Department of Defense

High Performance Computing Modernization Program

The Promise and Challenges of Computational Science and Engineering

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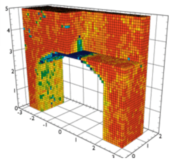
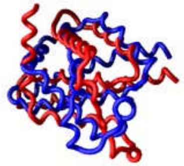
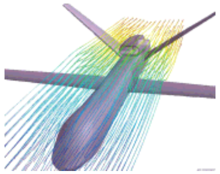
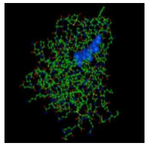
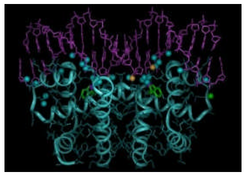
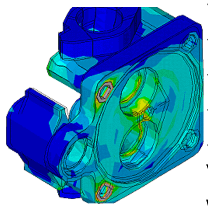
Overview

- High Performance Computing for Science and Engineering
  - The Progress and The Promise
  - The Challenges and The Opportunities
- Some examples
  - Goodyear
  - CREATE

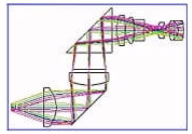
Computational Science And Engineering Is Becoming an Essential Tool for Theoretical Science And Engineering

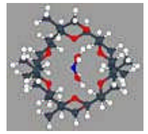
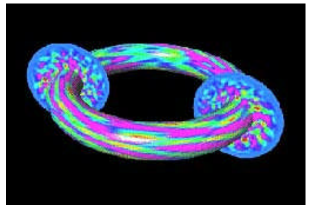
Accelerator Design
Aircraft Design
Archaeology
Armor Design
Astrophysics
Atomic And Molecular Physics
Automobile Design
Bioengineering And Biophysics
Bioinfomatics
Chemistry
Civil Engineering
Climate Prediction
Computational Biology
Computational Fluid Dynamics
Cosmology
Cryptography
Data Mining
Drug discovery
Earthquakes
Economics
Engineering Design And Analysis
Finance
Fluid Mechanics
Forces Modeling And Simulation
Fracture Analysis
General Relativity Theory
Genetics
Geophysics

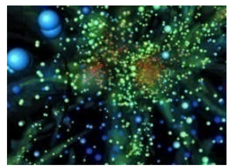






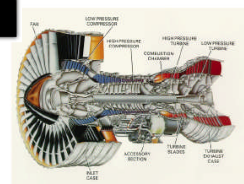




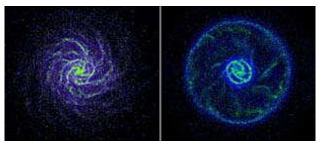
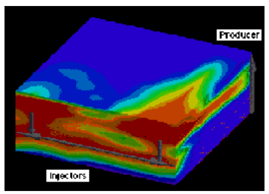
Groundwater And Contaminant Flow
High Energy Physics Research
Hydrology
Image Processing
Inertial Confinement Fusion
Integrated Circuit Chip Design
Magnetic Fusion Energy
Manufacturing
Materials Science
Medicine
Microtomography
Nanotechnology And Nanoscience
Nuclear Reactor Design And Safety
Nuclear Weapons
Ocean Systems
Petroleum Field Analysis And Prediction
Optics and Optical Design
Political Science
Protein Folding
Radar signature and antenna analysis
Radiation Damage
Satellite Image Processing
Scientific Databases
Search Engines
Shock Hydrodynamics
Signal Processing
Space Weather
Volcanoes
Weather Prediction
Wild Fire Analysis

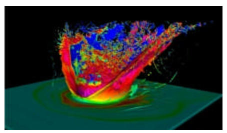
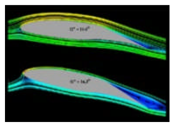
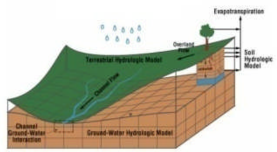
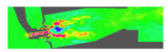


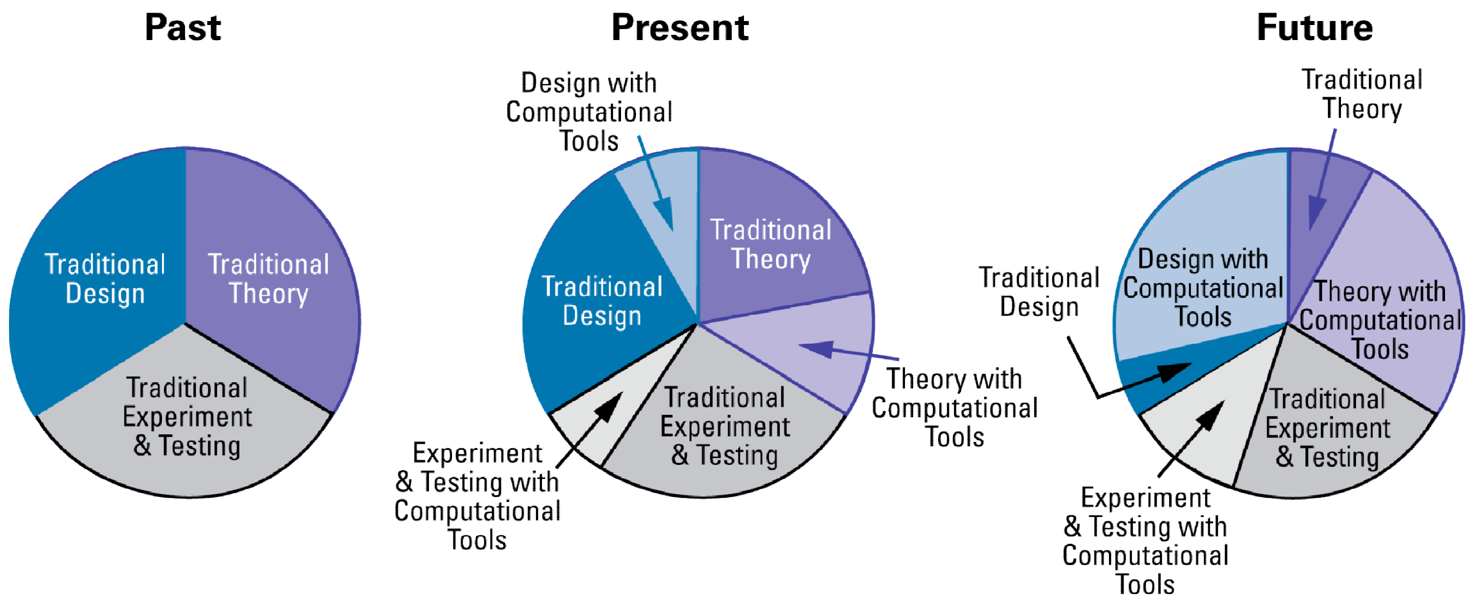




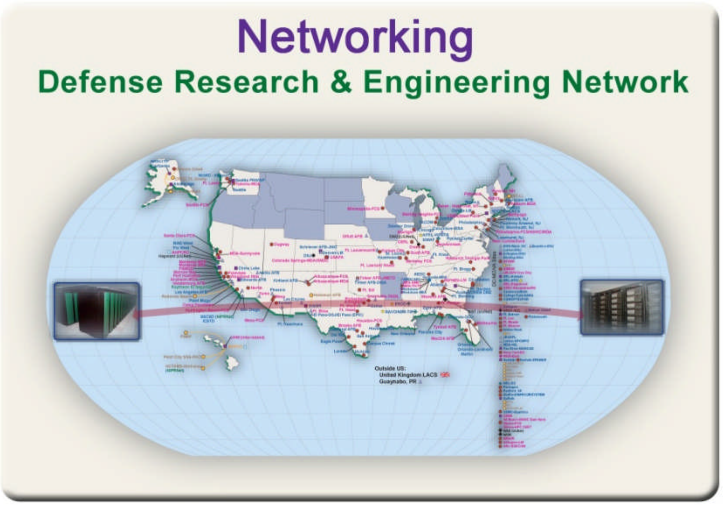





Computational Tools Are Becoming "Tools of the Trade" In Science And Engineering



	Past	**Present**	**Future**
Theory	Pencils, paper; slide rules	New: symbolic math; computational solutions	New: Almost all computional
Experiments	Physical hardware; notebooks; chart recorders; polariod film, …	New: computerized data collection & analysis; little V&V of computations; simple simulations & experimental design	New: Extensive V&V of computations; simulations are a part of experimental methodology
Eng. Design	Pencils, paper; slide rules	New: CAD-CAM; computational design analysis	New: Computational design & optimization

DoD HPC Modernization Program



Army HPCMP Participation

ARL & ERDC DSRCs
1,343 Users/24 Organizations/ 108 Projects
50 DREN Sites
15 Challenge Projects/2 DHPIs
5 Institutes

Navy HPCMP Participation

Navy DSRC
942 Users/16 Organizations/ 197 Projects
40 DREN Sites
13 Challenge Projects/2 DHPIs
1 Institute

Air Force HPCMP Participation

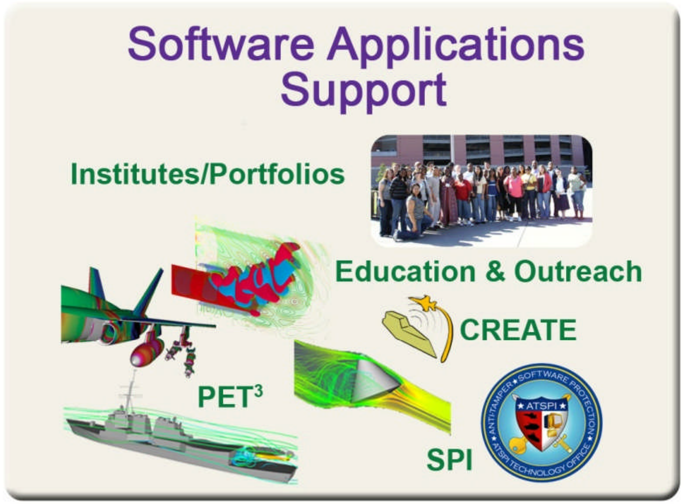
AFRL & MHPCC DSRCs
1,330 Users/25 Organizations/ 199 Projects
21 DREN Sites
11 Challenge Projects/3 DHPIs
3 Institutes

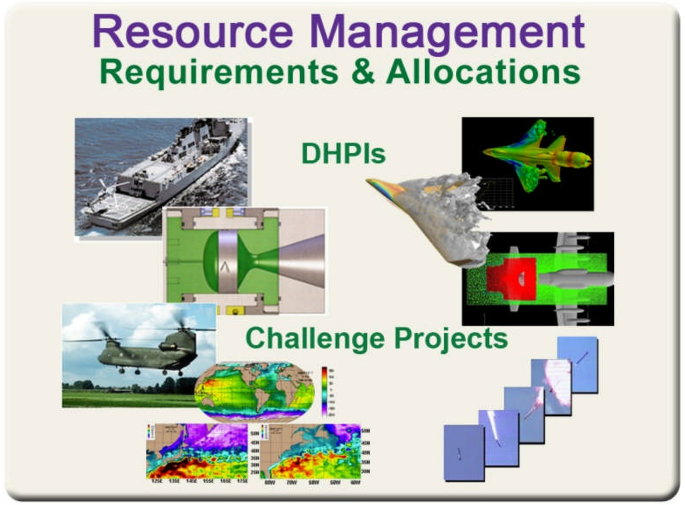
Defense Agencies Participation

DARPA, DTRA, JNIC, JFCOM, MDA, PA&E & OTE
537 Users/4 Organizations/ 25 Projects
28 DREN Sites
2 Challenge Projects/2 DHPIs

Other

ARSC DSRC
56 DREN Sites

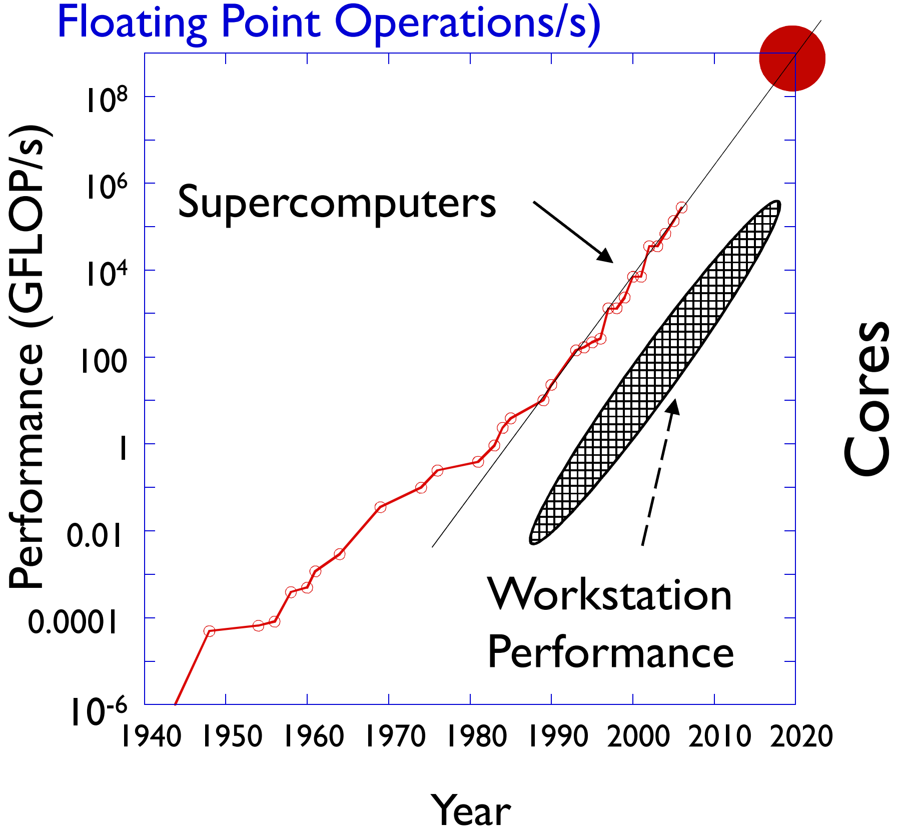




Next Generation Computers Offer Society Unparalleled Power to Address Important Problems

- Next generation computers (2020) will enable us to develop and deploy codes that are much more powerful than present tools:
  - Utilize accurate solution methods
  - Include all the effects we know to be important
  - Model a complete system
  - Complete parameter surveys in hours rather than days to weeks to months
- In ~ 10 years, workstations will be as powerful as today's supercomputers
- Greatest opportunities for 2020 (and 2010) include large-scale codes that integrate many multi-scale effects to model a complete system

Computing Power For The World's Fastest Computer Floating Point Operations/s)

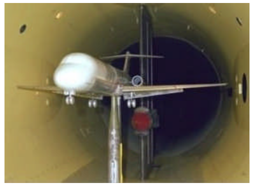


Physics-based Computational Engineering has great opportunities!

- Computational Science won’t grow exponentially
  - Everyone involved in theoretical physics, theoretical chemistry, theoretical material science, etc. already use supercomputers
- Physics-based Computation Based Engineering—New frontier
  - Only a small fraction of engineers now use Computation Based Engineering (CE)
- Replace physical design-build-test iterations with computational “Design Through Analysis” , i.e. CAD-mesh-analyze iterations validated with a final physical test

Design-build-test describes many product cycles




Requirements → Design → Build Physical Product → Test Physical Product → Market

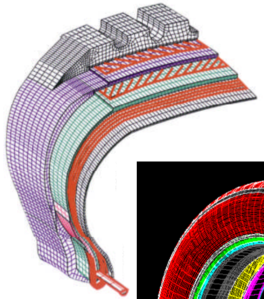
(Many) Design iterations

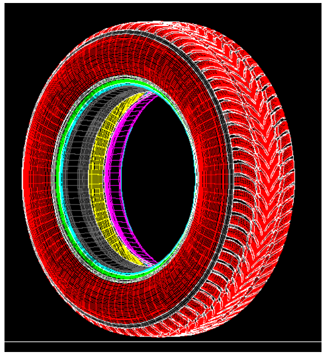
- Requires many lengthy and expensive design/build/test iteration loops
- Process converges slowly, if at all
- Design flaws discovered late in process

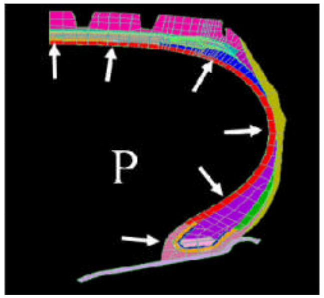
→ Long time to market

Replace physical design-build-test with computational design-build-test

GOODYEAR







Inflation and Seating

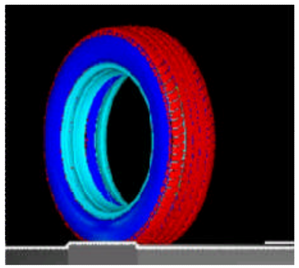
G949 RSA
Regional Hwy &City

Requirements → Design and Build Virtual Product → Analyze and Test Virtual Product → Build and Test Physical Product → Market

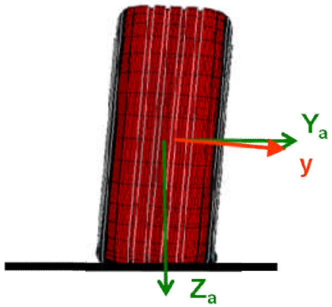
Design iterations

- Reduced time to market from 3 years to 9 months
- Increased new products delivery from 1 every 3 years to 5 per year
- Saved the company

G971
Off Road Drive



Running Over Obstacles

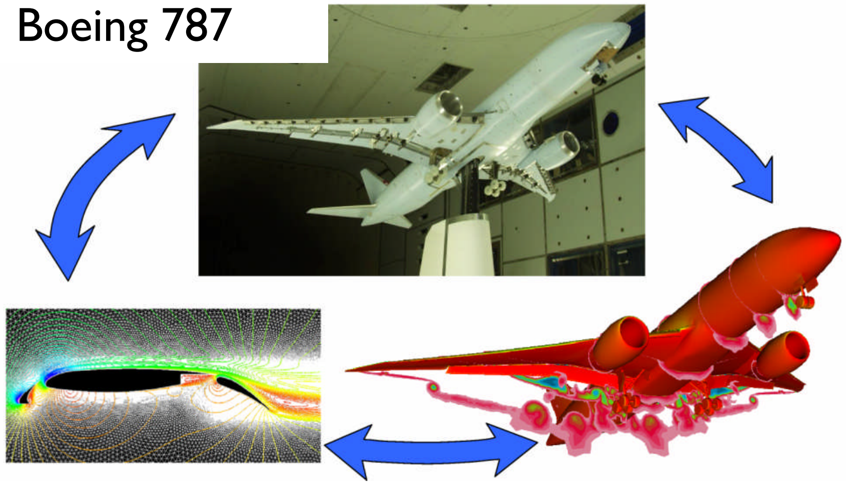


Camber

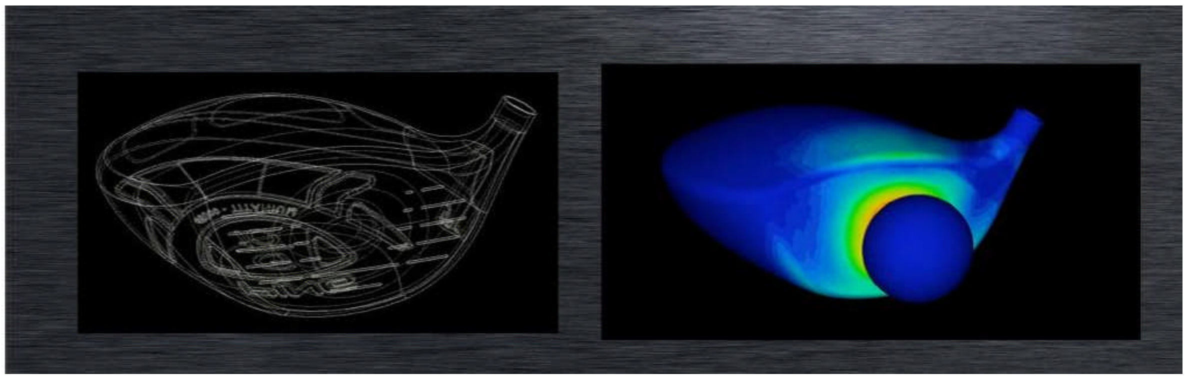
Industry Beginning to Replace Physical Design-build-test With Computational Design Through Analysis: "CAD→Mesh→Analyze"

- Boeing-New 747, 20% improvement lift/drag, 787 better, quieter
- Whirlpool designs washers, stoves, refrigerators,….
- Proctor and Gamble uses CE extensively
- Ping Golf
- Auto industry…..

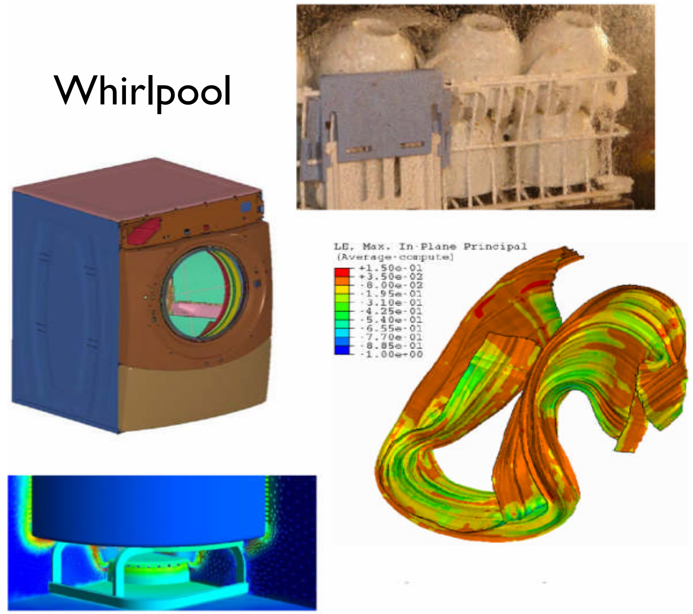
Boeing 787



Golf Clubs (and golf balls)



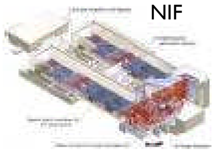
Whirlpool



Physics-based Computational Engineering helped the US build nuclear weapons and win the cold war.

- Nuclear weapons are complex, expensive, and hard to test
  - ~ 5 to 10 tests per system
- DOE NNSA uses computational tools for:
  - Design development, optimization, & analysis.
- DOE NNSA labs own the biggest supercomputers

Testing + Computer Power + Computational Design → Weapon Capability



Test ban

Underground

Air Tests

1,000,000 GigaFlops/s

0.000000001 GigaFlops/s

2010

Increasing Computational Design Capability

Improvements over time:

- Solution methods
- Spatial resolution
- Temporal resolution
- Geometric fidelity
  - 1-D to 2-D to 3-D
- Physics models
- …….

1945

Improved safety

Improved robustness

Improved yield to weight

MIRV (even lighter, smaller)

SLBM (even lighter, smaller)

ICBM (Lighter,smaller)

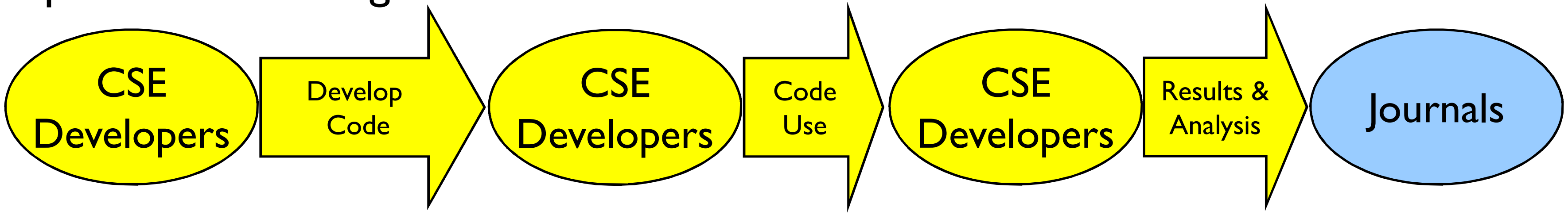
Heavy Hydrogen Bombs

Atomic Bombs

CSE and CE are very different, and CE has different challenges

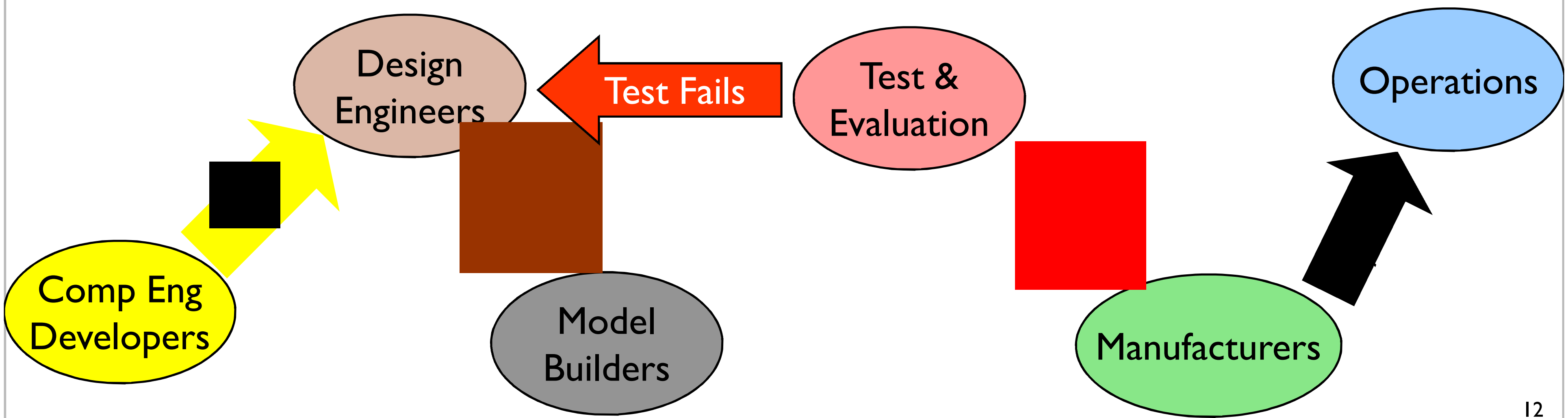
Computational Science and Engineering (CSE) is challenging:

- Develop a complex code, apply it to study a scientific research problem, and publish the findings.



Physics-Based Computational Engineering (CE)has different challenges:

- Develop a complex code, and support its use by other groups



It Takes A Village!

- **Sponsors** → Provide mission, resources and support
  - **Designers—End-users**

    → Engineers to use the tools to design products

    - **Codes**

      → Takes a good team ~ 10 years and ~ $100M to develop a complex code

    - **V&V**

      → Dedicated experiments and tests

    - **Computers**

      → Capability to develop codes and run the problems quickly and conveniently

What are the challenges? What can we do about them?

At Least Four Challenges arise from Complexity → Cope with it.

1. Complex physics and engineering
   – Integrated modules, scalable algorithms, best practices, **V&V**
2. Complex computers and computer architectures

   Multidisciplinary teams; good **tools**, design, practices, V&V
3. Complex customer organizations and culture

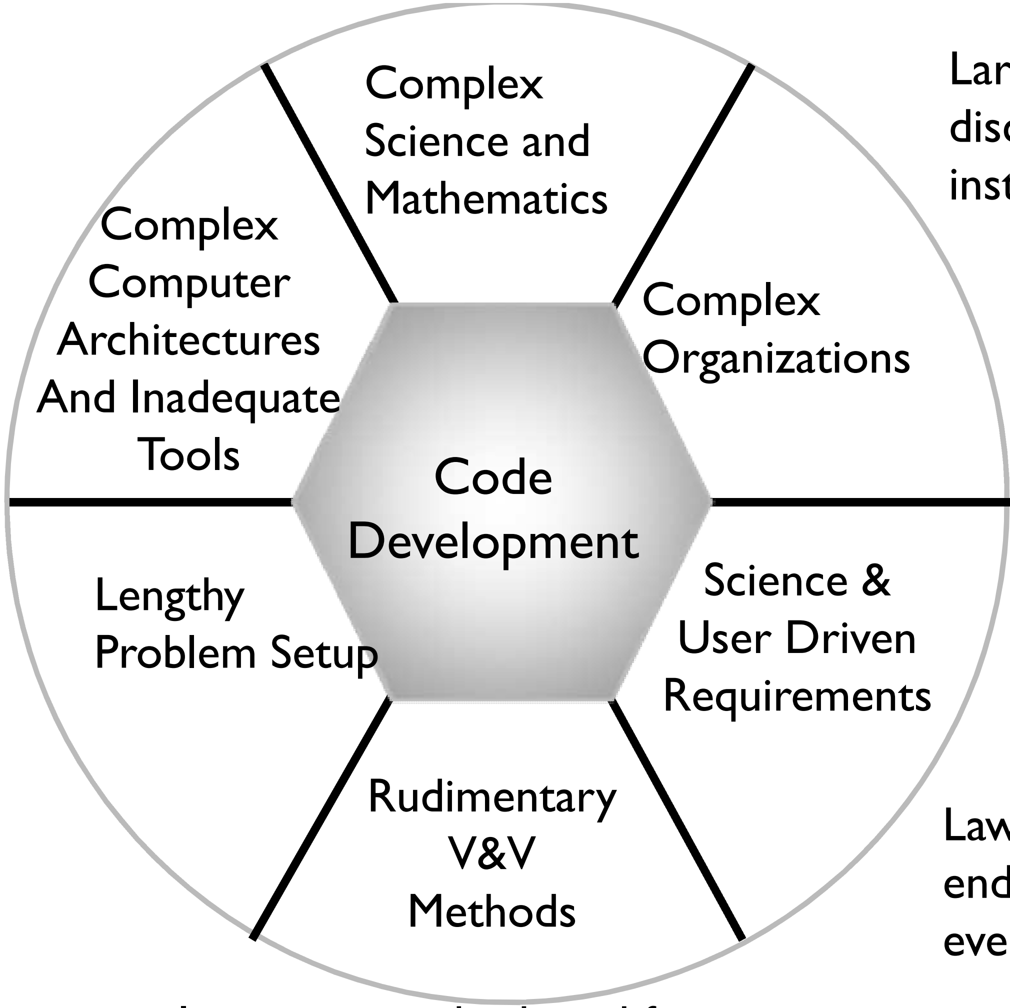
   Connect with stakeholders, deliver products early and continually during life of program, design for whole life cycle
4. Complex Development Organizations → "Code development will no be longer a cottage industry!"—Brendan Godfrey, AFOSR
   – Big codes require explicit funding for code development→ large funding brings lots of management attention, oversight, reporting and guidance, whether it helps or not!

Computational Engineering Code Developer's World – Six Major Challenges

Many strongly coupled effects and massively parallel computers

Zillions of complex processors linked with complicated and slow networks + Little help for dealing with this complexity

Problem setup (e.g. mesh generation) takes too long for rapid design development



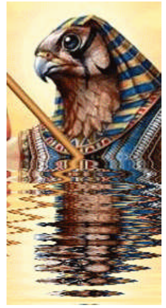
Large, multi-disciplinary, multi-institutional teams

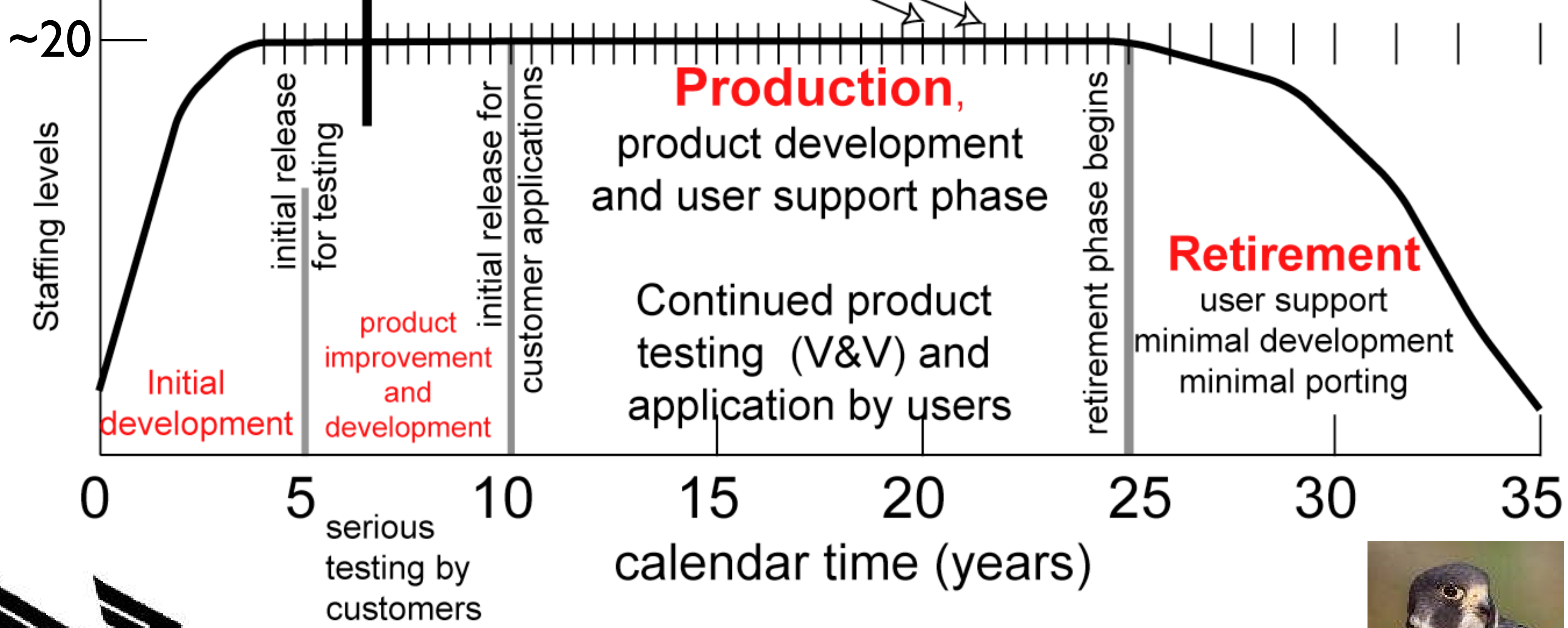
Computer security and high fuel costs pose major barriers

Laws of nature & end-user needs win every time

Immature methods and few validation experiments

Developing a Large, Multi-scale, Multi-physics CE Code Takes a Large Team a Long Time

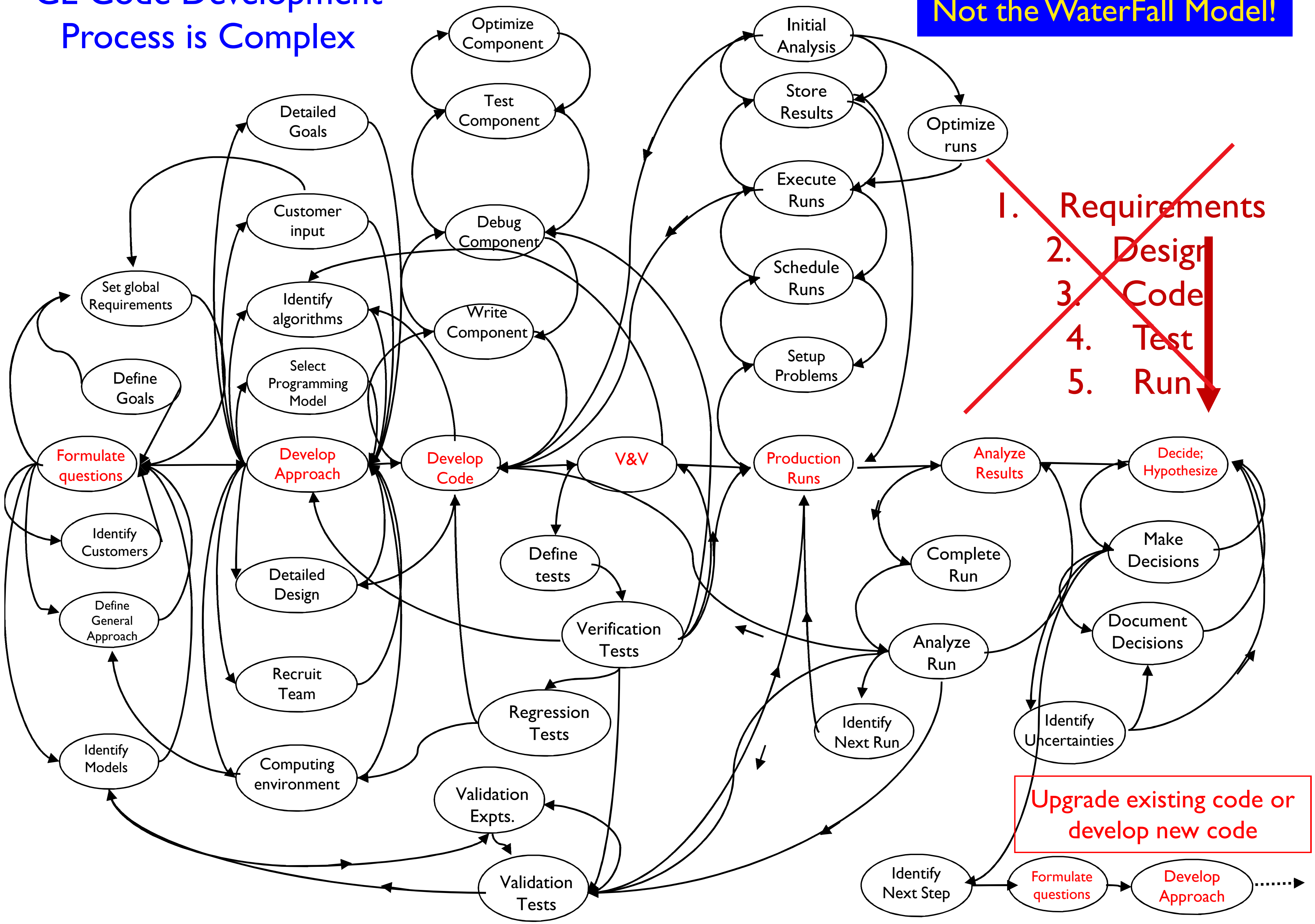




From: D. Post, R. Kendall and E. Whitney, "Case Study of the Falcon Code Project", Proceedings of the Workshop on Software Engineering for High Performance Computing, International Conference on Software Engineering, May 15, 2005, St. Louis, Missouri.

CE Code Development Process is Complex

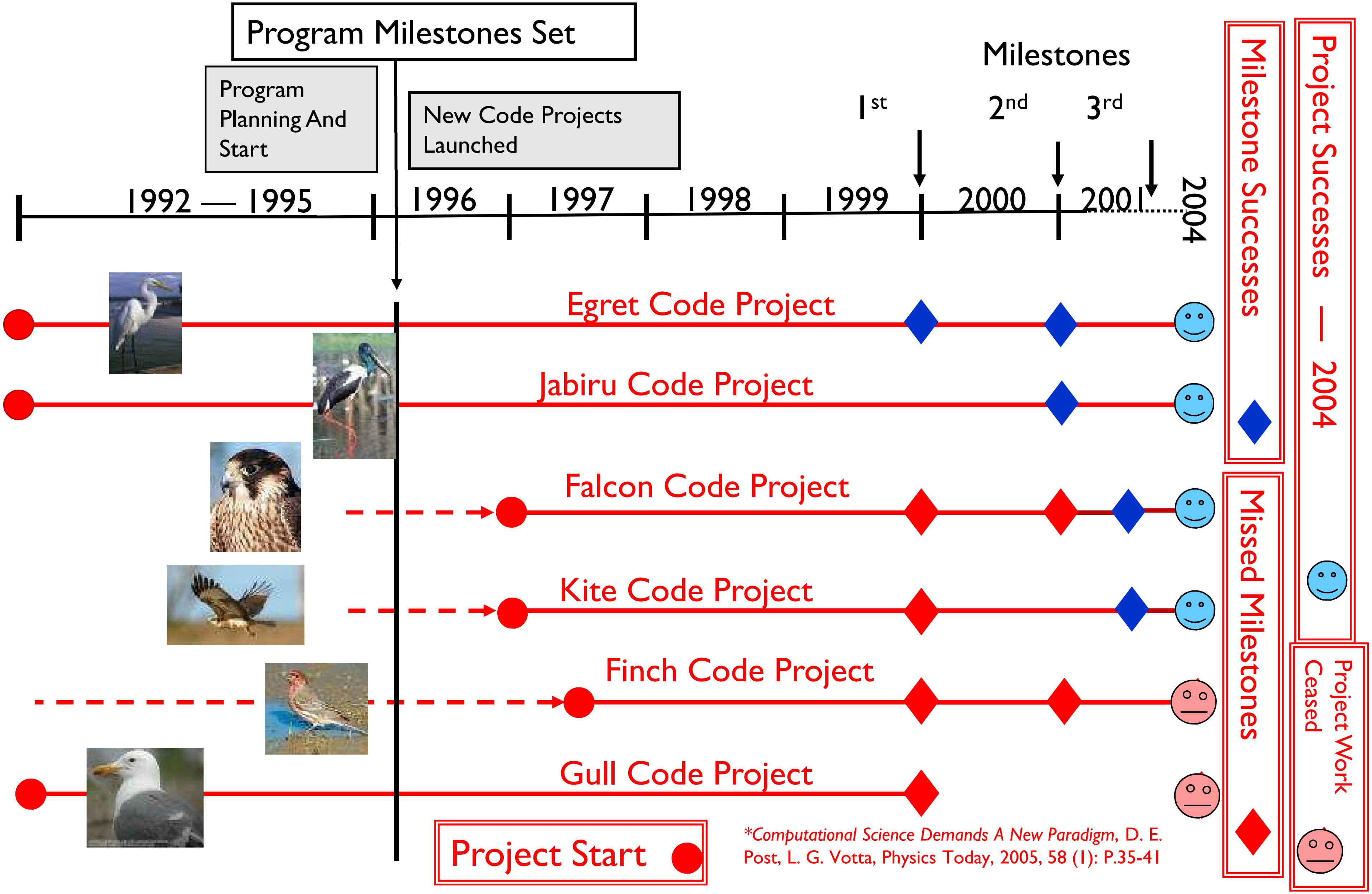
Not the WaterFall Model!



—D. E. Post, R. P. Kendall, Large-Scale Computational Scientific and Engineering Project Development and Production Workflows, CTWatch (2006), vol.2-4B,pp68-76.

Computational Engineering Code Development is Risky!

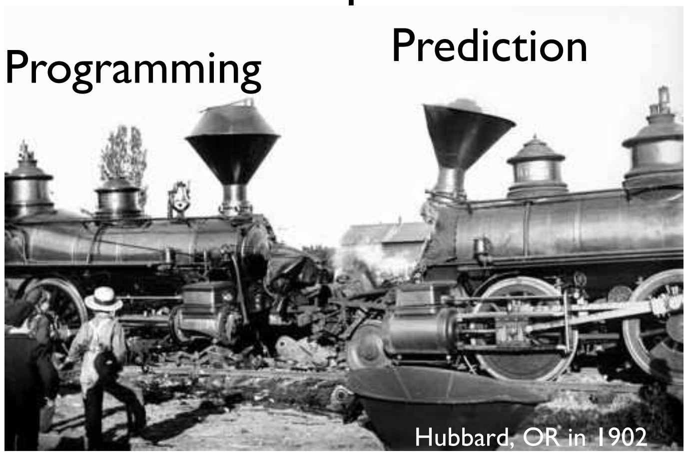
Code Project Schedule For Six Large-scale Physics-based CBE Codes



**Computational Science Demands A New Paradigm*, D. E. Post, L. G. Votta, Physics Today, 2005, 58 (1): P.35-41

Another Perspective---Three Challenges
Performance, Programming and Prediction

1. Performance Challenge - Computers power increasing through growing complexity
   - Massive parallelization, multi-core & heterogeneous (CELL, FPGA, GPU…) processors, complex memory hierarchies…..
2. Programming Challenge -Program Massively Parallel Computers
   - Rapid code development of codes with good performance
3. Prediction Challenge —Developing predictive codes with complex scientific models
   - Develop accurate predictive codes
     - Verification
     - Validation
     - Code Project Management



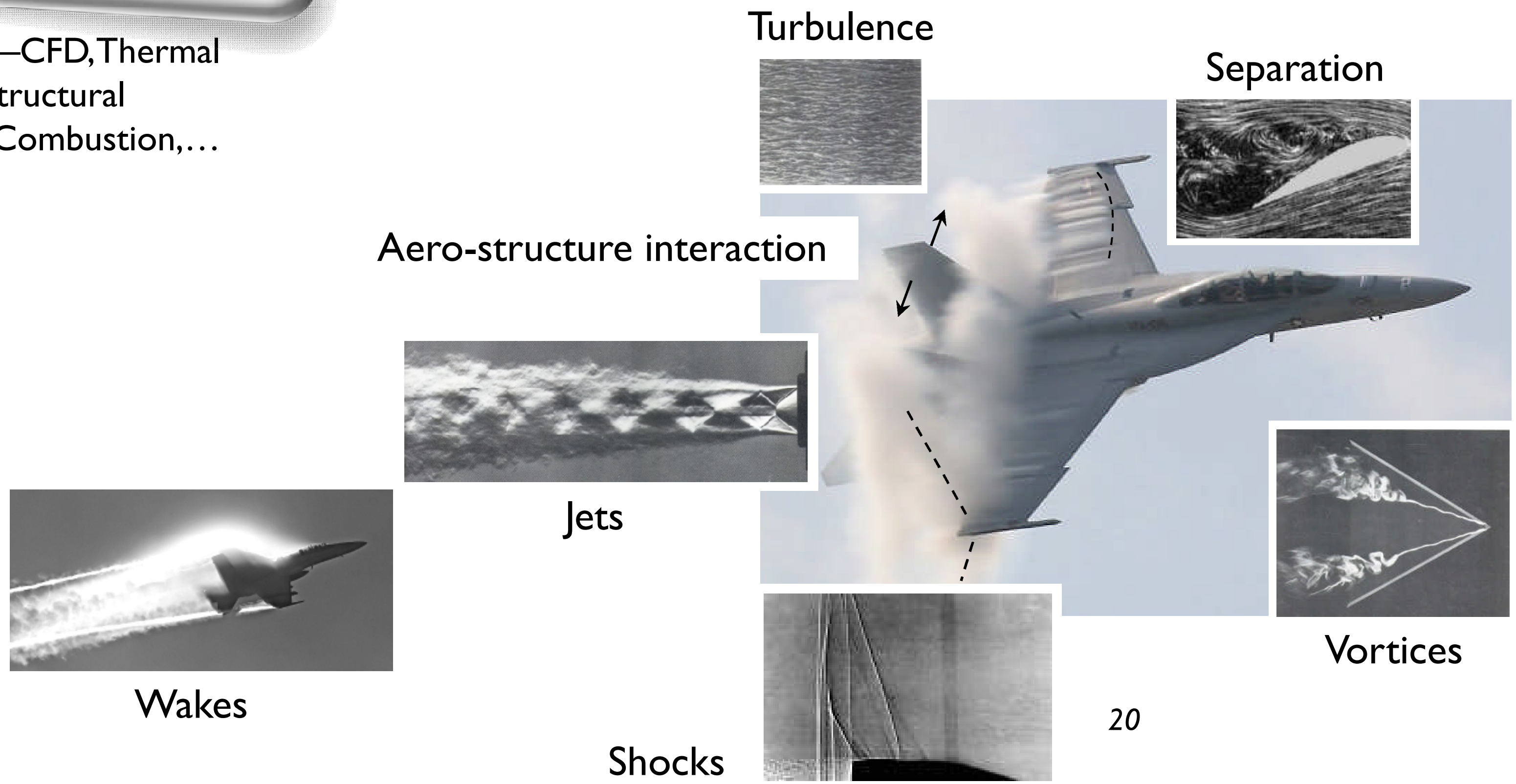
- Train wreck coming between the last two
- Better software development and production tools are desperately needed for us to take full advantage of computers

Multi-Disciplinary Optimization Challenge → Integrate Many Multi-Scale Physics Effects

Many different physics elements govern aircraft behavior

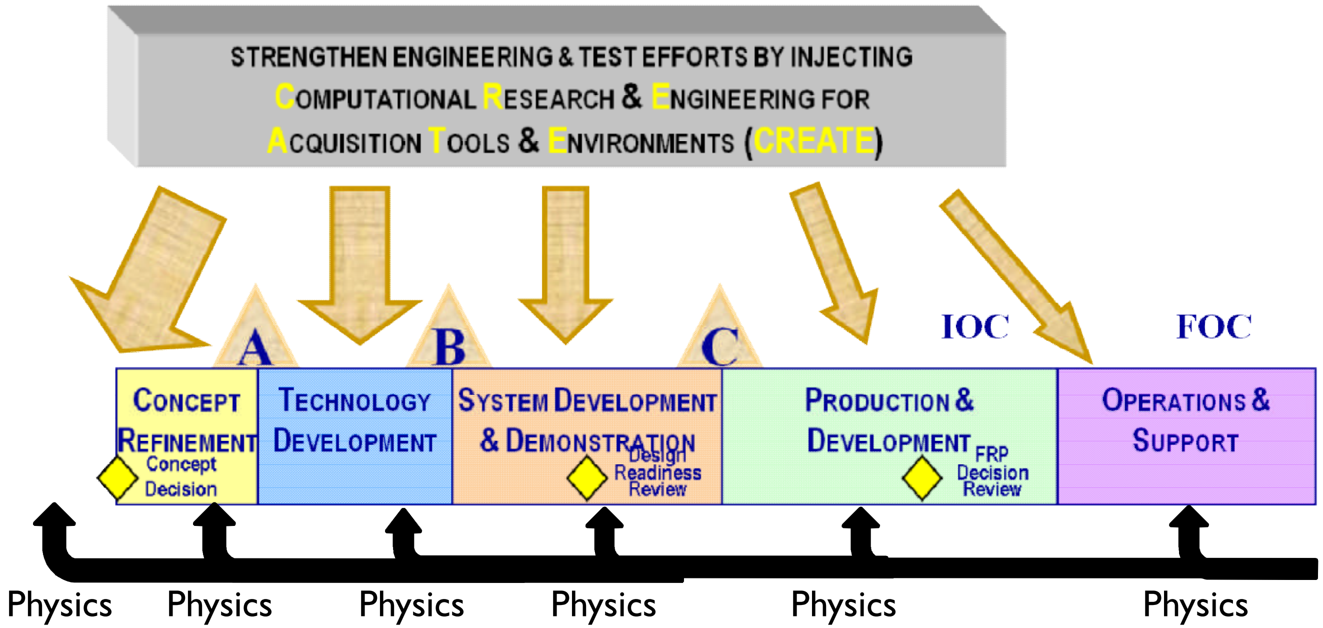
Propulsion—CFD, Thermal transport, Structural Mechanics, Combustion,…

- Turbulent CFD, structural layout, structural mechanics, flight control, structural layout, signatures, sensor design and integration, materials strength, response, crack propagation…..



Computational Research and Engineering Acquisition Tools and Environments (CREATE)

- **CREATE goal is to enable major improvements in the DoD acquisition process**
  - **Replace design paradigm based on historical data and experimental testing with physics-based computational design validated with experimental testing**
  - **Detect and fix design flaws early in the design process**
  - **Develop optimized designs for new concepts**
  - **Begin system integration earlier in the acquisition process**
  - **Increase acquisition program flexibility and agility to respond to rapidly changing requirements**
  - **Enhance the productivity of the DoD engineering workforce**
  - **Establish DoD capability to develop and Deploy these tools**

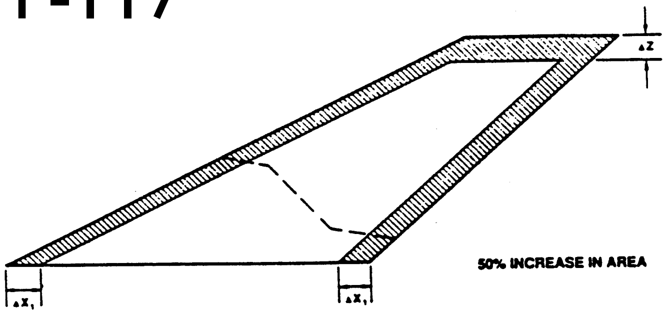


Acquisition Challenge Examples

Fighters– Vertical Tail Size; Ships-Capsize Stability

- F-100, F102, F-105, F7U, F11F, F-16, F117
- All Needed to increase tail fin size between 25% to 50% after initial design

F-117



Defense News 04/02/07

"Is New U.S. Destroyer Unstable?"

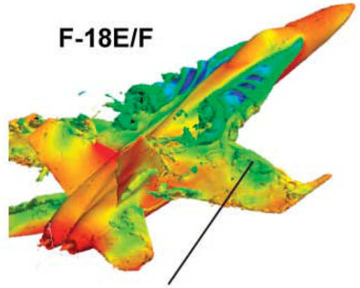
- Lesson Learned: Can't base radically new designs on historical experience, it's not a good guide
- Need physics-based design tools to extrapolate

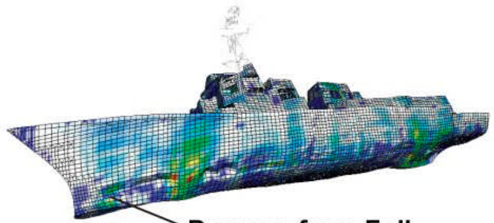
Computational Research and Engineering Acquisition Tools and Environments

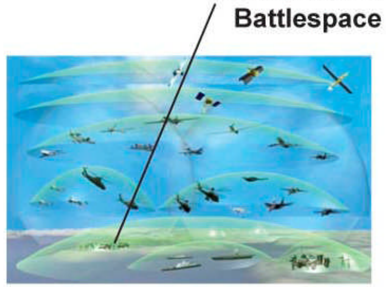
CREATE

Computational Research & Engineering for Acquisition Tools & Environments

- **$360M 12-year program to develop & deploy 3 computational engineering tool sets for acquisition engineers**
- **Air Vehicle design tools**: Aerodynamics**, air frame, propulsion, control,** early rapid design
- **Ship design tools: Early-stage design, shock damage and hydrodynamics performance**
- **RF Antenna design tools: RF Antenna performance and integration with platforms**
  - + **Geometry and Mesh Generation**







CREATE Air Vehicles Projects address major aircraft design challenges

Proposed Computational Engineering Software Products and Activity

Technical & Development

- DaVinci: Conceptual Design, next generation software to enable CSE insertion into early phase acquisition, advanced conceptual design, and virtual prototyping

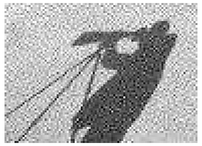
- KESTREL: Next generation high-fidelity multi-physics simulation for *FIXED-WING* air vehicles

- HELIOS: Next generation high-fidelity multi-physics simulation for *ROTARY-WING* air vehicles

- Firebolt: Next generation software to enable high-fidelity analysis of AIRFRAME/PROPULSION INTEGRATION

Transition & V&V

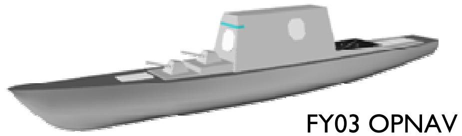
- SHADOW-OPS: Primary mechanism to validate AV CSE software products and process changes to targeted acquisition workflows; transition CREATE-AV technology into acquisition workforce; and to build bridges between AV CSE software development teams and targeted acquisition organizations.



CREATE-Ships Goal: Develop Optimized Total Warship Designs

Develop computational tools for:

1. **Rapid Design Capability and Design Synthesis**
   – Rapid development, assessment, and integration of candidate ship designs to avoid cost versus capability mismatches
2. **Ship Hydrodynamics**
   – Accelerate and improve all stages of ship hydrodynamic design
3. **Ship Shock & Damage**
   – Provide analysis of shock and damage effects and reduce need for tests to assess ship shock and damage effects



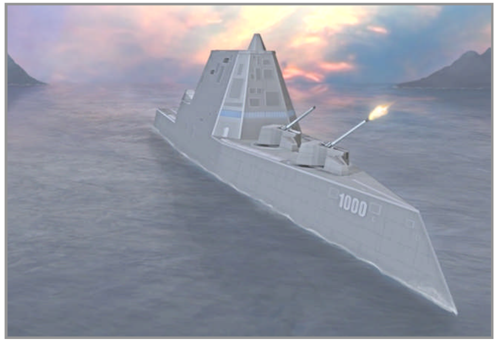
FY03 OPNAV Sponsored Cruiser Concept

CREATE-RF Tool Vision

Geometry Creation
Commercial CAD Tools

Mesh Generation
CREATE-MG

Boundary Condition &
Material Specification
SENTRI / Pre-Processing



First-Order Codes
Waveguides,
Infinite Periodic Structures,
Antenna Apertures in Ground Plane,
Small Antenna Systems

SENTRI / Workstation

High-Fidelity Codes

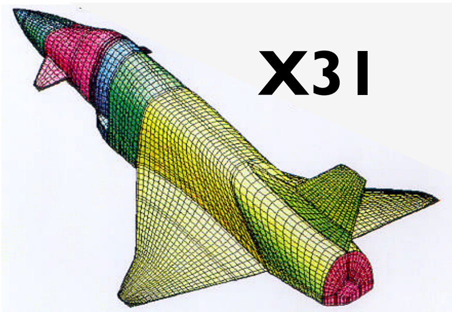
Large Antennas,
Antennas on Platforms,
Antenna Interference

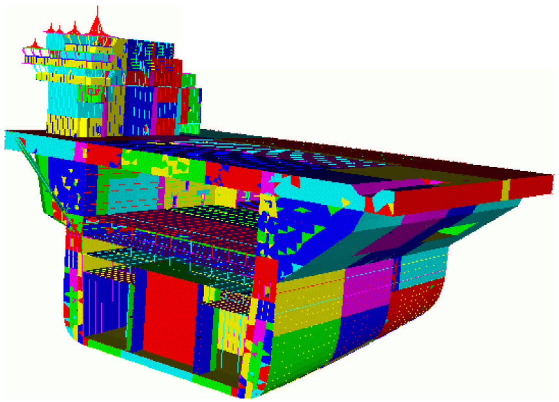
SENTRI / HPC

Near Field Imaging
SENTRI / Post-Processing

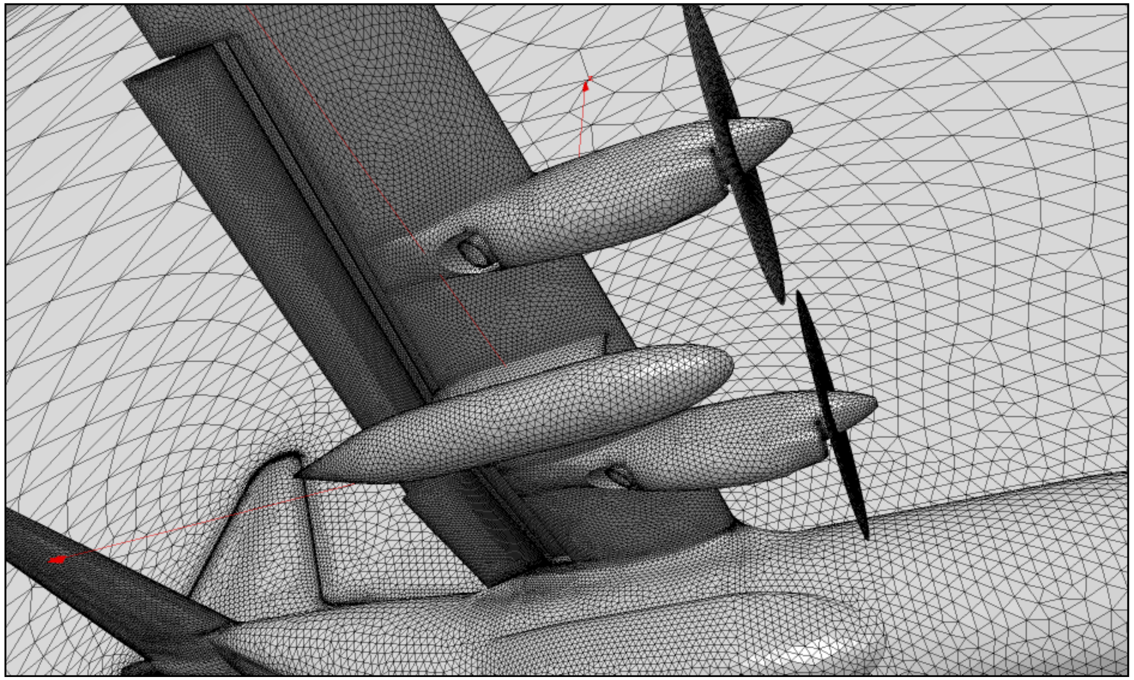
Mesh and Geometry Generation (MG) Project being launched

- Problem Generation takes up to 90% of the calendar time
- Every project needs geometry and mesh generation
- Modeling and Geometry Interactive (MG) will provide the geometry and meshing tools needed by all the projects

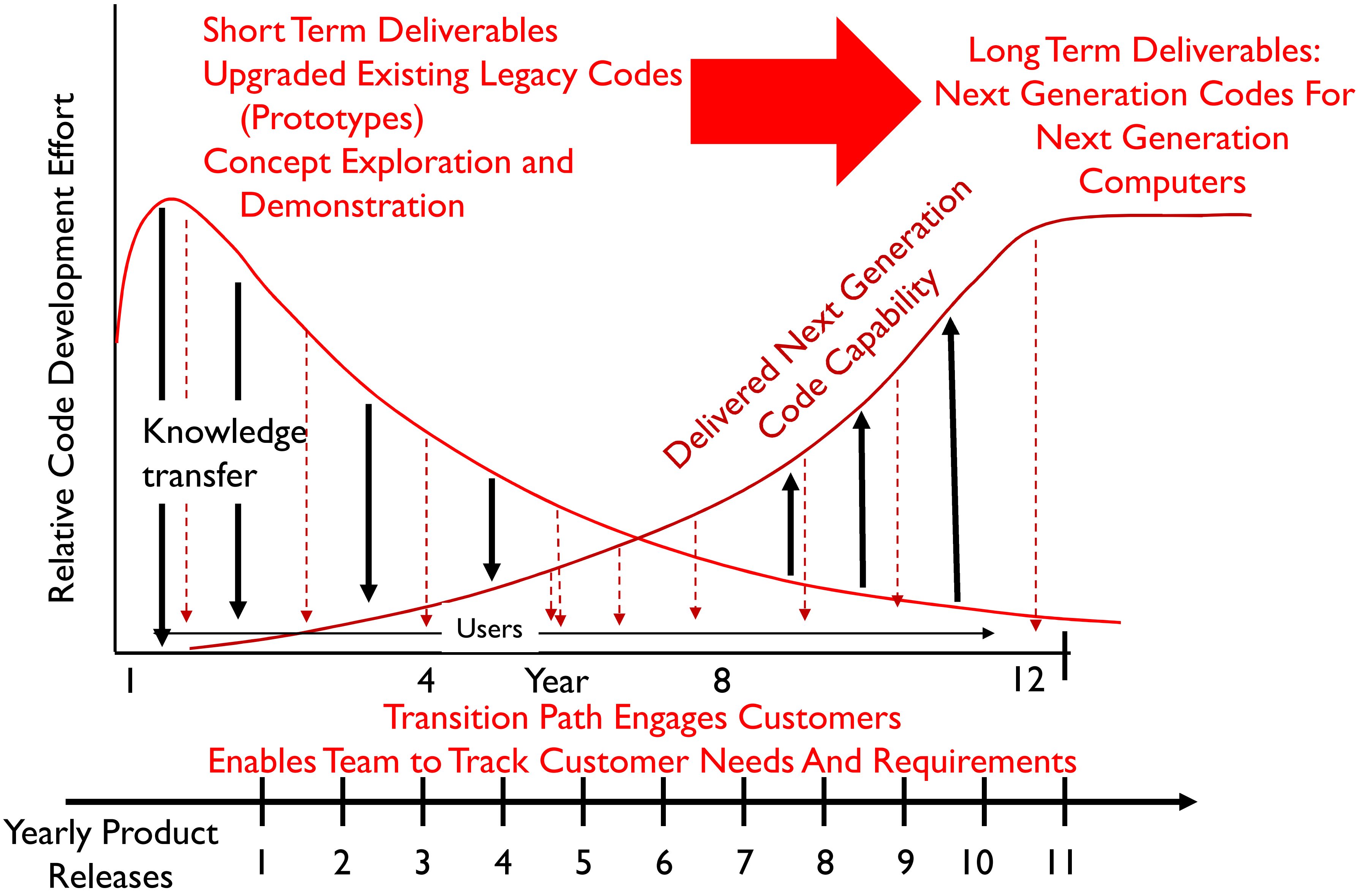




C-130



Systems Engineering and Acquisition Approach: Begin With Prototype Codes and Replace Them With Next Generation Codes



CREATE Status

- Project Teams formed
- Requirements developed and validated
- Initial plans developed and development started
- First deliverables planned for this summer and fall (upgraded legacy codes)
- Software Engineering Practices and Plans being formed
- Six version 1.0 releases this calendar year

Our Community is Beginning to Work Out How to Develop Software

Software Engineering Practices

Goal is maintainable, extensible, portable and reliable software products

1. Requirements Management and Stakeholder Engagement
2. Software Quality Attributes
3. Design and Implementation
4. Software Configuration Management
5. Verification and Validation of CREATE Products
6. Software Release
7. Customer Support

Documents: Manuals: Technical, Developers, Users

Plans: Test, V&V, Risk, Development (EVMS), Financial, Management

You have an exciting future!!!!

- Computational Science is revolutionizing scientific discovery
- Physics-based Computationally engineering will revolutionize the way we design and build machines
- You are coming in on the ground floor!!!!
- Your generation has the computer skills and cultural orientation
- You need only to acquire the subject matter skills, be fanatic about Verification and Validation and customer focus,
  - and the world is yours