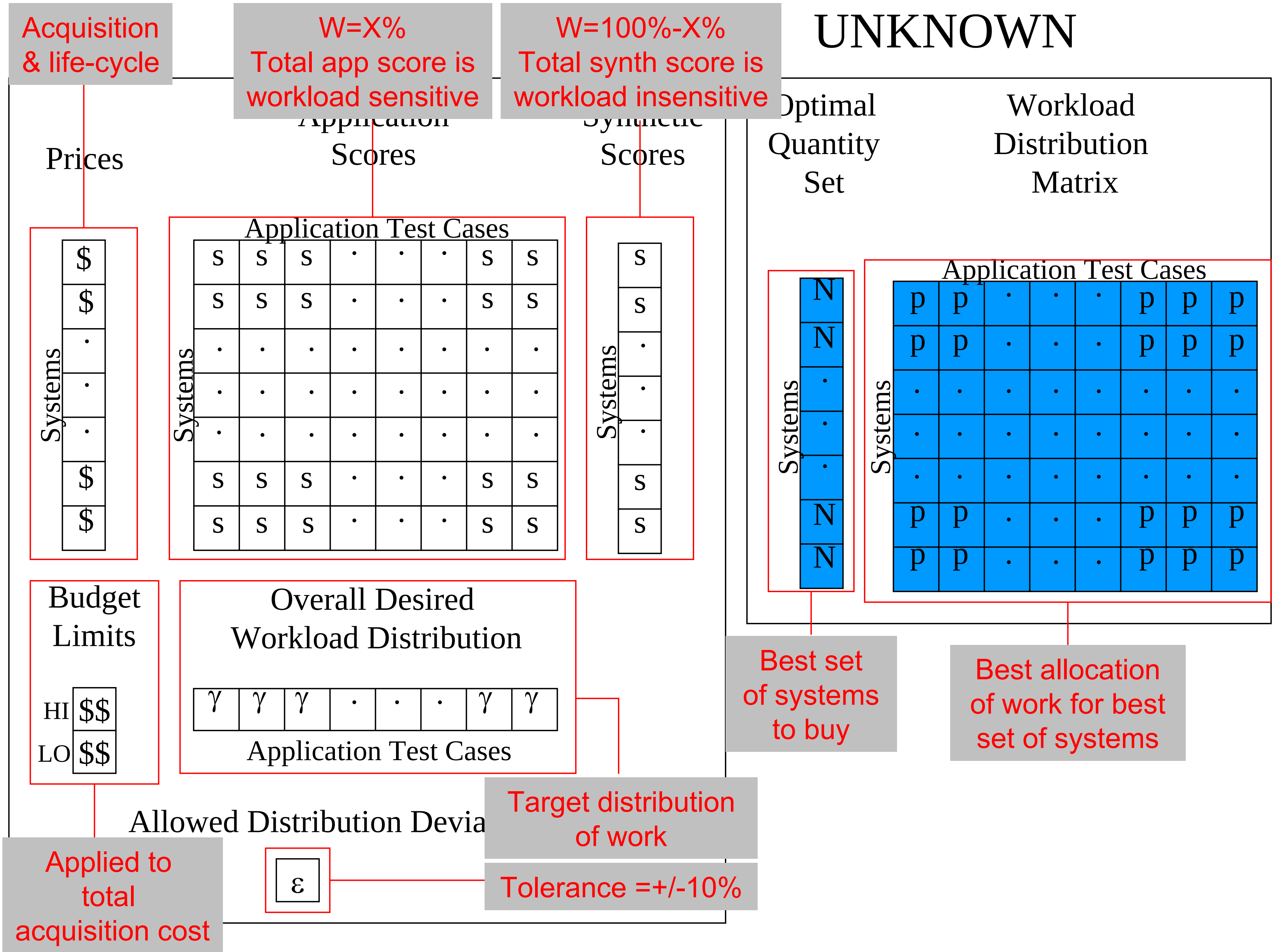


TI-08 Synthetics Benchmark Suite

- CPUBench – Single processor tests
- ICBench - 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)


UNKNOWN
Acquisition & life-cycle
W=X% Total app score is workload sensitive
W=100%-X% Total synth score is workload insensitive
Prices
Application Scores
Synthetic Scores
Optimal Quantity Set
Workload Distribution Matrix
Application Test Cases
Systems
Budget Limits
HI $$
LO $$
Overall Desired Workload Distribution
Allowed Distribution Deviation
ε
Best set of systems to buy
Best allocation of work for best set of systems
Target distribution of work
Tolerance =+/-10%
Applied to total acquisition cost

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

Validation Check for GAMESS Standard Case

- 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

Validation Check for Overflow2 Standard Case

- 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
  - ../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.

Validation Check for Overflow2 Standard Case (Continued)

- 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?

Performance Modeling 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, …, the uncertainty in a calculated function q (x, y, z …) can be expressed as

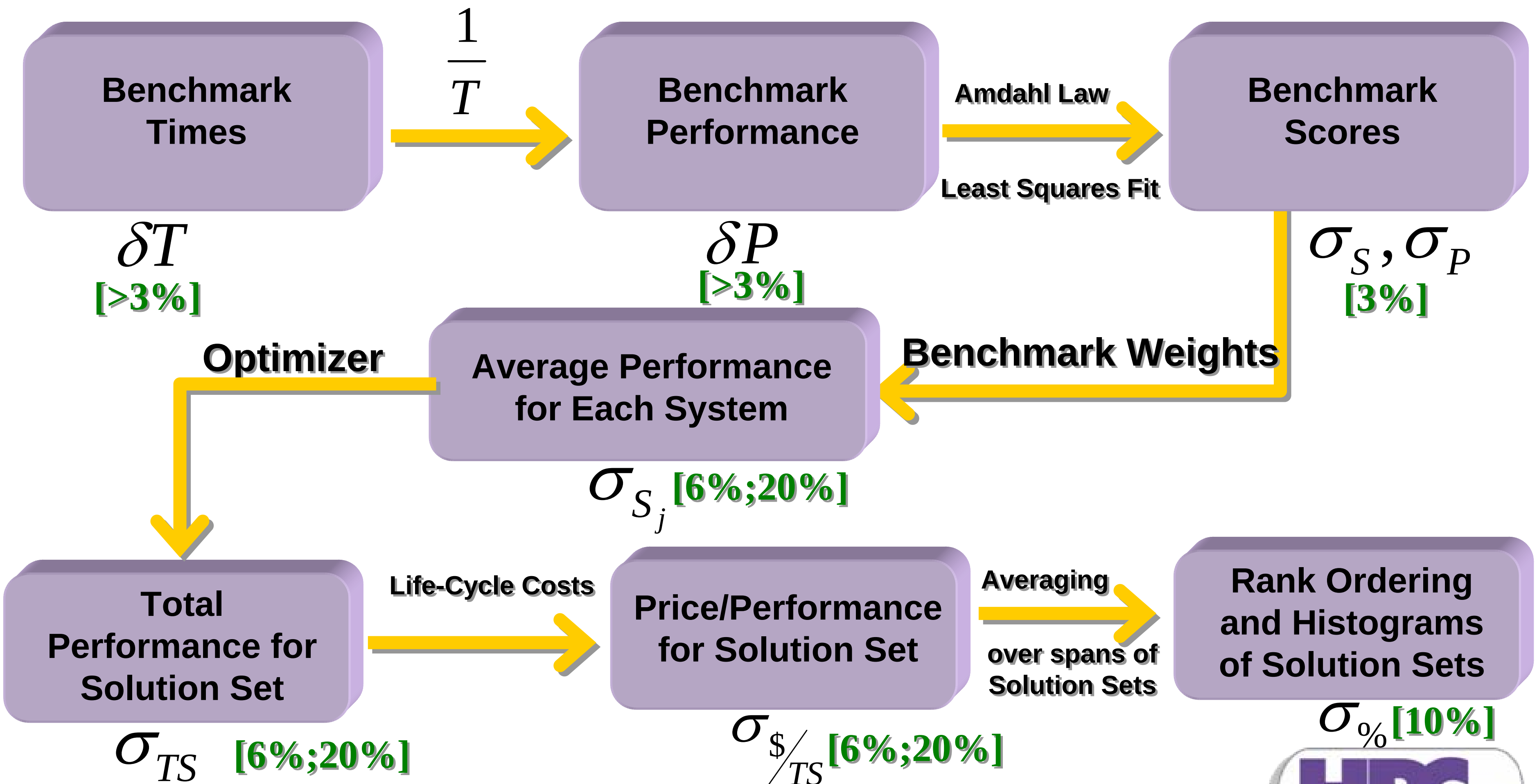
$$\delta q = \sqrt{\left(\frac{\partial q}{\partial x}\delta x\right)^2 + \cdots + \left(\frac{\partial q}{\partial z}\delta z\right)^2}$$

- Systematic errors need careful consideration since they cannot be calculated analytically

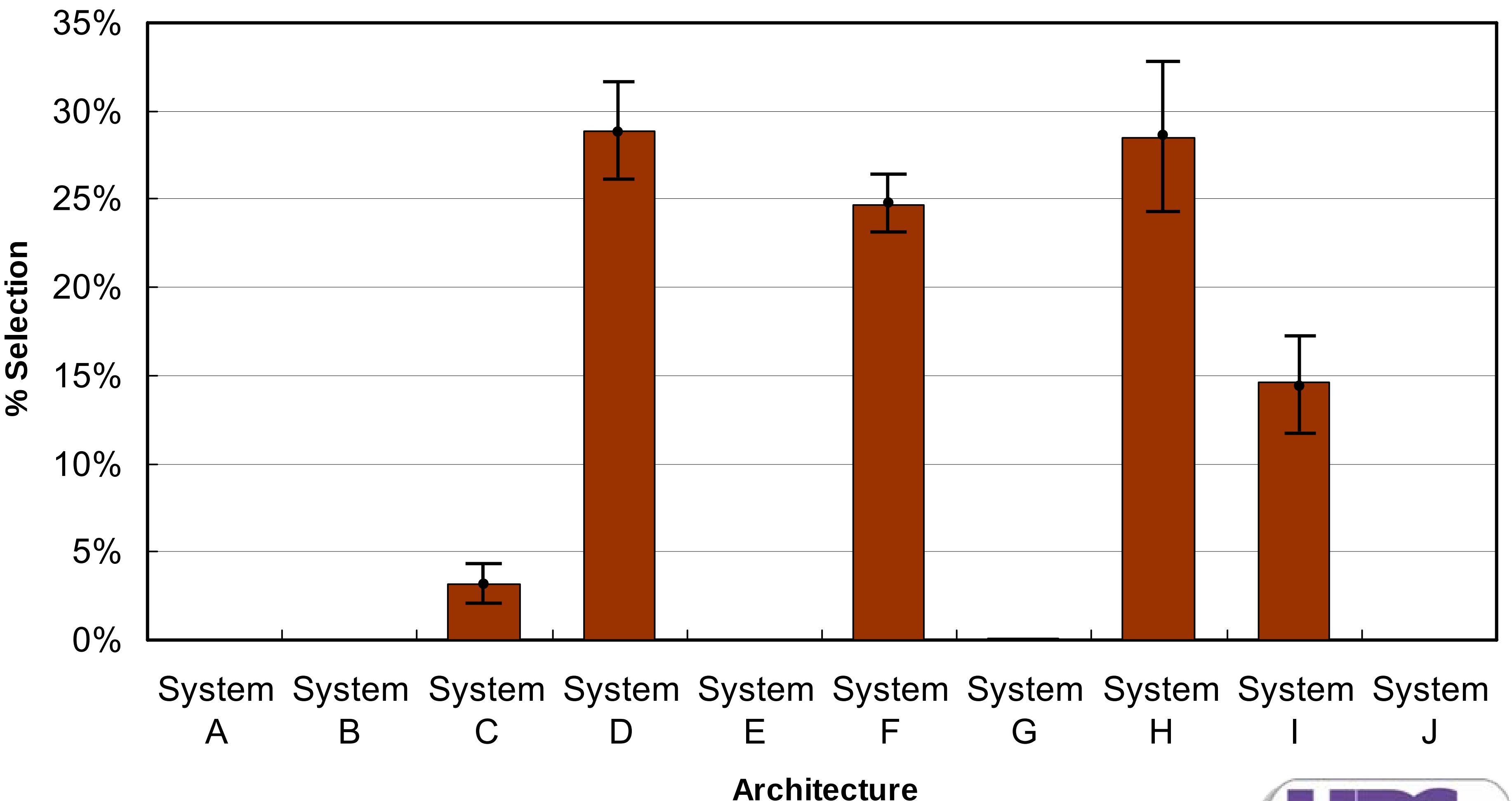
Benchmarking and Performance Prediction Uncertainty Analysis

- 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



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