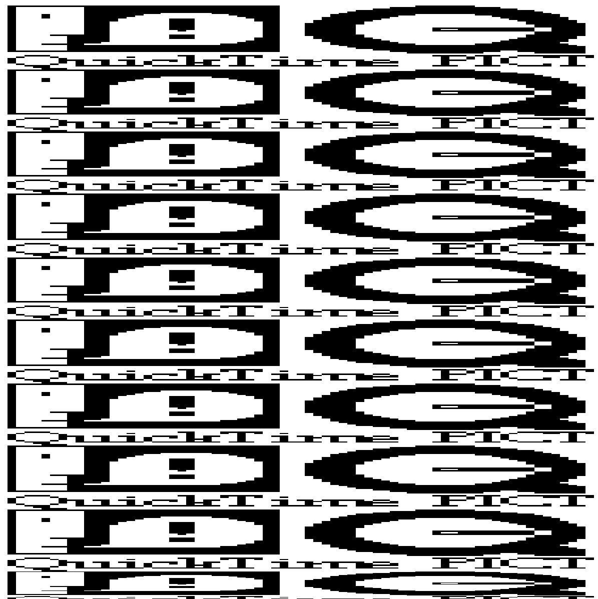
Independent Assessment

High Performance Computing & Communications Program

Earth and Space Sciences (ESS) Project



Jim Fischer/GSFC, Project Manager

Robert Ferraro/JPL, Associate Project Manager

June 19-21, 2000

NASA Ames Research Center

Overview

ESS Presentation Agenda

- **Overview**
- **ESS Goal**
- **ESS Objectives**
- **Changes in ESS objectives since the last IAR**
- **ESS Implementation approach** (FY00-04)
- **ESS Management organization**
- **ESS Phase-II Program/Project milestone plan**
  - ESS Program Milestone "Roadmap" as a Component of the HPCC Goals and Milestones
  - Program/Project milestones organized by PCA
  - Program/Project milestones organized by WBS
- **ESS Phase-I Program milestone status**
  - 1997 Program Plan Milestone Crosswalk
  - ESS Accomplishments to the Prior PCAs since the last IAR
- **ESS Phase-II Program milestone status**
  - ESS Project Milestones as Components of the HPCC Program Goals and Milestones
  - Key ESS Project Milestones Share Metrics with Program Milestones
  - Program milestone status by PCA (X charts)
- **ESS Resource Summaries**
  - Budget by WBS (6-digit FY 00-04)
  - Budget by PCA (FY 00-04)
  - Workforce by __ (FY00-04)
- **Issues**
- **Backup Material**
  - ESS Guest Investigators (Groups-4 and 5)
  - CAS Investigators using the ESS Testbed (1999 selections)

Background Material

- ESS Project Plan, June 2000 draft - provided to IAR Panelists in a pre-IAR mailing

Goal of the ESS Project

Goal

Demonstrate the power of high-end and scalable cost-effective computing environments to further our understanding and ability to predict the dynamic interaction of physical, chemical, and biological processes affecting the Earth, the solar-terrestrial environment, and the universe. *- HPCC Program Plan - June 2000*

Objectives of the ESS Project

Customer Impact Objective

- *Infuse HPCCP technologies into mission critical stakeholder Enterprise/Office processes, document discernible improvements in the stakeholders' processes and, if possible, document discernible improvements in the final products as a result of the use of HPCC technologies.*

Computational and Communication Performance Objective

- *Dramatically increase the computer and communication performance available for use in meeting NASA mission requirements.*

Interoperability Objective

- *Dramatically increase the interoperability of application and system software operating on high-performance computing and communications systems available for use in meeting NASA mission requirements.*

Portability Objective

- *Dramatically improve the portability of application software and data to new or reconfigured high-performance computing and communications systems available for use in meeting NASA mission requirements.*

Customer Usability Objective

- *Dramatically improve the usability of high-performance computing and communications tools and techniques available for use in meeting NASA mission requirements.*

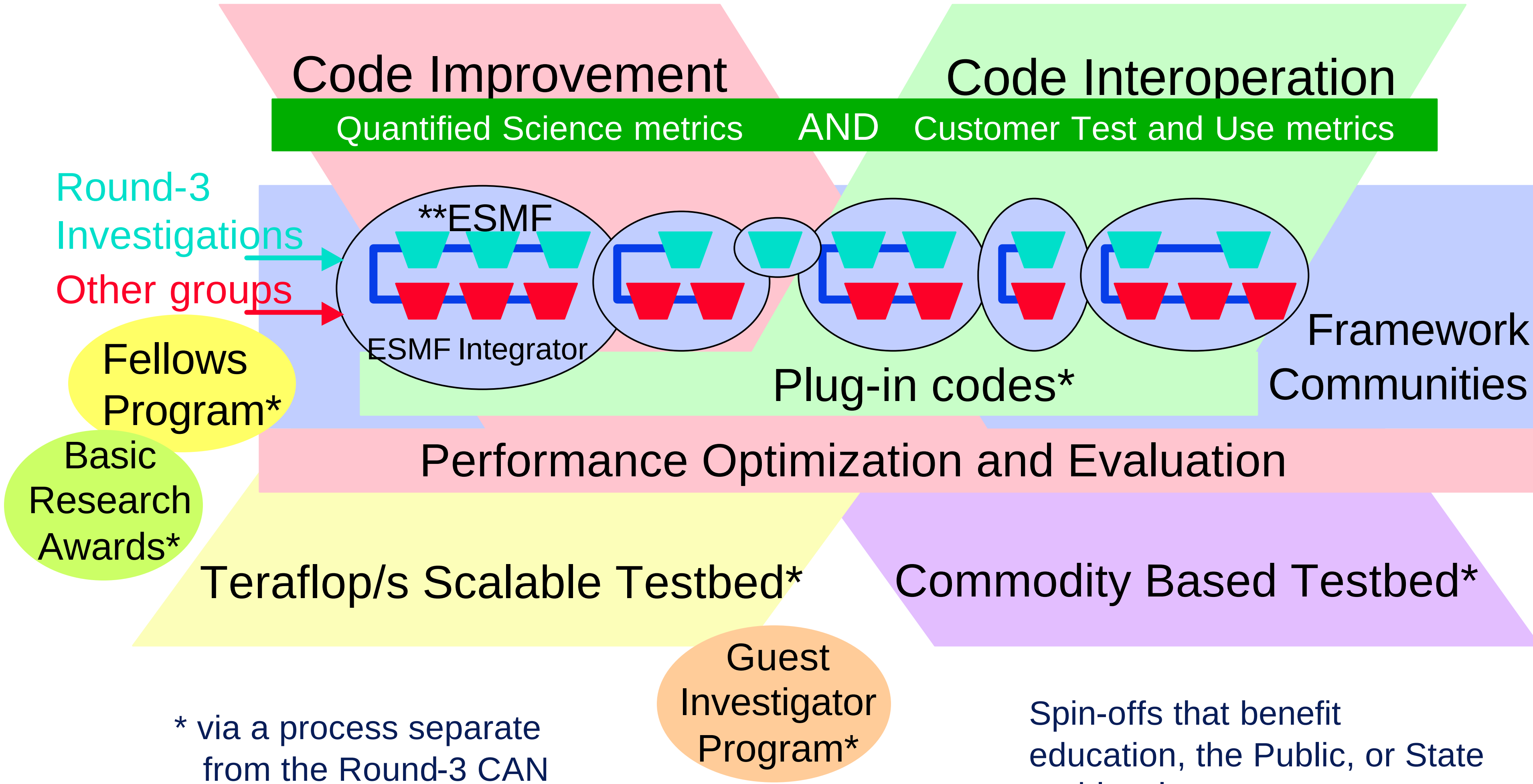
Changes in ESS Objectives Since the Last IAR

Increased emphasis on broad impact of developed technologies
- **Application code interoperability and portability**
- **Sustained customer use**
- **Software tools**
- **Impact to the public, education, state and local governments**

Increased emphasis on use of NASA data

To be presented as a 12 step animation

ESS Implementation Approach (FY00-04)

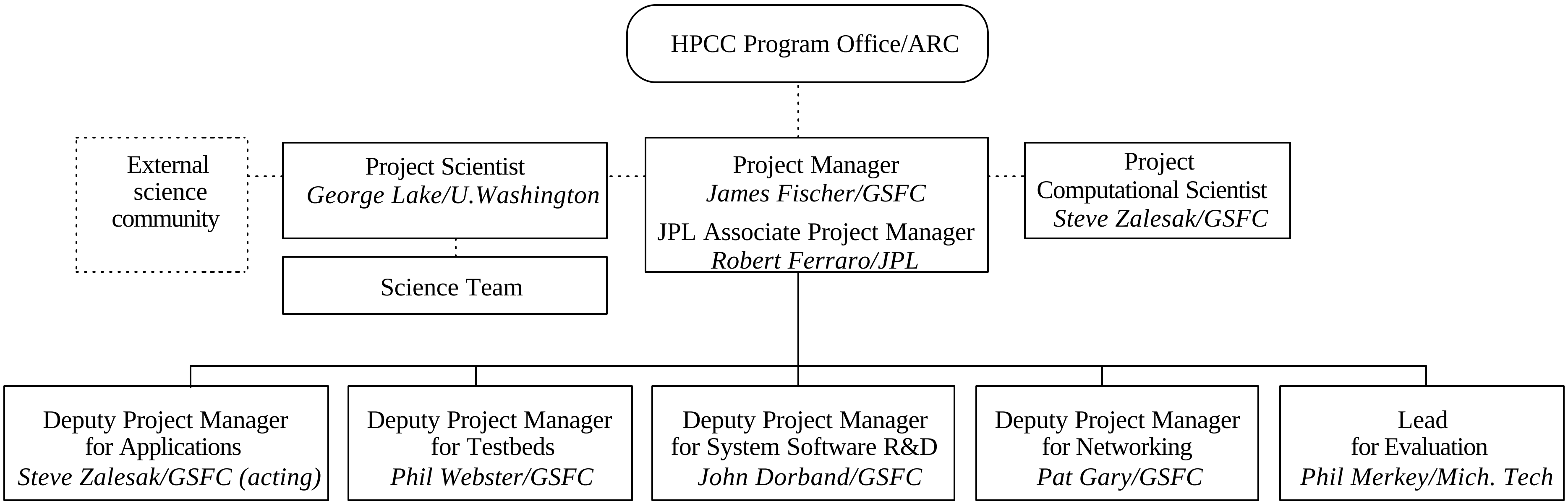


* via a process separate from the Round-3 CAN

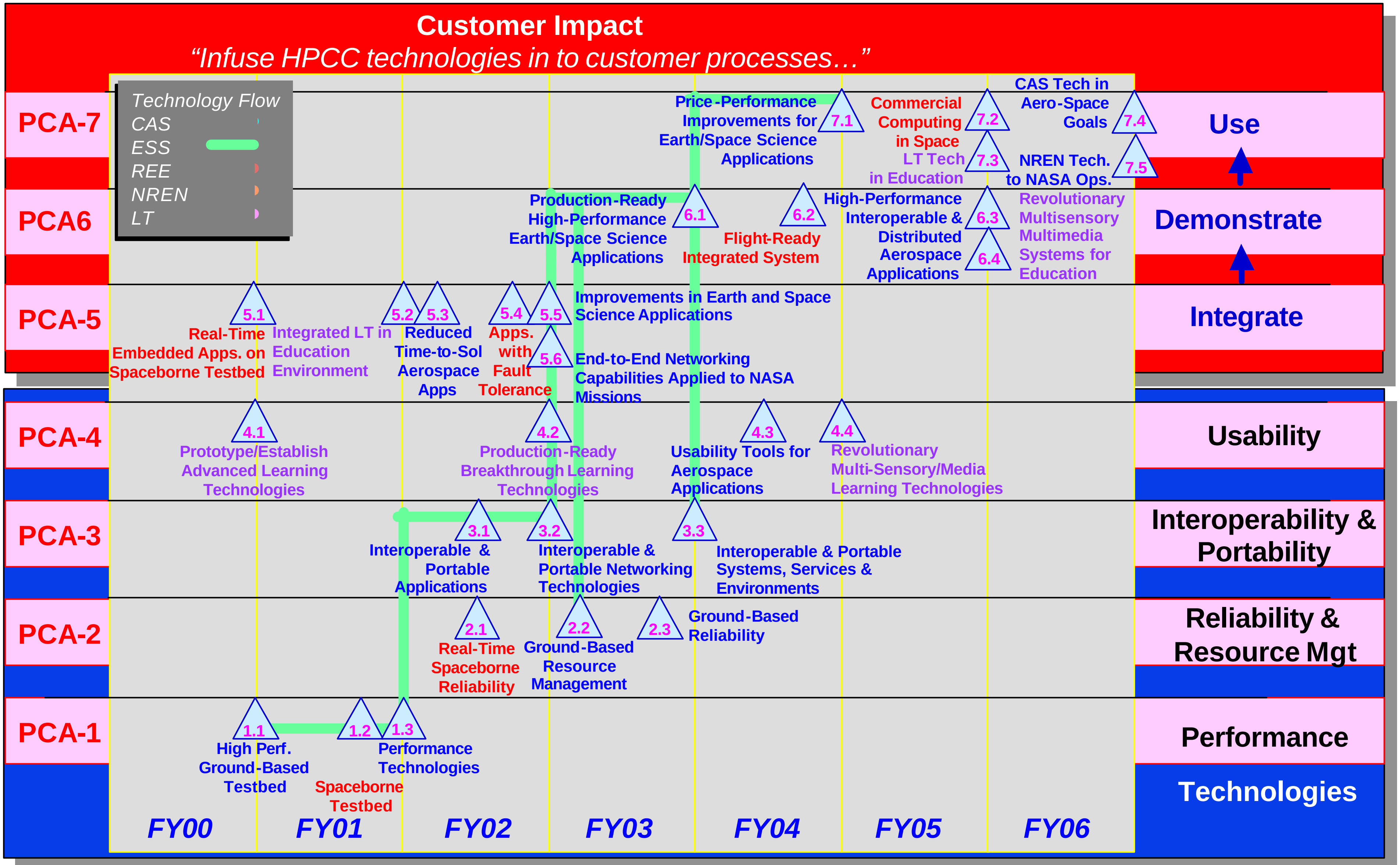
** Earth System Modeling Framework (ESMF)

Spin-offs that benefit education, the Public, or State and local governments.

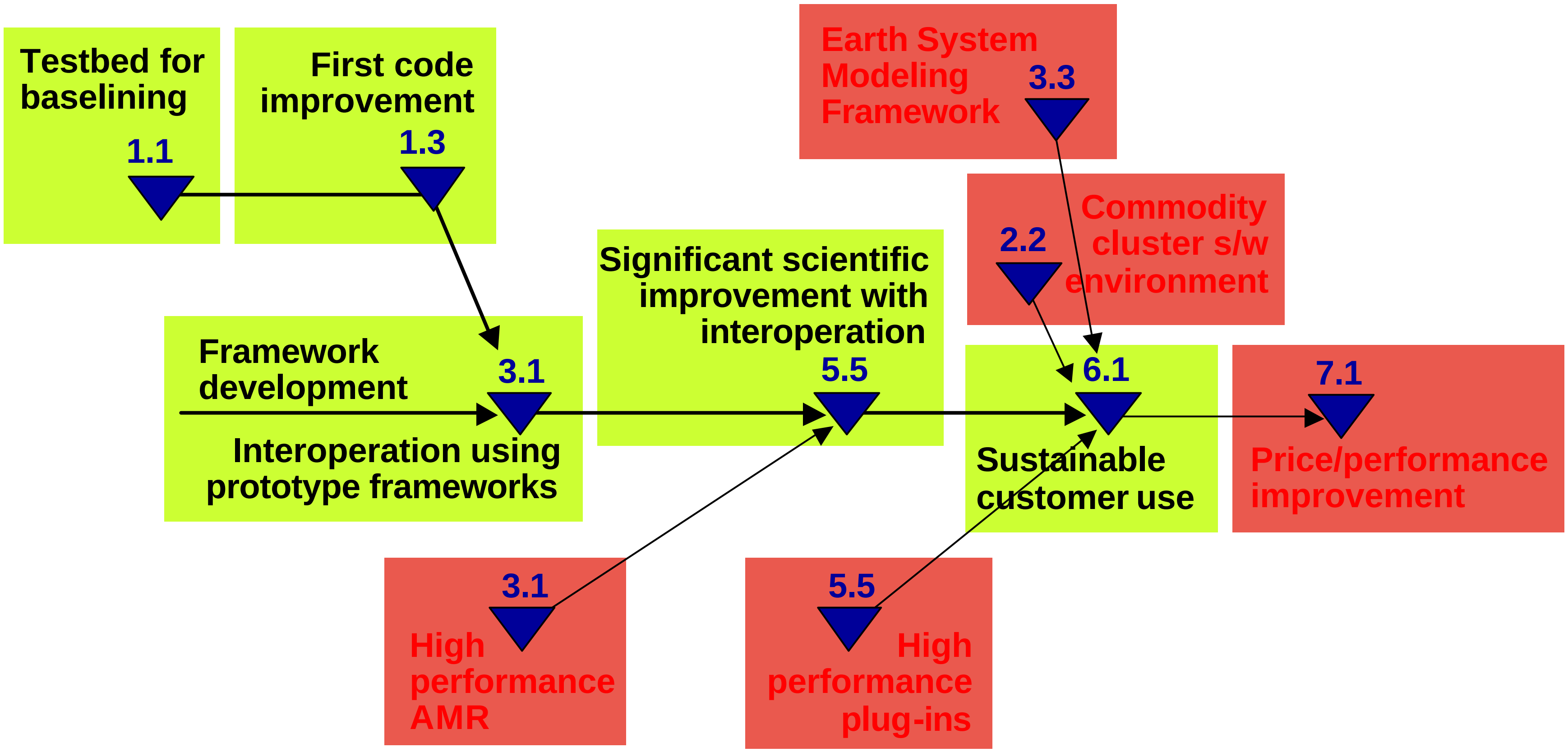
ESS Management Organization



HPCC Program Technology Flow
- ESS -



Roadmap
Program Milestones Organized by PCA



Legend:
Program milestone number (a.b = PCA.sequence#) 1.1
Involves **all** Investigators
Involves **some** Investigators

Program/Project Milestones Organized by PCA

PCA-1 Develop component technologies for performance

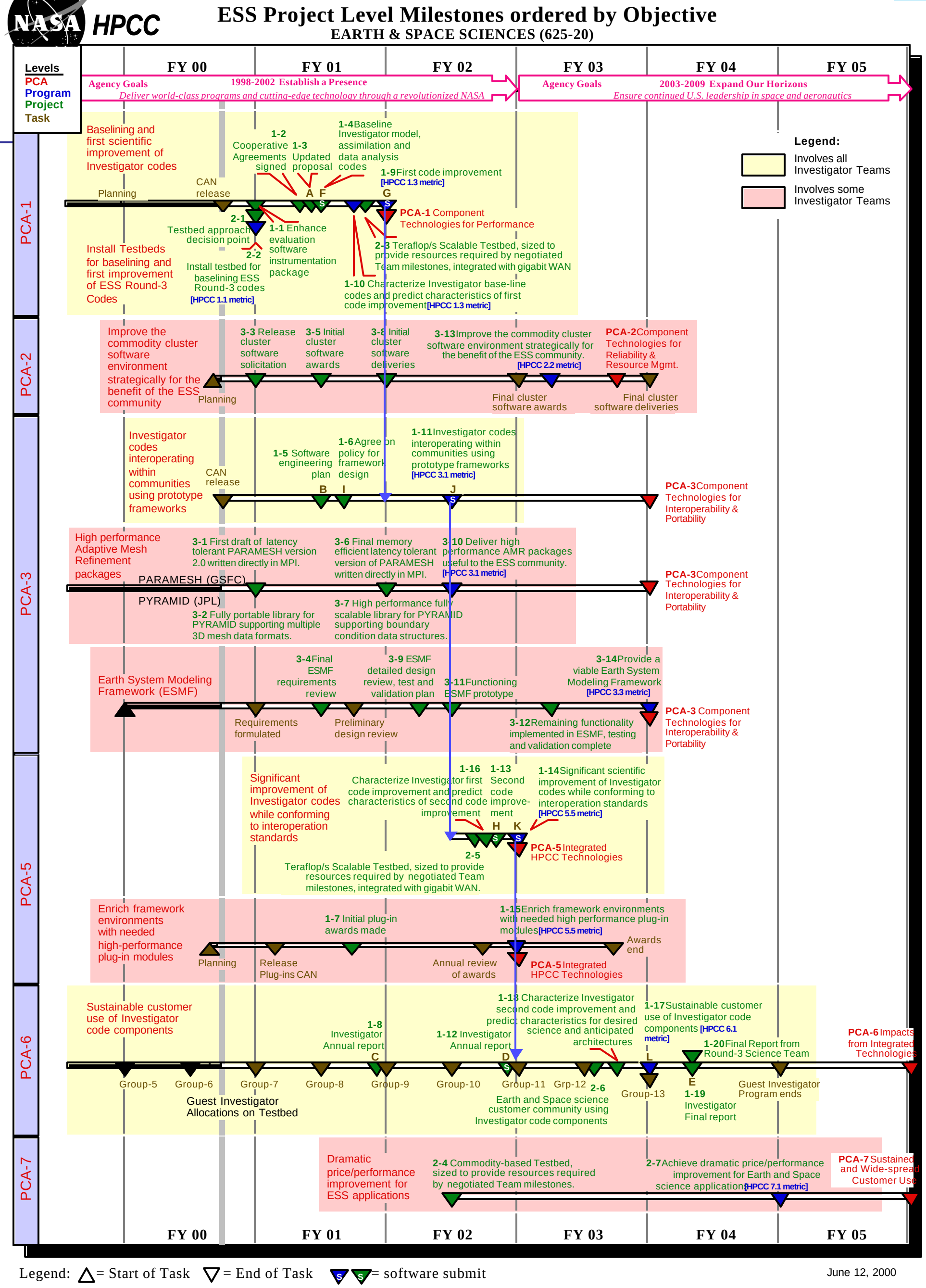
PCA-2 Develop component technologies for reliability and resources management

PCA-3 Develop component technologies for interoperability and portability

PCA-5 Demonstrate integrated HPCC technologies

PCA-6 Demonstrate significant engineering, scientific, and educational impacts from integrated HPCC technologies

PCA-7 Establish sustainable and wide-spread customer use of HPCC Program technologies



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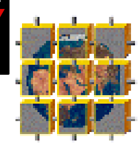
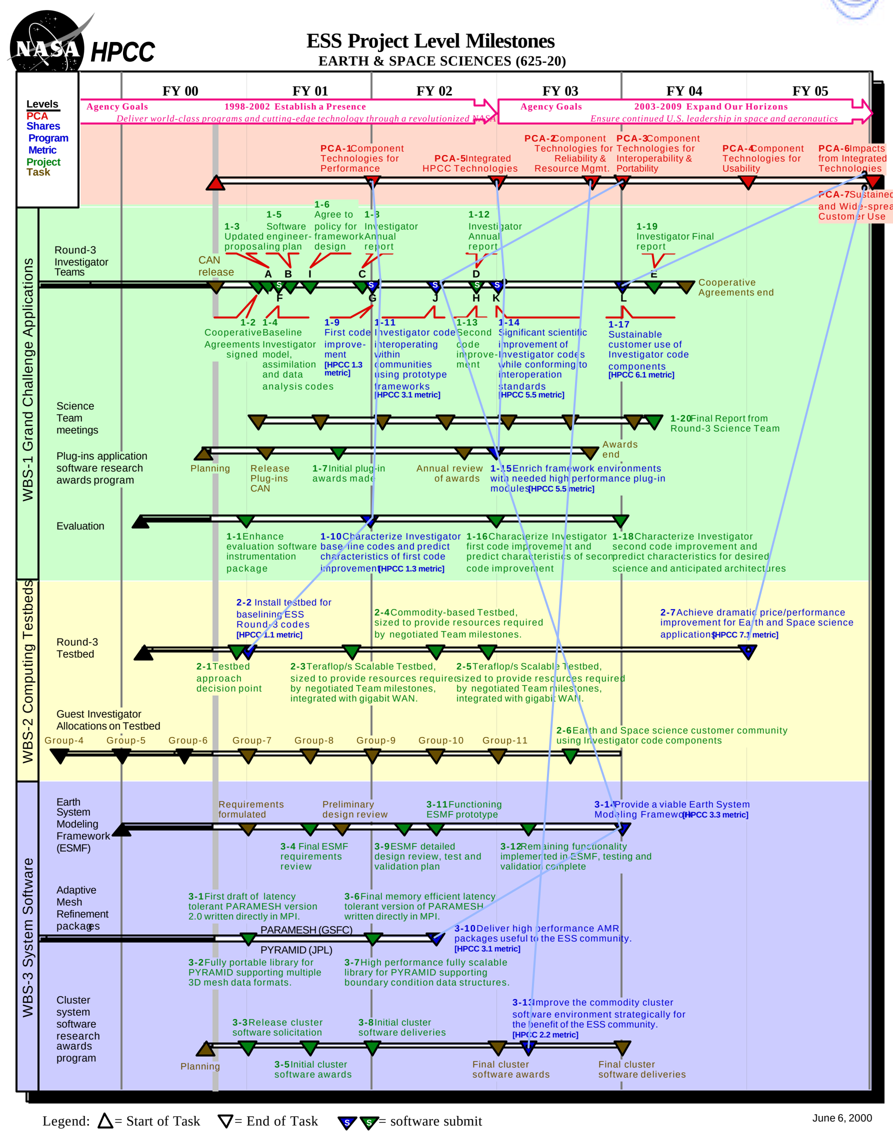


Program/Project Milestones Organized by WBS

1. Round-3 Investigator Teams
2. Round-3 Science Team
3. Plug-ins Application Software Research Awards Program
4. Evaluation
5. Round-3 Testbeds
6. Guest Investigator Allocations on Testbed
7. Earth System Modeling Framework (ESMF)
8. Adaptive Mesh Refinement Packages
9. Cluster System Software Research Awards Program



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Colorize background to distinguish the 9 threads to be presented

and

Identify each thread with an icon for later reference

ESS Phase-I

Phase I Program Milestone Status and Cross Walk

(Extracted from January 1997 Program Plan as updated by April 1999 PCA)

HPCC NASA

Grand Challenge Milestones

#	Due Date	Comp Date	IAR Review
GC1	6/93	6/93	Prior IAR
GC2	9/96	9/96	Prior IAR
GC3	9/97	9/97	Prior IAR
GC4	9/97	9/97	Prior IAR
GC5	6/99	3/99	IAR 2000-Phase I
GC6	3/00	Open	IAR 2000-Phase II
GC7	9/01		IAR 2000-Phase II
GC8	9/03		IAR 2000-Phase II
GC9	9/03		IAR 2000-Phase II

NASA Research and Education Network Milestones

#	Due Date	Comp Date	IAR Review
NR1	6/93	6/93	Prior IAR
NR2	9/94	12/94	Prior IAR
NR3	6/95	9/95	Prior IAR
NR4	9/95	9/95	Prior IAR
NR5	3/96	3/96	Prior IAR
NR6	9/97	9/97	Prior IAR
NR7	10/98	10/98	IAR 2000-Phase I
NR8	3/00	3/00	IAR 2000-Phase I
NR9	9/02		IAR 2000-Phase II
NR11	6/04		IAR 2000-Phase II

Computing Testbeds Milestones

#	Due Date	Comp Date	IAR Review
CT1	12/92	12/92	Prior IAR
CT2	9/93	9/93	Prior IAR
CT3	6/94	6/94	Prior IAR
CT4	9/96	6/97	Prior IAR
CT5	12/96	12/96	Prior IAR
CT6	9/97	9/97	Prior IAR
CT7	6/98	10/98	IAR 2000-Phase I
CT8	12/99	Open	IAR 2000-Phase II
CT9	9/00		IAR 2000-Phase II
CT10	6/02		IAR 2000-Phase II

Information Infrasstructure Technology and Applications Milestones

#	Due Date	Comp Date	IAR Review
II1	12/93	12/93	Prior IAR
II2	9/95	9/95	Prior IAR
II3	9/94	8/94	Prior IAR
II4	9/95	9/95	Prior IAR
II5	9/96	9/96	Prior IAR
II6	9/94	8/94	Prior IAR
II7	9/95	9/95	Prior IAR

Basic Research and Human Resources Milestones

#	Due Date	Comp Date	IAR Review
BR1	9/96	9/96	Prior IAR
BR2	9/97	9/97	Prior IAR
BR3	Yearly	Yearly	Prior/Phase I

System Software Milestones

#	Due Date	Comp Date	IAR Review
SS1	9/96	9/96	Prior IAR
SS2	9/97	9/97	Prior IAR
SS3	9/98	9/98	IAR 2000-Phase I
SS4	9/99	9/99	IAR 2000-Phase I
SS5	9/00		IAR 2000-Phase II
SS6	3/01		IAR 2000-Phase II
SS7	9/01		IAR 2000-Phase II
SS8	12/01		IAR 2000-Phase II

Learning Technologies Milestones

#	Due Date	Comp Date	IAR Review
LT1	9/01		IAR 2000-Phase II
LT2	9/02		IAR 2000-Phase II
LT3	9/03		IAR 2000-Phase II
LT4	9/04		IAR 2000-Phase II
LT5	9/05		IAR 2000-Phase II

Statistics	
34 Milestones Completed	
9%	Completed Ahead of Schedule
88%	Completed Ahead of or on Schedule
12%	Completed After Schedule (Average slip < 1 Quarter)

ESS Phase-I Milestone Status

Six Phase-I milestones met by ESS since the last IAR
- GC5 (due 6/99, met 3/99)
- CT7 (due 6/98, met 10/98)
- SS3 (due/met 9/98)
- SS4 (due/met 9/99)
- BR1 (due/met 1/99)
- BR2 (due/met 1/00)

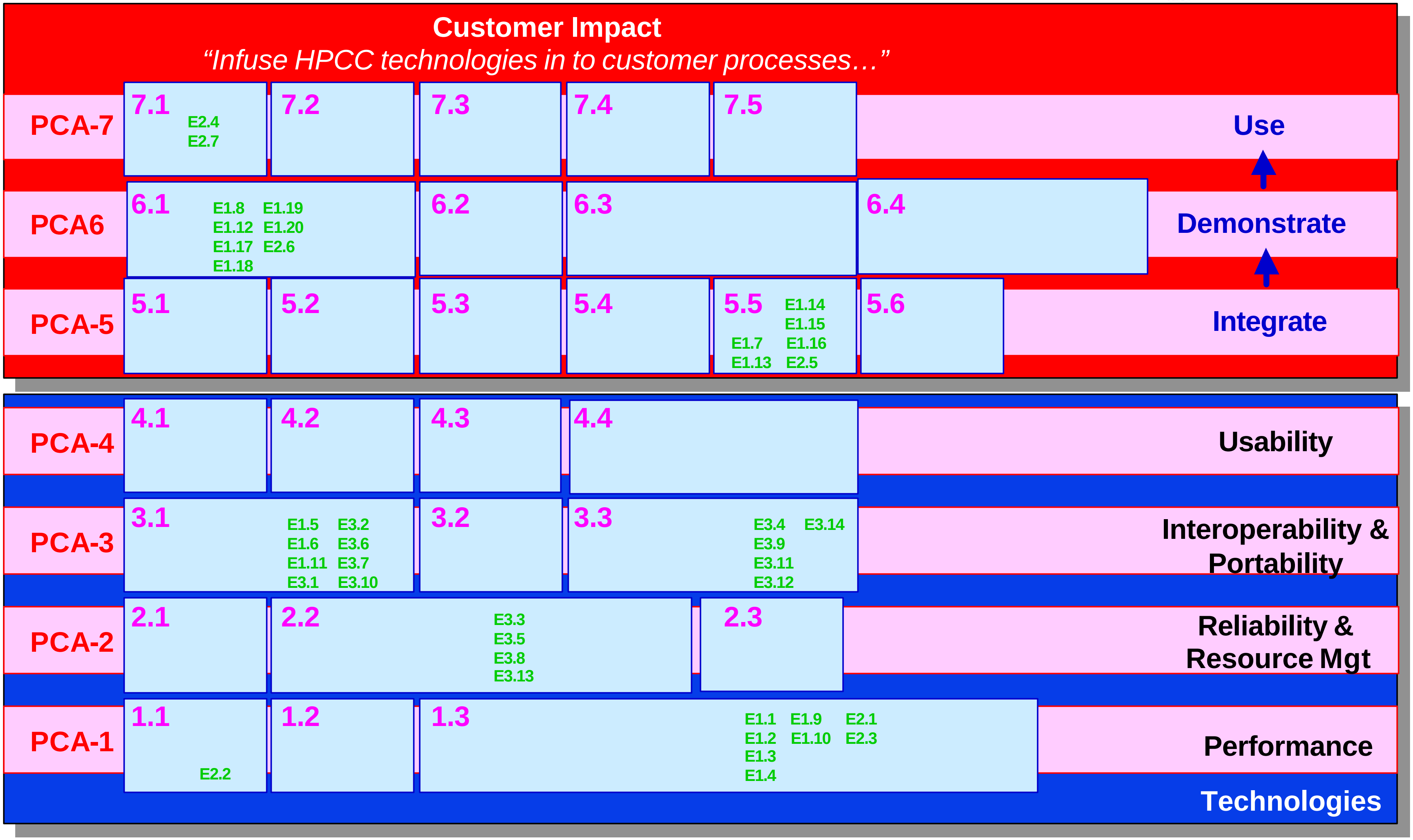
Level-1 Milestone GC5 "demonstrate 200-fold improvements over FY92 baseline in time to solution for GC applications on TFLOPS testbeds," was achieved with two codes:

AMRMHD3D achieves 250:1 reduction in time to solution over baseline. Its Adaptive Mesh Refinement (AMR) capability is extending spatial dynamic range in coronal MHD models by 1-2 orders of magnitude for the Principal Investigator group at the Naval Research Lab led by John Gardner.

DYNAMO demonstrates 300:1 increase in performance. The science Investigator, Gary Glatzmaier of U.C. Santa Cruz, can now simulate the core of the Earth with much higher fidelity, moving in resolution from 100km down to 20km.

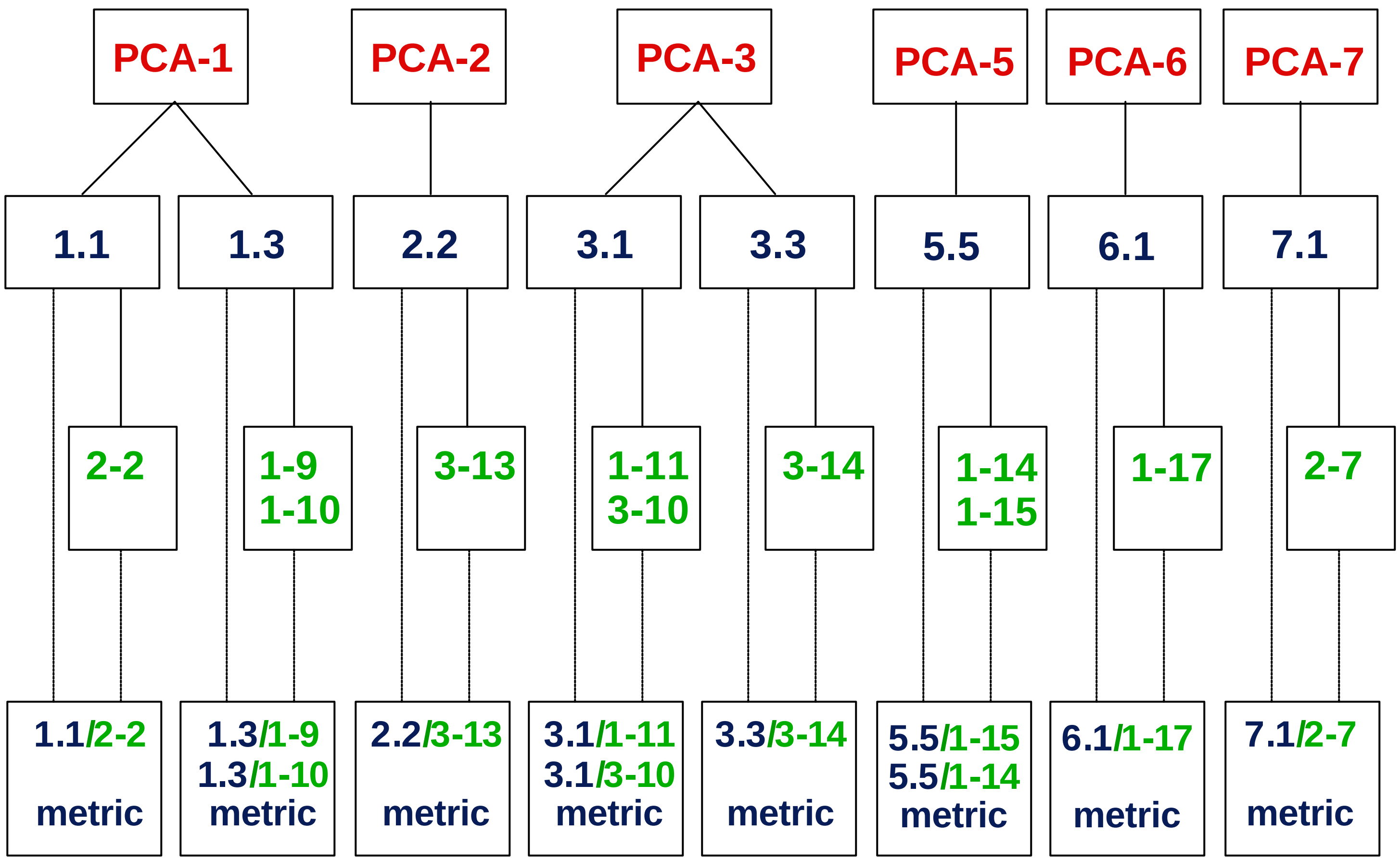
Level-1 Milestone SS4 "Demonstrate portable scalable distributed visualization of multi-Terabyte 4D datasets on Teraflop/s scalable systems," was achieved with ParVox, a scalable parallel volume rendering system capable of distributed visualization of 4D datasets. This system allows investigators to visualize data sets of arbitrary size (i.e. Terabytes) limited only by the available disk storage space. (Due 9/99; achieved 9/99)

ESS Project Milestones as Components of the HPCC Program Goals and Milestones



ESS Phase-II Program Milestone Status

11 Key ESS Project Milestones Share Metrics with Program Milestones



6 PCA Milestones supported by ESS

8 Program Milestones with ESS metrics

Legend:
a.b = (PCA).(sequence #)

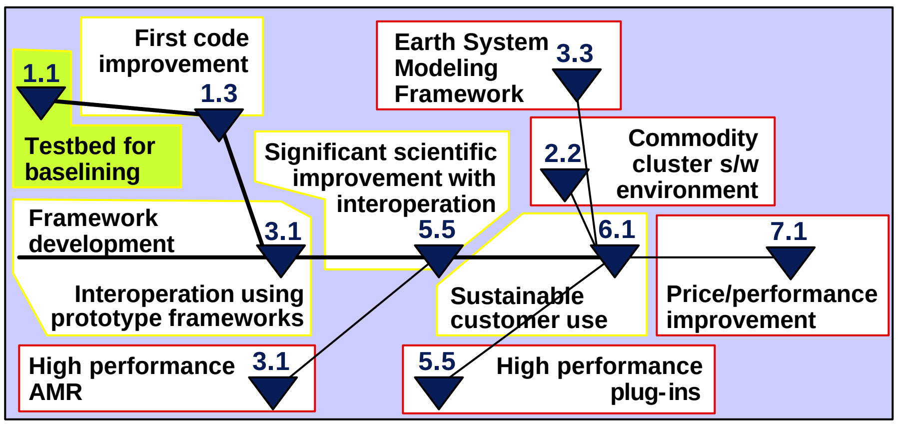
11 ESS Project Milestones sharing Program metrics

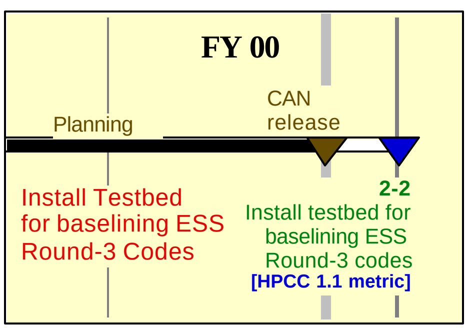
Legend:
c-d = (WBS)-(sequence #)

11 Shared Program/Project Metrics

HPCC 1.1: Establish high-performance Testbed for application performance

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-1	Develop component technologies for performance	9/01		on schedule
HPCC 1.1	Establish high-performance Testbed for application performance (CAS/ESS/NREN)	9/00	Integrated hardware and software to provide a computing and communications testbed for HPCC applications capable of 250 gigaflops (benchmarks) and 3 locations with gigabit WAN capability.	completed 1/00
ESS 2-2	Install Testbed for baselining ESS Round - 3 codes.	9/00		





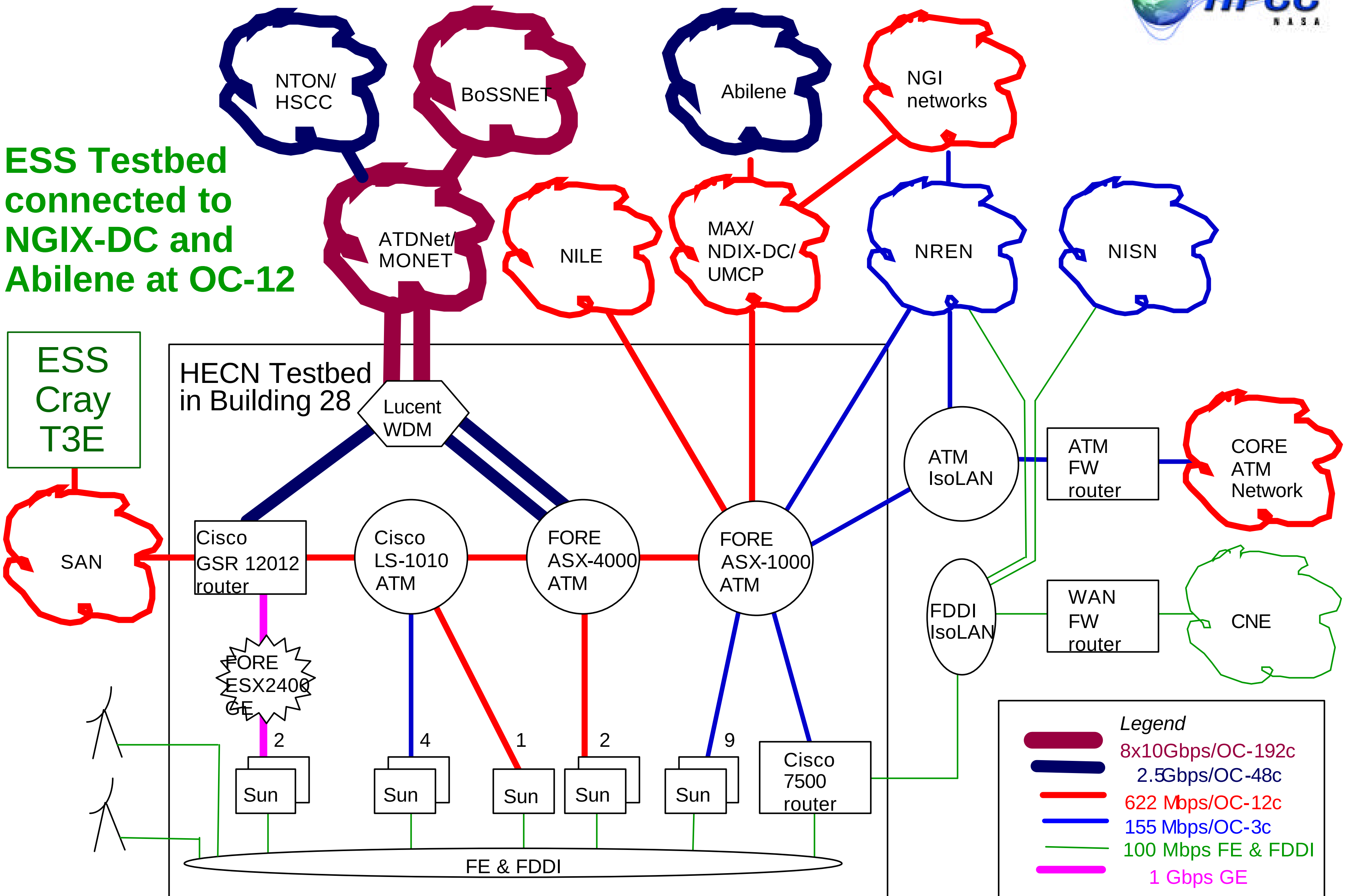
- **Upgraded ESS Cray T3E**
- **Connected it to NGIX-DC and Abilene at OC-12**

ESS 2-2: Install Testbed for Baselining ESS Round-3 Codes

- **Purchased upgrade to GSFC T3E-600 “jsimpson”**
  - **277 processors dedicated to ESS installed in January 2000**
  - **1,360 T3E processors available to ESS on a non-interference basis from the owner of the remainder of the system, the NASA Seasonal to Interannual Prediction Project (NSIPP). Total system has 162,000 Gbytes memory and 2.2 Tbytes of disk.**
  - **1,024 T3E processors sustained 261 Gflops on the DYNAMO code from the P.Olson/JHU ESS Round-2 Team running on a 1536x1536x129 grid.**

ESS 2-2: Install Testbed for Baselining ESS Round-3 Codes

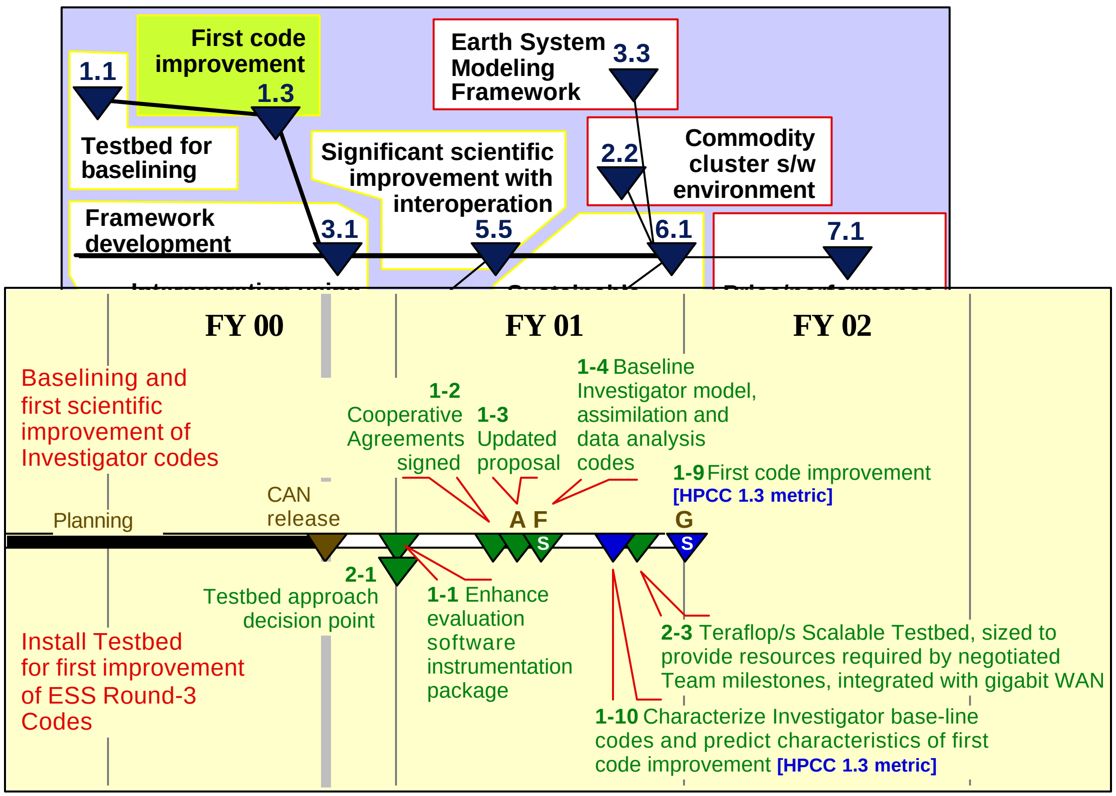
ESS Testbed connected to NGIX-DC and Abilene at OC-12



JPG 6/19/00

HPCC 1.3: Develop and apply technologies to measure and enhance performance on high performance testbeds

Number	Milestone	Due	Metric	Status
PCA-1	Develop component technologies for performance	9/01		on schedule
HPCC 1.3	Develop and apply technologies to measure and enhance performance on high performance testbeds (CAS/ESS/NREN)	9/01	90% of Round-3 codes with capabilities for automated performance monitoring and characterization. 30% of ESS Round-3 applications operating at 3X improvement using negotiated science metrics over baseline at the start of Round-3. Tallies Investigator milestone-G and commodity optional milestones.	on schedule
ESS 1-10	Characterize Investigator baseline codes and predict characteristics of first code improvement	6/01		on schedule
ESS 1-9	Investigator first code improvement	9/01		on schedule



- **Round-3 CAN process**
- **Investigator selection**
- **First code improvement**
- **Code characterization**

  (7 charts)

ESS 1-9: Investigator first code improvement

Round-3 CAN Process

Goal:

- Enable the science community to make production-ready high-performance ESS computational applications that model, analyze, or interpret NASA enterprise observational mission data.

Approach:

- Headquarters issues a CAN requesting proposals for scientific Investigations to develop significant high-end computing applications using accepted software engineering practices that:
  - Address a significant element of one of the NASA Enterprises' Strategic Plans, and
  - Incorporate the use of NASA data to understand Earth, Space, Life, or Microgravity science phenomena.
- Headquarters oversees a peer review including scientific and technical peers.
- Following selection for negotiation, ESS negotiates cooperative agreements with teams, where the work is defined by milestones and payments are tied to achievement of the milestones.
- ESS provides a variety of support technologies to the Investigator Teams.

Scope: Approximately 10 Teams with award values totalling $18M over 3 years.

Status: NASA Cooperative Agreement Notice (CAN) CAN–23456-253 "Increasing Interoperability and Performance of Grand Challenge Applications in the Earth, Space, Life, and Microgravity Sciences" in final approval at Headquarters.

ESS 1-9: Investigator first code improvement

Approach to Select ESS Round-3 Investigators

Proposals are requested from potential Investigators to work collaboratively with a selected Testbed vendor to:

- **Prepare high performance scalable parallel codes for use by NASA for research and mission support;**
- **Build sustainable common frameworks within Earth and Space science communities enabling interoperation of code components;**
- **Achieve code interoperation and high performance simultaneously;**
- **Fill community priority needs for code components compatible with agreed on software framework interfaces;**
- **Enable science communities to leverage code interoperation by testing, comparing and using alternative code implementations; and**
- **Provide spin-offs from Round-3 Investigations that benefit education, the Public, or State and local governments.**

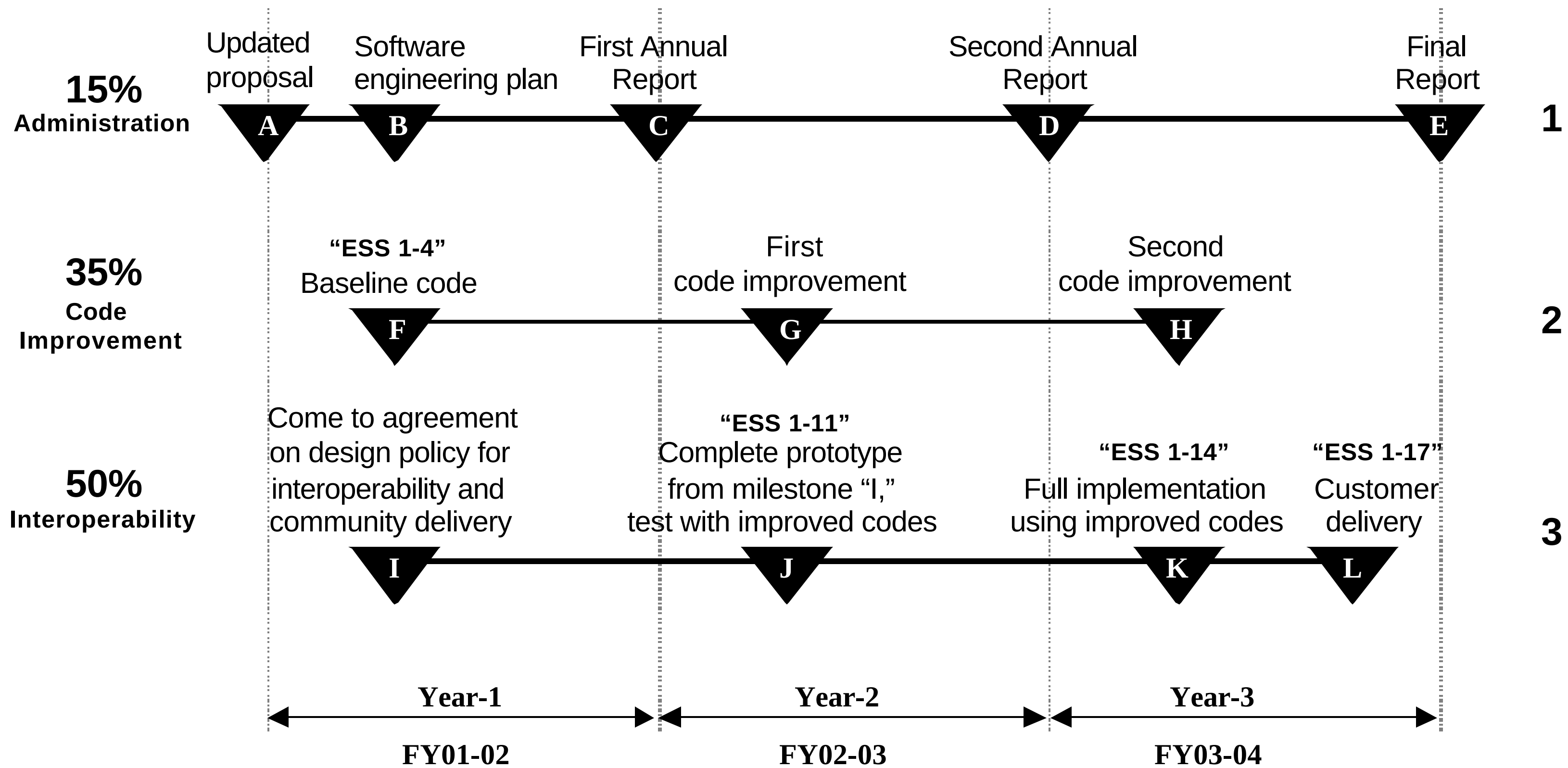
CAN Evaluation Criteria

- **Scientific quality 40%**
- **Technical quality 40%**
- **Cost 20%**

ESS 1-9: Investigator first code improvement

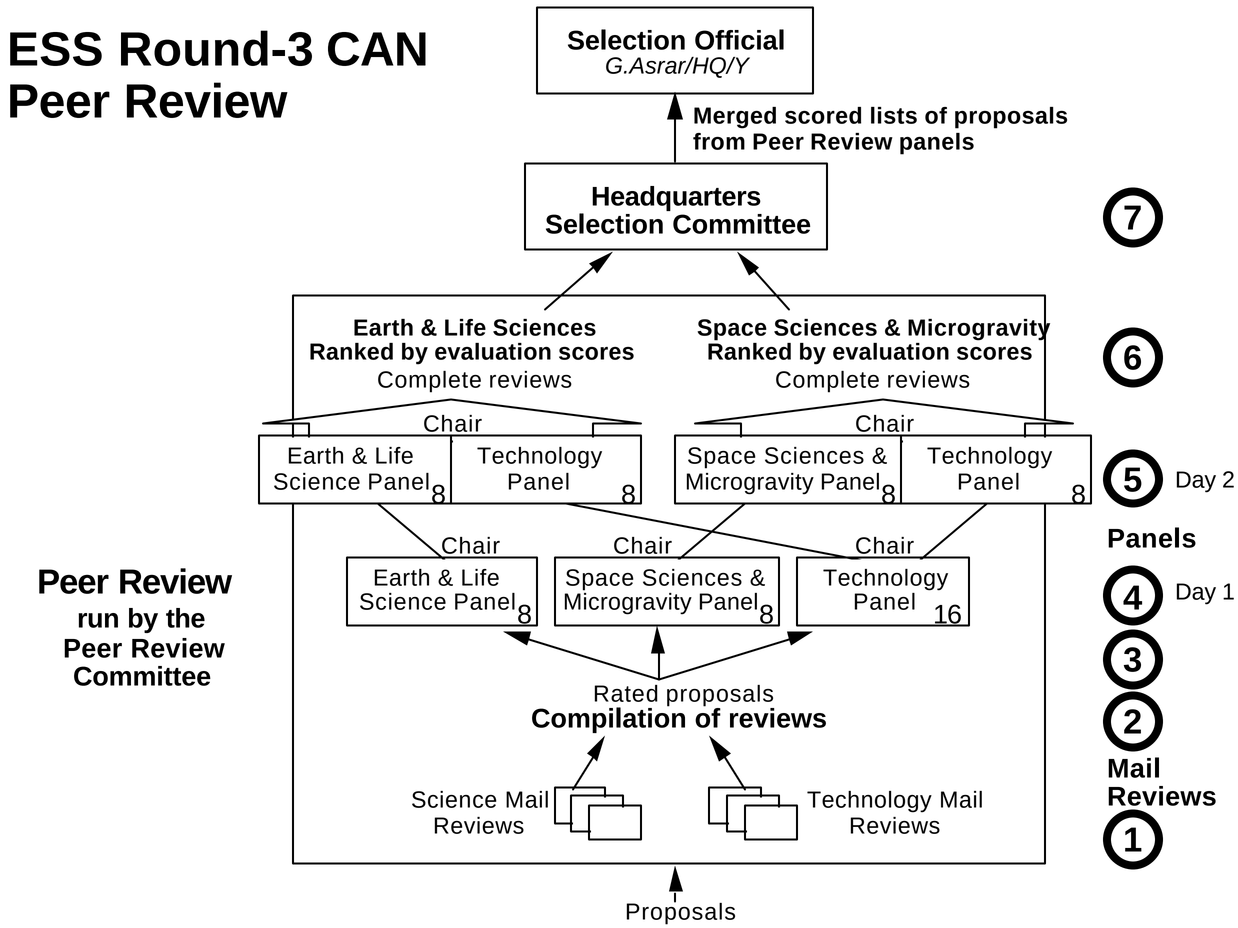
Approach to Select ESS Round-3 Investigators (cont.)

Required milestones for ESS Round-3 Team proposals



ESS 1-9: Investigator first code improvement

Approach to Select ESS Round-3 Investigators (cont.)



ESS 1-9: Investigator first code improvement

Approach to Select ESS Round-3 Investigators (cont.)

CAN Timeline

Schedule for review and selection of Round-3 Investigator Teams:

Release of the CAN	*tbd*
Preproposal Conference	21 days after release
Letter of Intent to Submit Proposal due	30 days after release
Proposals due	60 days after release
Announcement of selections for negotiation	120 days after release
Announcement of award (target date)	180 days after release
Cooperative agreements signed	200 days after release

ESS 1-9: Investigator first code improvement

Following selection of Round-3 Investigators

Approach

- **Investigator Teams identify the code they will improve in their proposals.**
- **The improvement must be gauged by a scientific metric of quality.**
- **This improvement must require high performance computing.**

This objective tracks Investigator milestones A, F, and G.

Milestone A: Each Investigator Team provides an updated proposal, internally consistent with the results of the negotiations.

Milestone F: Each Team provides a baseline measurement of the code that it will improve.

Milestone G: Each Team achieves its negotiated initial code improvement, as gauged by a scientific metric of quality.

ESS 1-10: Characterize Investigator Baseline Codes and Predict Characteristics of First Code Improvement

System Evaluation Activities

Goal

- Identification and understanding of the critical success factors for the selected Grand Challenge Investigations.
- Understanding of the characteristics and interactions among the computational platform, the application code, and the underlying model.

Round-2 Achievements: (T.Pratt)

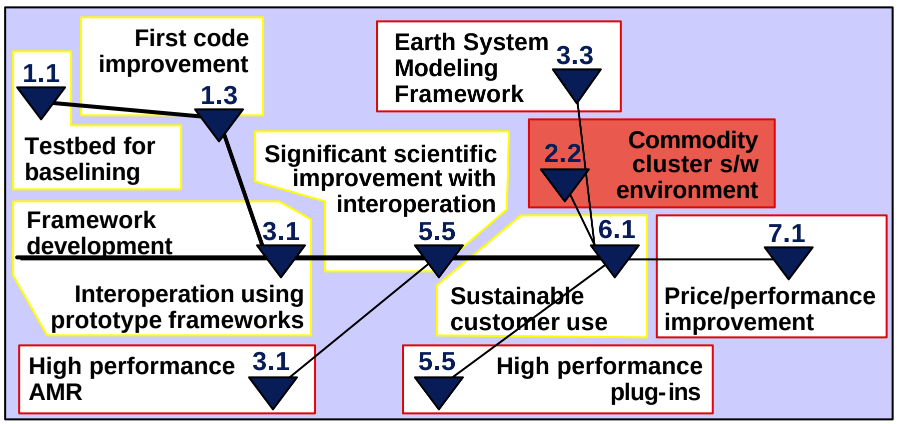
- Developed Software Instrumentation package GODIVA. Displayed its validity by applying it to science codes and selected benchmarks. Published results in technical notes and conference papers

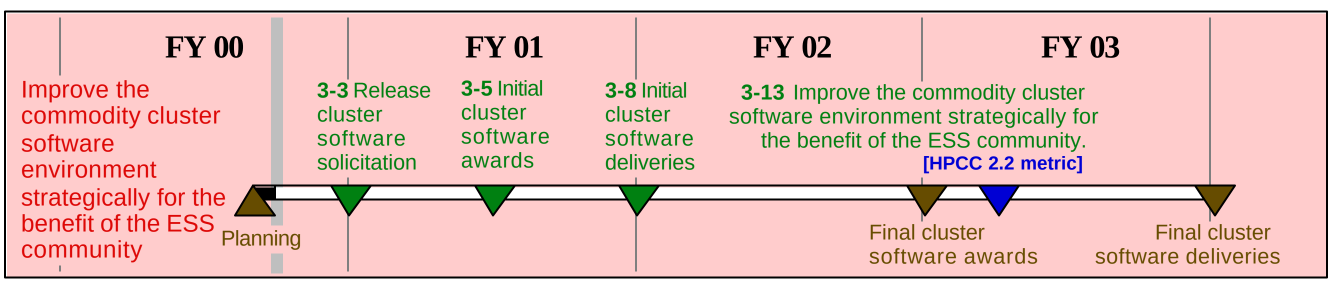
Current Activities and Round-3 Approach: (P.Merkey)

- Adopted the research and develop of the GODIVA tools. Studying the internals and extending the capabilities to facilitate F90 and C++ and eventually frameworks.
- Make measurements using these software instrumentation tools, conventional performance measurement on the testbeds, and the PI teams chosen metrics.
- Develop and refine our understanding of relationships among the key parameters quantified by these measurements and predict the scientific impact of proposed PetaFLOPS architectures.

HPCC 2.2: Develop embedded tools and services for autonomous resource estimation/request of local and distributed ground based systems

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-2	Develop component technologies for reliability and resources management	6/03		on schedule
HPCC 2.2	Develop embedded tools and services for autonomous resource estimation/request of local and distributed ground based systems (CAS/ESS/NREN)	12/02	Production-ready commodity-based cluster computing runtime and development environments portable to three Linux-based testbeds from different vendors.	on schedule
ESS 3-13	Improve the commodity cluster software environment strategically for the benefit of the ESS community	12/02		on schedule





Cluster System Software Research Awards Program

ESS 3-13: Improve the Commodity Cluster Software Environment Strategically for the Benefit of the ESS Community

Cluster System Software Research Awards Program

Goal:

- Provide the equivalent motivation to the open-source, cluster based, research and development community that supporting Grand Challenge science projects has traditionally placed on vendors.

Approach:

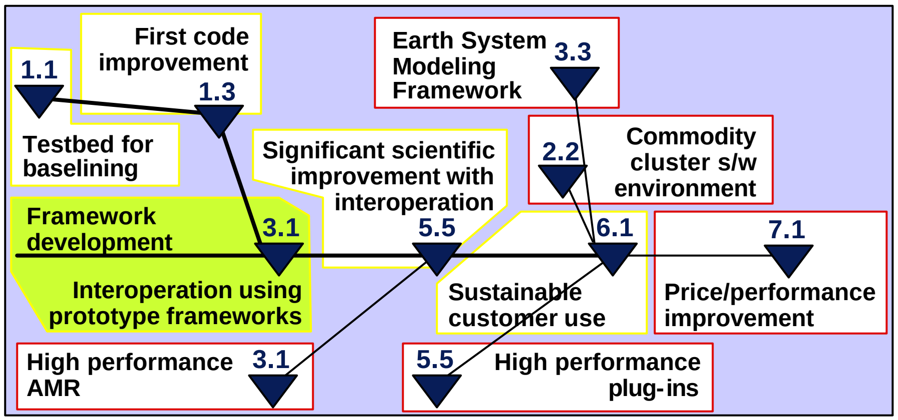
- Issue a series of CANs listing Investigator needs in improved cluster open source software. ESS maintains a prioritized list based on PI requirements. The list is probably predictable: libraries, performance tools, debuggers, schedulers, batch systems, etc.
- Peer review proposals twice a year. Rate and rank proposals based on responsiveness to PI requirements and on basic research potential.
- The resulting cooperative agreement will schedule at least two deliveries: an initial delivery of beta software or proof of concept, and a finally delivery.
- Allow for course corrections or second tries. The initial finding could be: The proposed approach is not quite right and we will correct it in the final delivery, or the proposed approach won't work and as a result we have a modified approach.

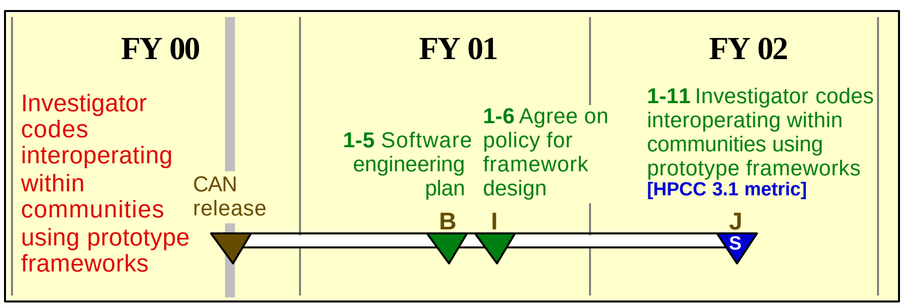
Scope: Dynamic with an average of 8 projects at 125K/yr in the pipeine at a time.

Status: CAN preparation beginning.

HPCC 3.1: Tools and techniques for interoperable and portable applications in aerospace, Earth science, and space science communities

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-3	Develop component technologies for interoperability and portability	9/03		on schedule
HPCC 3.1	Tools and techniques for interoperable and portable applications in aerospace, Earth science, and space science communities (CAS/ESS)	3/02	Prototype Earth and space science frameworks impacting at least 5 scientific communities with interoperability among 2 or more applications per framework. 3 applications interoperating within a prototype Earth System Modeling Framework. Integration of new module into framework within 1 day; portability to new computing system within 1 week.	on schedule
ESS 1-11	Investigator codes interoperating within communities using prototype frameworks	3/02		on schedule





Integration of the first code improvement with the framework

ESS 1-11: Investigator Codes Interoperating Within Communities Using Prototype Frameworks

Integration of the first code improvement with the framework

Goal

Achieve Integration of the first code improvement with the framework

Approach

- **Assist the Investigator Teams to move in the direction of a solid software engineering infrastructure if they do not have it.**
- **Write the CAN to select scientific Investigator Teams needing to achieve both performance and interoperability within a community of application codes**
- **Teams facilitate, within their application communities, the adoption of an existing framework or definition of a modified or new framework (ESS facilitates definition of the Earth System Modeling Framework).**
- **Teams show their improved code interoperating with this framework**

This objective tracks Investigator milestones B, I, and J.

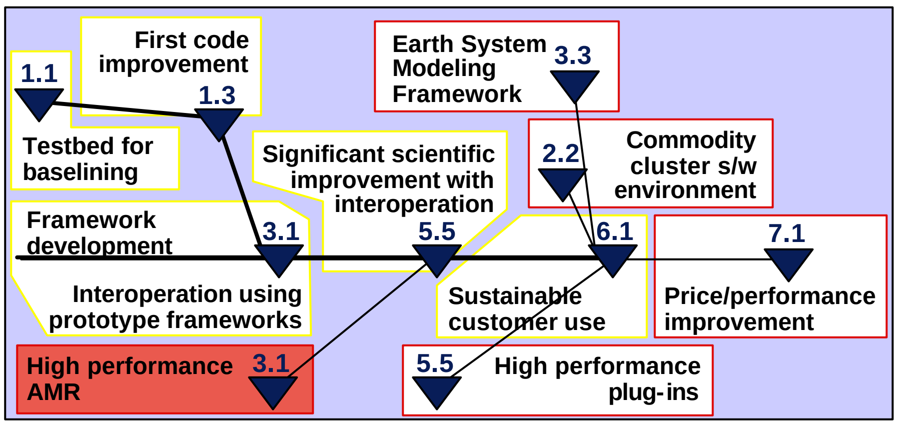
Milestone B: Validates that Investigator Teams have a serious plan for maintaining a software infrastructure

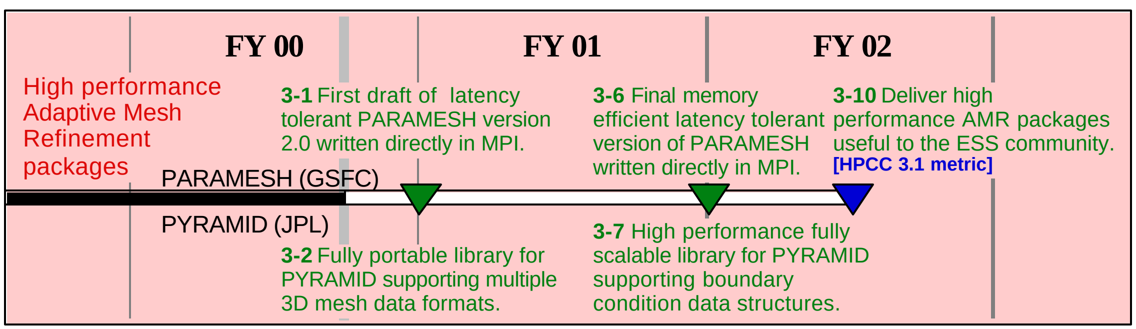
Milestone I: Brings Investigator Teams and their application community to agreement on design policy for interoperability and community delivery

Milestone J: Shows that the improved codes developed by Investigator Teams work with their prototype framework developed under Milestone I.

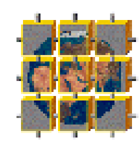
HPCC 3.1: Tools and techniques for interoperable and portable applications in aerospace, Earth science, and space science communities

Number	Milestone	Due	Metric	Status
PCA-3	Develop component technologies for interoperability and portability	9/03		on schedule
HPCC 3.1	Tools and techniques for interoperable and portable applications in aerospace, Earth science, and space science communities (CAS/ESS)	3/02	Two portable parallel latency-tolerant adaptive mesh refinement packages.	on schedule
ESS 3-10	Deliver high-performance AMR packages useful to the ESS community	3/02		on schedule





- Structured Grid AMR Package PARAMESH
- Unstructured AMR package PYRAMID



ESS 3-10: Deliver high-performance AMR packages useful to the ESS community

Motivation

Adaptive Mesh Refinement (AMR) is increasingly popular for Grand Challenge scale applications which cannot achieve the dynamic range they require with uniform grids. Techniques for uniprocessor computers have been investigated for many years, but parallel AMR algorithms and software tools are still a relatively new research area.

Impact

Performing parallel AMR in an application requires both a deep understanding of advanced numerical analysis (local error estimates) and sophisticated software development techniques. The ESS packages, PARAMESH and PYRAMID, will provide this capability for scientists through a set of practical parallel AMR software tools.

ESS 3-10: Deliver high-performance AMR packages useful to the ESS community

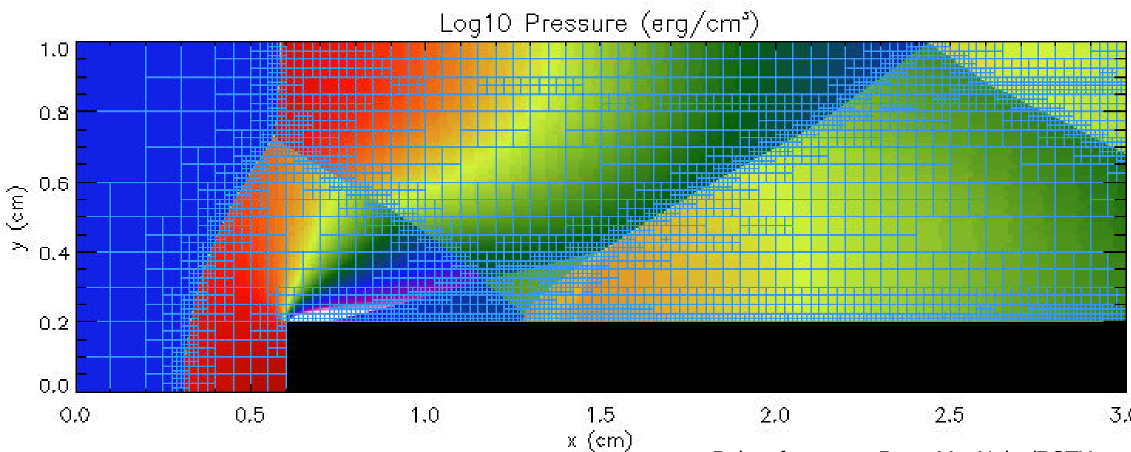
GSFC Structured Grid AMR Package PARAMESH

Goal:

– **Develop a parallel AMR package (PARAMESH) to support multi-dimensional user applications which compute on logically cartesian meshes.**

Approach:

– **Enable users to decompose their computational domain into logically cartesian sub-blocks with varying spatial resolution. Manage the creation and modification of the sub-blocks and the communications which are required between them.**



Point of contact: Peter MacNeice/RSTX, <macneice@alfven.gsfc.nasa.gov >

– **Use Fortran 90 and either the Cray SHMEM library or a combination of MPI and MMPI for interprocessor communications.**

Status:

– **Version 2.0 is available from http://sdcd.gsfc.nasa.gov/RIB/repositories/inhouse_gsfc/Users_manual/amr.html**

– **An efficient version for high latency architectures (eg Beowulf) is being developed. This version will support MPI based communication without use of MMPI. The communication efficiency of this design has been validated.**

ESS 3-10: Deliver high-performance AMR packages useful to the ESS community

JPL Unstructured AMR package PYRAMID

Goal:

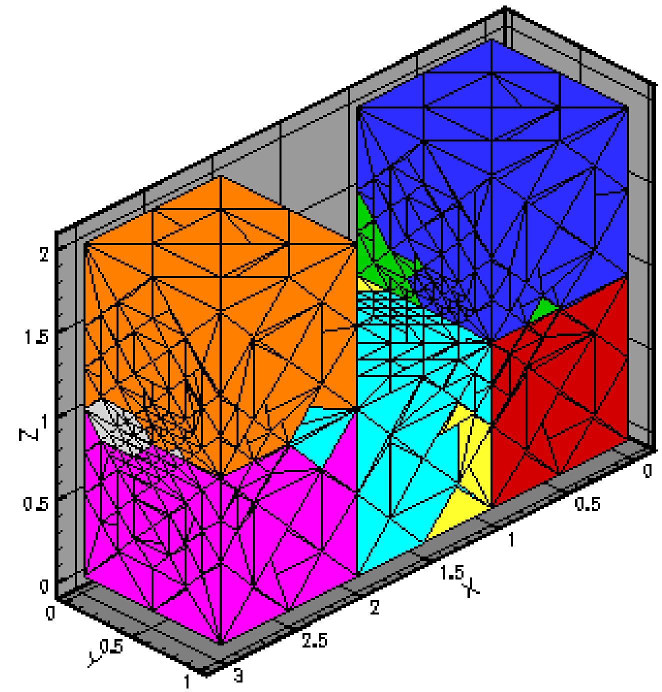
- Develop a comprehensive parallel unstructured AMR Problem-Solving Package (PYRAMID) which can be easily integrated into existing mesh-based parallel applications running on massively parallel computers and computer clusters.

Approach:

- Deliver a fully portable library (including the Origin 2000) that supports multiple 3D mesh data formats
- Deliver a high performance fully scalable library that includes support for boundary condition data structures

Status:

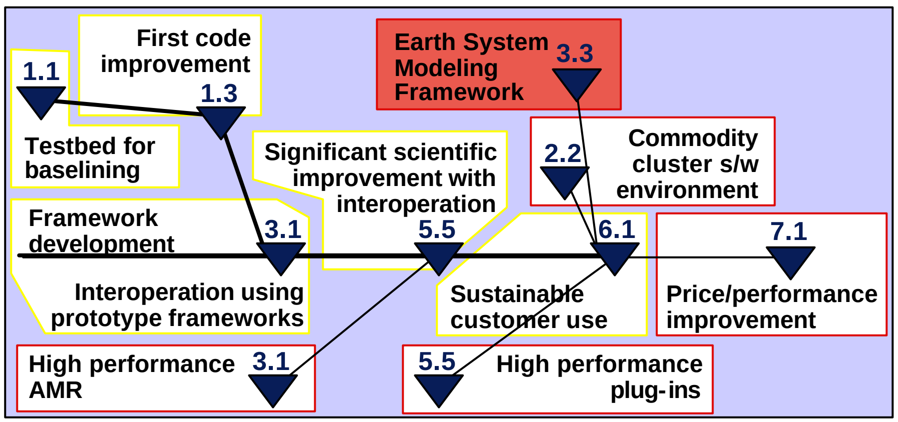
- On schedule
- In discussion with U.Texas and NCSA to become first users outside JPL and Caltech community

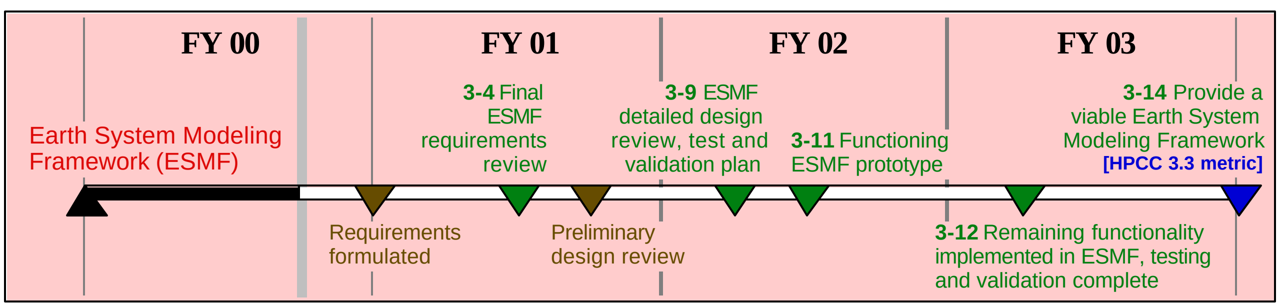


Point of contact: Tom Cwik/JPL, <cwik@jpl.nasa.gov >

HPCC 3.3: Interoperable and portable systems, services and environments

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-3	Develop component technologies for interoperability and portability	9/03		on schedule
HPCC 3.3	Interoperable and portable systems, services and environments (CAS/ESS)	9/03	Portable production-ready Earth System Modeling Framework incorporating 5 disciplines.	on schedule
ESS 3-14	Provide a viable Earth System Modeling Framework	9/03		on schedule

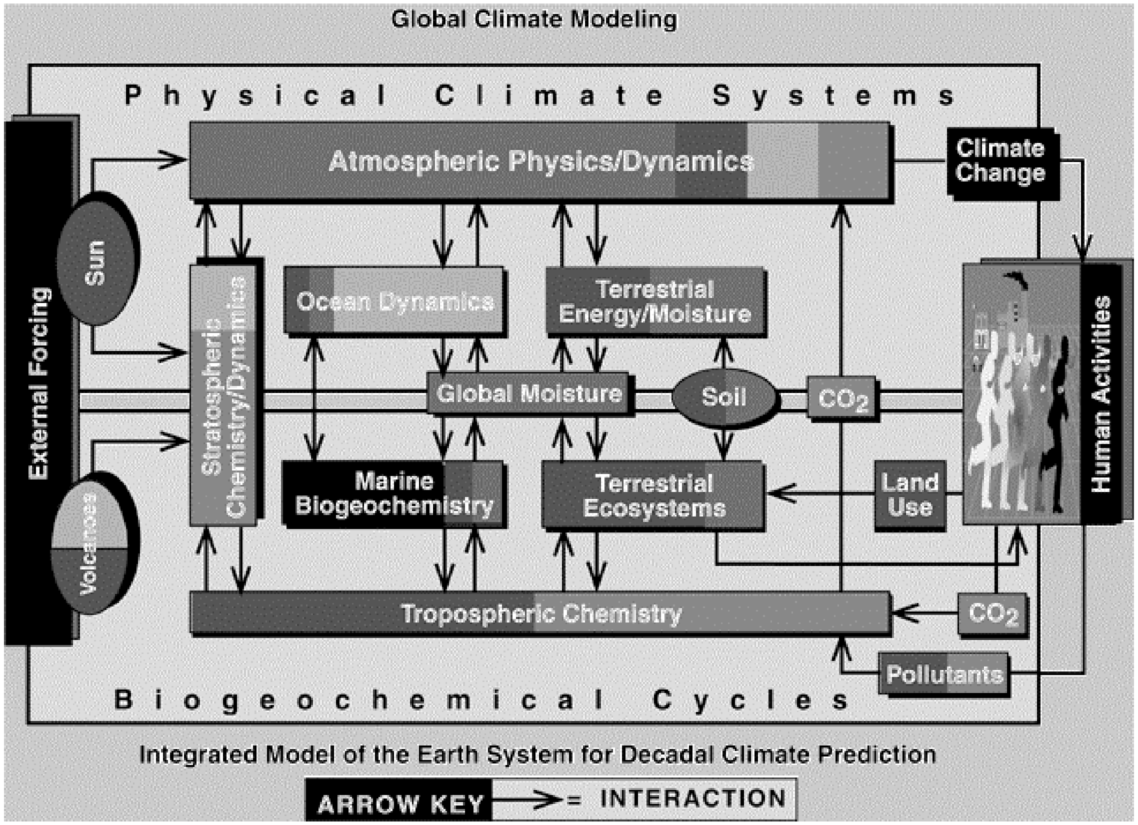




Earth System Modeling Framework

ESS 3-14: Provide a viable Earth System Modeling Framework

The Earth Science Enterprise needs to achieve interoperation of many model systems



The Earth System and Its Interactions - from page 3 of the Earth Science Strategic Enterprise Plan 1998-2002

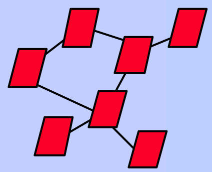
How can ESS enable this bold vision?

ESS 3-14: Provide a viable Earth System Modeling Framework

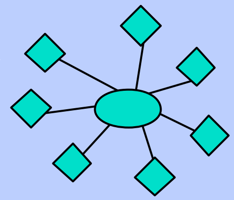
Current Situation:

Even though several major atmospheric models employ modern software engineering involving frameworks, none of the frameworks interoperate.

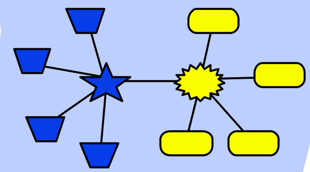
Model A



Model B



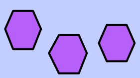
Model & Analysis C



Running under various systems
- Flux Coupler (NCAR)
- GEMS (GSFC)
- Flexible Modeling System (GFDL)
- Data Broker (UCLA)
... and others

Making it very hard for:

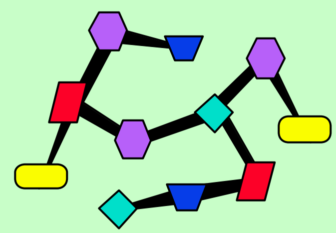
- Models to incorporate advances from outside their framework;



3rd party objects

- Other intellectual communities to help the modeling communities.

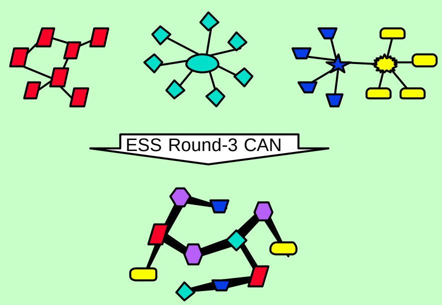
The need is for a Common Framework Infrastructure



Some significant Code Y communities such as weather and climate modeling are ready to adopt a common infrastructure.

ESS intends to facilitate this evolutionary step

in Round-3 for a key Code Y community.



Earth System Modeling Framework

There is significant risk:

1) That high performance and interoperability will not be achieved together.
2) That a sub-critical mass of the community will participate in the design and convert to it.

Mitigation:

1) Milestones must be constructed to require both.
2) Other solicitations must help to populate the framework.

Earth System Modeling Framework

Goal:

- Facilitate creation of the common software infrastructure called for by the U.S. Earth system modeling and data assimilation community

Approach:

- Round-3 Teams and inhouse staff will scope and design the Earth System Modeling Framework (ESMF).
- An ESMF Science Team will provide oversight.
- ESS will provide a neutral software engineering organization, termed the ESMF Integrator, to facilitate the specification, design, and prototyping.
- Most technical contributions will come from the Investigator Teams.
- Teams will migrate their codes to the ESMF.
- Other Round-3 awardees build/use frameworks as part of their own community interoperation/software engineering plans.

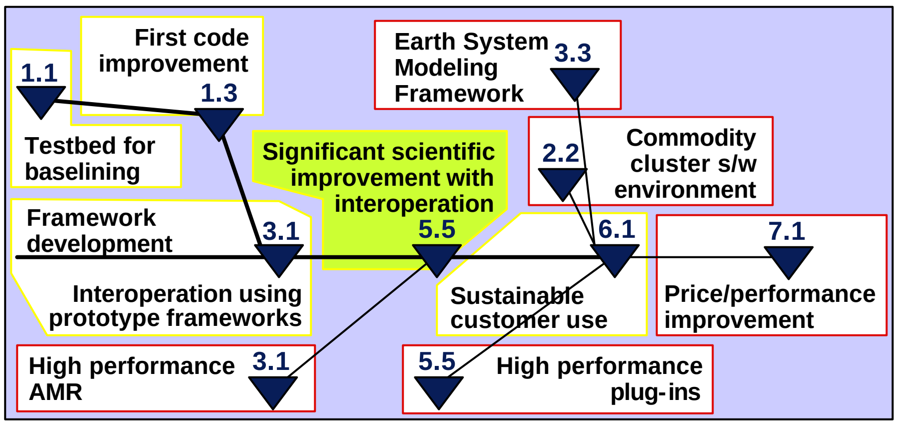
Scope: Determined by the interest shown in the Round-3 CAN proposals.

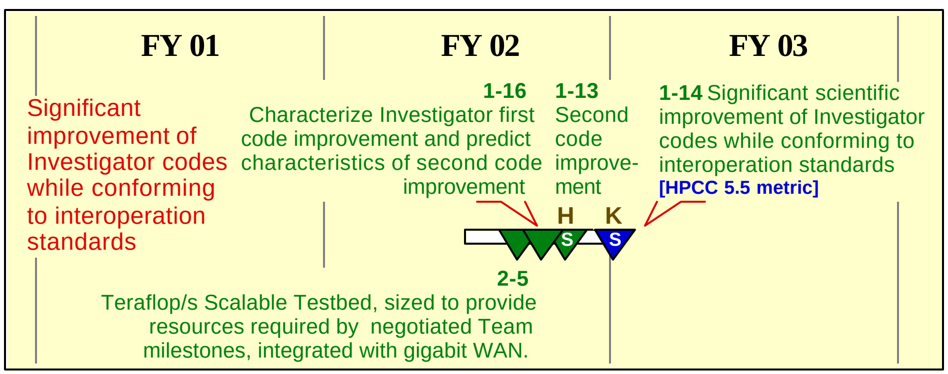
Status:

- The ESMF Integrator is obtaining and becoming familiar with key Earth system modeling code interoperability systems and is developing an analysis of the code and interoperability characteristics.
- The ESMF Integrator has begun to look at existing high performance framework systems.

HPCC 5.5: Demonstrate significant improvements in Earth and space science applications codes

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-5	Demonstrate integrated HPCC technologies	9/02		on schedule
HPCC 5.5	Demonstrate significant improvements in Earth and space science application codes (ESS)	9/02	10X improvement using negotiated science metrics over baseline at start of Round -3 in 50% of all applications while interoperating among 2 codes.	on schedule
ESS 1-14	Significant scientific improvement of Investigator codes while conforming to interoperation standards	9/02		starts 3/02





- **Second code improvement**
- **High performance interoperation**
- **Code characterization**

ESS 1-14: Significant scientific improvement of Investigator codes while conforming to interoperation standards

Goal

Achieve performance AND interoperability for Investigator codes

Approach

Augment the Teraflops Scalable Testbed to provide resources required by negotiated Team milestones integrated with the gigabit WAN.

Assist scientific Investigator Teams to achieve their code improvement goal and integrate the resulting code with their framework, achieving both performance and interoperability within a community of codes

Refine performance evaluation technology by characterizing the Investigator's first code improvement and predicting characteristics of the second improvement.

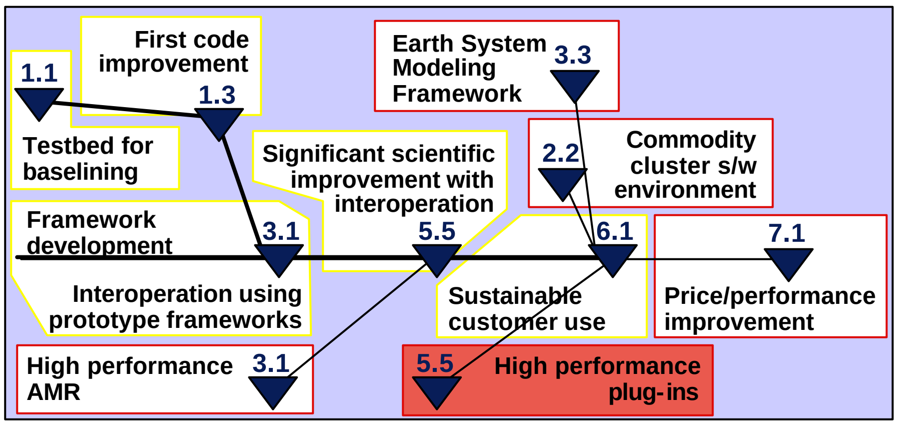
This objective tracks Investigator milestones H and K.

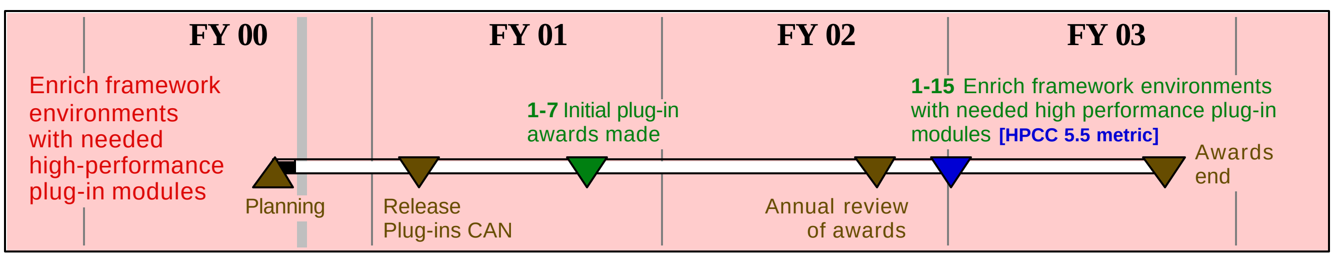
Milestone H: Each Team achieves its negotiated final code improvement goal, as gauged by a scientific metric of quality.

Milestone K: Teams demonstrate that their significantly improved scientific codes achieve high performance while conforming to framework interoperation standards.

HPCC 5.5: Demonstrate significant improvements in Earth and space science applications codes

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-5	Demonstrate integrated HPCC technologies	9/02		on schedule
HPCC 5.5	Demonstrate significant improvements in Earth and space science application codes (ESS)	9/02	20 high-performance modules compatible with existing frameworks.	on schedule
ESS 1-15	Enrich framework environments with needed high-performance plug-in modules	9/02		on schedule





Plug-ins Development Awards Program

ESS 1-15: Enrich framework environments with needed high-performance plug-in modules

Plug-ins Development Awards Program

Goal:

– Enrich the environment of the frameworks developed by the selected Investigator Teams with needed compatible high performance software components.

Approach:

– Release a series of CANs following the start of work by the Round-3 Investigators.

– CANs list Investigator needs in framework compatible software components. ESS maintains a prioritized list based on PI requirements.

– Enlist the Round-3 Investigators to assist in evaluating plug-in proposals, to provide their frameworks to awardees, and to potentially work with the awardees. Round-3 Investigators may not compete for a plug-in award where there is an organizational conflict of interest.

– Peer review proposals twice a year. Rate and rank proposals based on responsiveness to PI requirements and on technical quality.

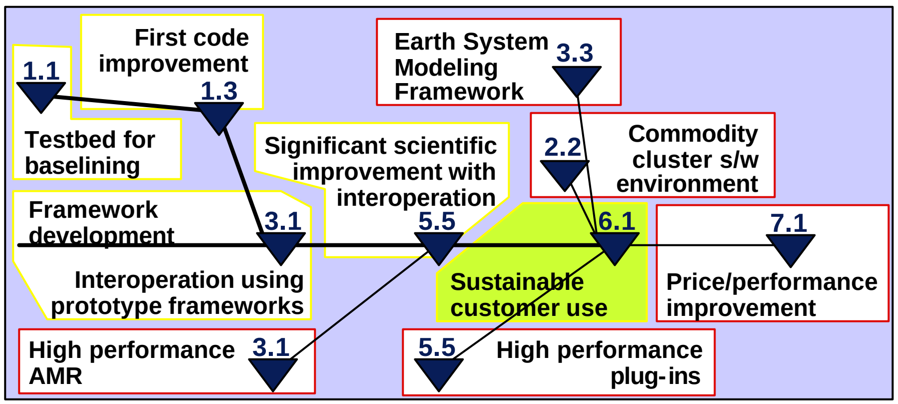
– The resulting cooperative agreements will schedule at least two deliveries: an initial delivery of beta software or proof of concept, and a finally delivery.

Scope: Dynamic with an average of 8 projects at 125K/yr in the pipeline at a time.

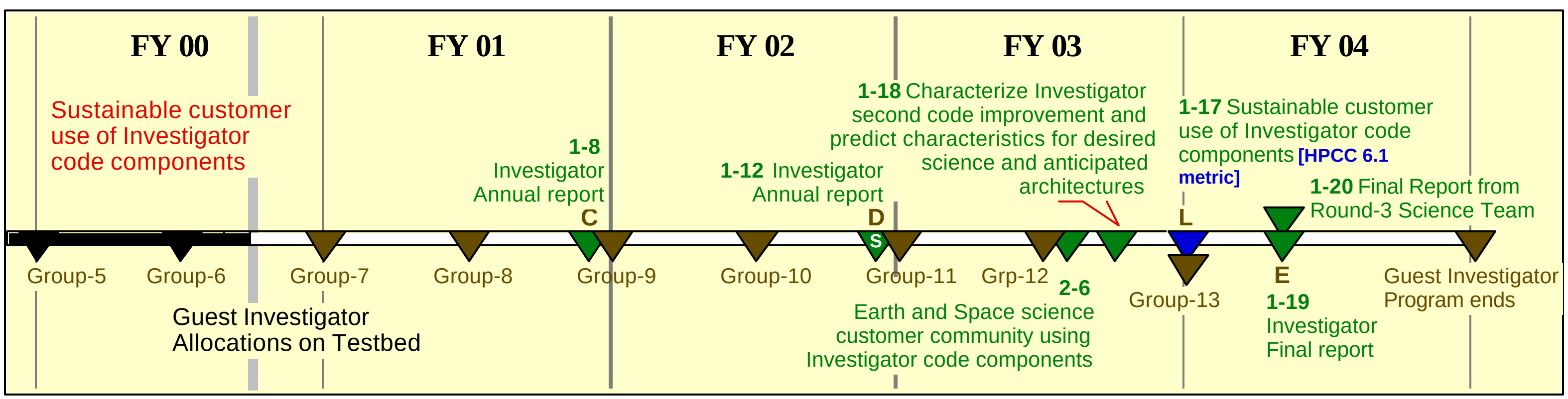
Status: CAN preparation beginning.

HPCC 6.1: Establish impact on Earth and space sciences through the demonstration of production ready high-performance Earth and space science computational simulations validated by NASA Enterprise observational mission data

Number	Milestone	Due	Metric	Status
PCA-6	Demonstrate significant engineering, scientific, and educational impacts from integrated HPCC technologies	9/05		on schedule
HPCC 6.1	Establish impact on Earth and space sciences through the demonstration of production ready high-performance Earth and space science computational simulations validated by NASA Enterprise observational mission data (ESS/NREN)	9/03	25 scientific research groups using applications supporting NASA science objectives operating at 10X improvement using negotiated science metrics over baseline at start of Round-3; 10 groups interoperating with stable Earth and space science frameworks impacting 5 scientific communities (2 per framework; 3 for Earth System Modeling Framework).	on schedule
ESS 1-17	Sustainable customer use of Investigator code components	9/03		on schedule



- **Customer use of codes**
- **Guest Investigator Program**
- **Code characterization**



ESS 1-17: Sustainable customer use of Investigator code components

Goal

Achieve sustainable customer use of Investigator code components

Approach

- **Write the CAN to select scientific Investigator Teams that want to provide high performance and interoperabe codes which they develop and maintain for use by other groups within their scientific community.**
- **Carry out a Guest Investigator program providing allocations of Teraflops Scalable Testbed resources and limited user support, but no funding, to Investigators with peer reviewed NASA science awards, in response to twice annual proposal calls.**
- **Refine performance evaluation technology by characterizing the Investigator's second code improvement and predicting characteristics of desired science and anticipated architectures.**

This objective tracks Investigator milestones C, D, L, and E.

Milestone C: Collects the first Investigator Annual Report delivered via the Web

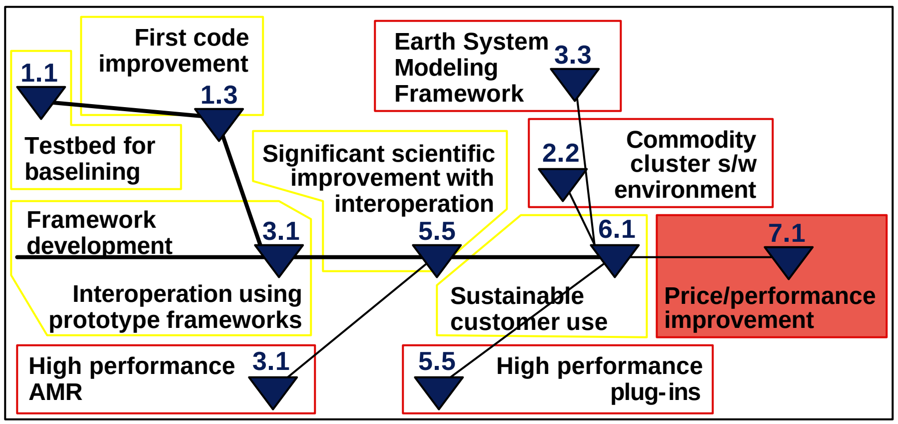
Milestone D: Collects the second Investigator Annual Report delivered via the Web

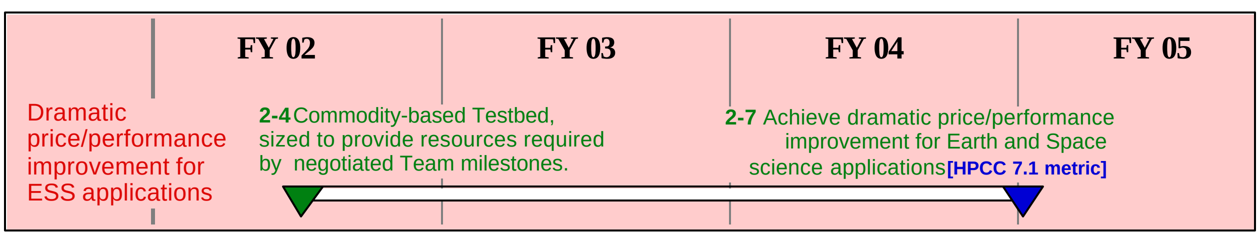
Milestone L: Shows sustainable customer use of Investigator code components. Customer delivery is being planned from the proposal stage.

Milestone E: Collects the Investigator Final Report delivered via the Web

HPCC 7.1: Establish sustained price performance improvements for Earth and Space science applications

Number	*Milestone*	*Due*	*Metric*	*Status*
PCA-7	Establish sustainable and wide-spread customer use of HPCC Program technologies	9/06		on schedule
HPCC 7.1	Establish sustained price performance improvements for Earth and space science applications (ESS)	9/04	Demonstrate 50 gigaflops sustained applications performance at $250K for 50% of Round-3 Investigations.	on schedule
ESS 2-7	Achieve dramatic price/performance improvement for Earth and space science applications	9/04		on schedule





Facilitate movement of Round-3 codes to commodity clusters

ESS 2-7: Achieve dramatic price/performance improvement for Earth and Space science applications

Facilitate movement of Round-3 codes to commodity clusters

Goal:

- Demonstrate dramatic price/performance improvement for Earth and Space science applications

Approach:

- Determine which Round-3 codes can meet Investigator milestone when run on clusters of commodity PCs.
- Include options in the Round-3 CAN which allow proposers to negotiate milestones formalizing this approach.
- Provide a commodity-based testbed sized to provide resources required by negotiated Team milestones.
- Provide technical support to assist Teams to achieve negotiated cluster based milestones.

Scope: Determined by the interest shown in the Round-3 CAN proposals.

Status: Round-3 CAN nearing release.

ESS Funding Allocation by Major WBS areas in $ Thousands

NASA HPCC/ESS Funding Requirements in $ Thousands

Center	FY99	FY00	FY01	FY02	FY03	FY04	Total
GSFC	9,216						
JPL	2,384						
ARC	0	7,050	0	0	0	0	7,050
Total ESS	11,600	19,667					

ESS Funding Allocation by Major WBS areas in $ Thousands

Funding Allocations	FY00	FY01	FY02	FY03	FY04	Total
GSFC	9,797	18,200	18,200	18,200	7,900	72,297
WBS-1 Applications	*1,490*	*6,864*	*6,761*	*6,761*	*1,735*	*23,611*
WBS-2 Testbeds	*6,012*	*6,875*	*6,875*	*6,875*	*3,000*	*29,637*
WBS-3 System Software	*938*	*1,373*	*1,373*	*1,373*	*736*	*5,793*
WBS-5 Basic Research and Human Development	*220*	*1,770*	*1,873*	*1,873*	*1,243*	*6,979*
WBS-6 Management	*1,137*	*1,318*	*1,318*	*1,318*	*1,186*	*6,277*
JPL	2,820	2,700	2,700	2,700	2,400	13,320
WBS-1 Applications	*995*	*995*	*995*	*995*	*995*	*4,975*
WBS-2 Testbeds	*808*	*808*	*808*	*808*	*646*	*3,878*
WBS-3 System Software	*644*	*772*	*777*	*777*	*644*	*3,614*
WBS-5 Basic Research and Human Development	*246*	*0*	*0*	*0*	*0*	*246*
WBS-6 Management	*127*	*125*	*120*	*120*	*115*	*607*
ARC	7,050	0	0	0	0	7,050
WBS-2 Testbeds	*7,050*	*0*	*0*	*0*	*0*	*7,050*
Total ESS	19,667	20,900	20,900	20,900	10,300	92,667

ESS Workforce Summary

ESS/NASA HPCC/ESS Workforce Summary (FTE)

Category	FY99	FY00	FY01	FY02	FY03	FY04
GSFC Civil Service	11.5	15.0	15.0	15.0	16.0	15.0
GSFC SSC and PBC Contractors (non-CS)	23.4	21.4	20.5	20.5	20.5	20.5
JPL Contracted R&D (non-CS)	10.5	11.5	10.5	10.5	10.5	9.5
Total	45.4	47.9	46.0	46.0	47.0	45.0

ESS/GSFC Civil Service Workforce Summary by WBS (FTE)

Workforce Allocations	FY00	FY01	FY02	FY03	FY04
GSFC	15.0	15.0	15.0	16.0	15.0
WBS-1 Applications	*1.5*	*1.6*	*1.6*	*1.9*	*1.6*
WBS-2 Testbeds	*6.8*	*7.4*	*7.4*	*7.7*	*7.4*
WBS-3 System Software	*2.0*	*2.1*	*2.1*	*2.3*	*2.1*
WBS-5 Basic Research and HumanDevelopment	*0*	*0*	*0*	*0*	*0*
WBS-6 Management	*4.7*	*3.9*	*3.9*	*4.1*	*3.9*

Science Highlights from ESS Round-2

Science highlights follow from:
- A.Malagoli/U.Chicago
- P.Saylor/U.Illinois U.C.
- T.Gombosi/U.Mich

Potential science highlights:
- P.Lyster/UMD
- P.Olson/JHU
- R.Mechoso/UCLA
- D.Curkendall/JPL
- G.Carey/UT
- J.Gardner/NRL

Technical highlights follow for:
- P.Olson/JHU, Three-Dimensional Spherical Simulations of Earth's Core and Mantle Dynamics
- The NSIPP atmospheric model: a cluster of commodity PC's provides performance similar to commercial products, but at significantly lower cost.
- The Beowulf Project - the GSFC-centric time line

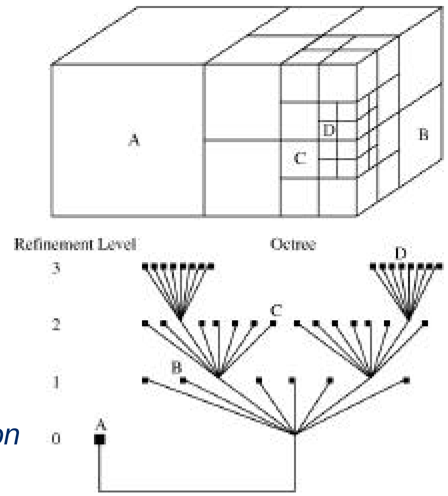
Additional summaries to be added:
- ESS Round-3 Investigator milestone tally
- Groups of ESS Guest Investigators given testbed allocations since the last IAR
- Groups of CAS Investigators given testbed allocations since the last IAR

Multiscale Modeling of Heliospheric Plasmas

Tamas Gombosi, University of Michigan
http://hpcc.engin.umich.edu/HPCC/

Goal: *To accurately simulate the dynamic Heliosphere, propagating the solar wind from the surface of the Sun to the interstellar shock for a complete solar cycle.*

Simulation performed using Block Adaptive Tree Solar-wind Scheme code (BATS-R-US)

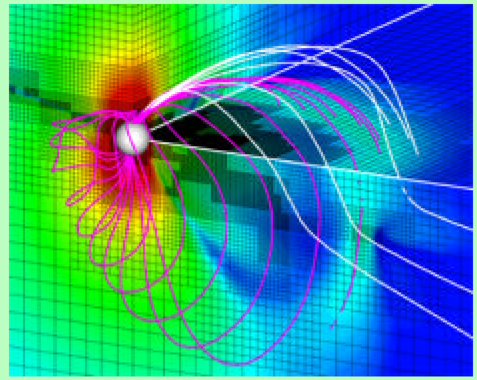


BATS-R-US is:

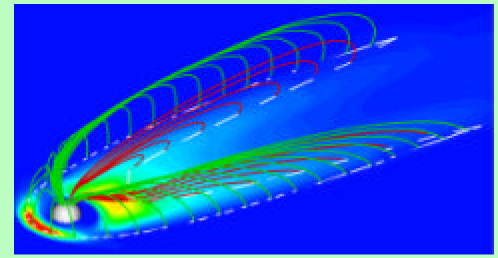
- *Cell-centered upwind finite volume formulation with high-resolution Godunov-type scheme.*
- *Block-based Adaptive Mesh Refinement (AMR):*
  - *Physics-based refinement and coarsening criteria*
  - *Resolution of multiple solution scales*
- *Parallel implementation:*
  - *Multiscale domain decomposition*
  - *Portable implementation (FORTRAN90/MPI)*
  - *Achieved 345 Gflops on a 1,490 processor Cray T3E-1200 with near-perfect scalability*
  - *Simulation ran for 80 hours on 512 processors. This was about 50% faster than real time (the simulation time was 125 hours).*

First ever "Sun to Mud" Space Weather Simulation

Generation of a Coronal Mass Ejection (CME), its interplanetary propagation and its interaction with the Earth's magnetosphere-ionosphere system.

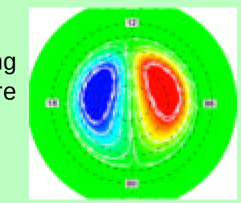


CME near the Sun 9-hours after its initiation



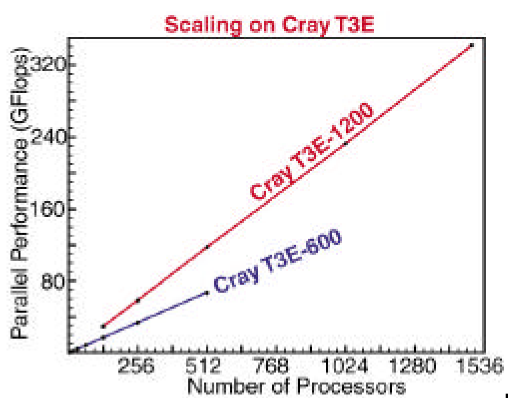
Magnetosphere of the Earth interacting with the CME;

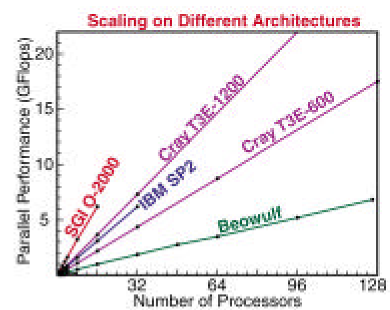
and the corresponding ionosphere



Other Applications of BATS-R-US:

- *Solar wind interaction with planets and comets.*
  - *Solar wind interaction with Mercury, Venus, Mars and Saturn*
  - *Solar wind interaction with comets and simulation of cometary x-rays*
- *Interaction of planetary satellites with planetary magnetospheres.*
  - *Interaction of Io and Europa with Jupiter's magnetosphere*
  - *Titan's interaction with Saturn's magnetosphere*





Earth and Space Science (ESS) Round-2 Grand Challenge

Turbulent Convection and Dynamos in Stars

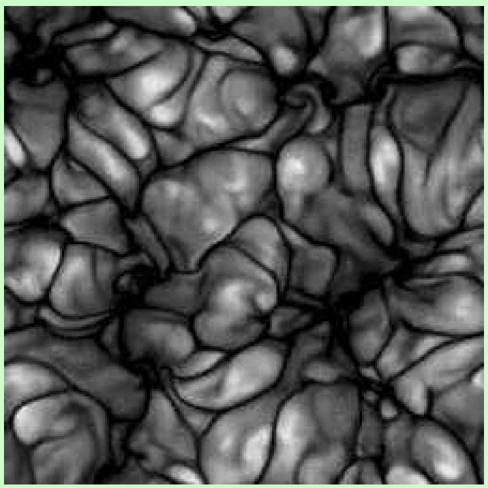
Andrea Malagoli, University of Chicago
http://astro.uchicago.edu/Computing/HPCC/

Goal: *To understand the structure and evolution of both large- and small-scale magnetic fields near the surface of the Sun.*

For the first time the resolution of simulations of turbulent convection on the Sun's surface can exceed the resolution of the observations.

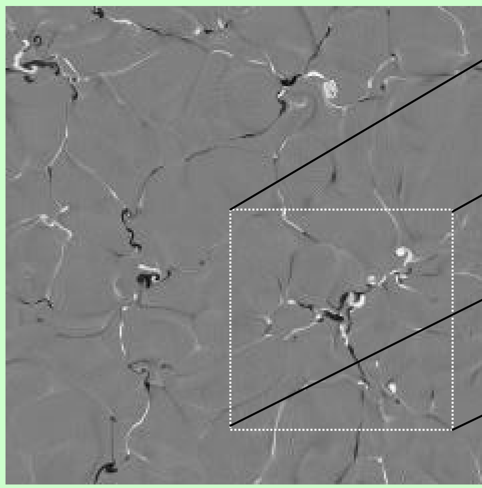
- Provides an important framework for the analysis of observations by eliminating incorrect interpretations.
- Provides robust theoretical guidelines for the planning of future missions like Solar-B.

Temperature of top layer

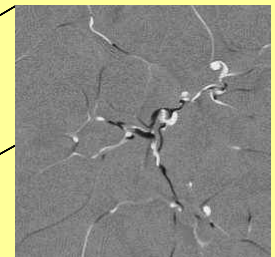


Light color represents hotter fluid moving up out of the page; dark color represents colder, sinking fluid.

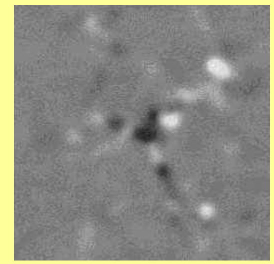
Magnetic Flux of top layer



Light color represents large positive flux pointing up out of the page; dark color represents large negative flux.



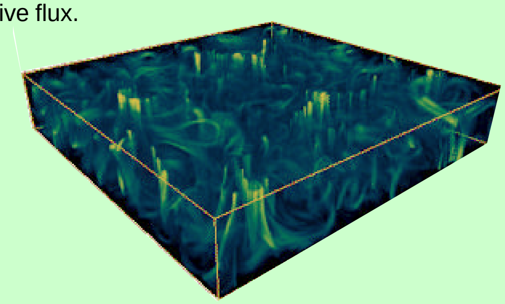
"actual" distribution produced by simulation



"blurred" distribution that would be observed by an instrument. It may be interpreted incorrectly as an emerging coherent flux tube.

Results from MPS, a MHD PseudoSpectral code simulating magnetic fields in the Sun

- *Carried out on a 512x512x97 grid.*
- *The size of the simulation enables it to contain several coherent structures that can be associated with the sun's granules.*
- *Run at 50 Gigaflop/s on 512 processors of the ESS Cray T3E at GSFC.*
- *100,000 iterations*



Magnetic enstrophy (the square of the magnetic field) near the surface of the solar convection zone

Earth and Space Science (ESS)
Round-2 Grand Challenge

J.Fischer 990419

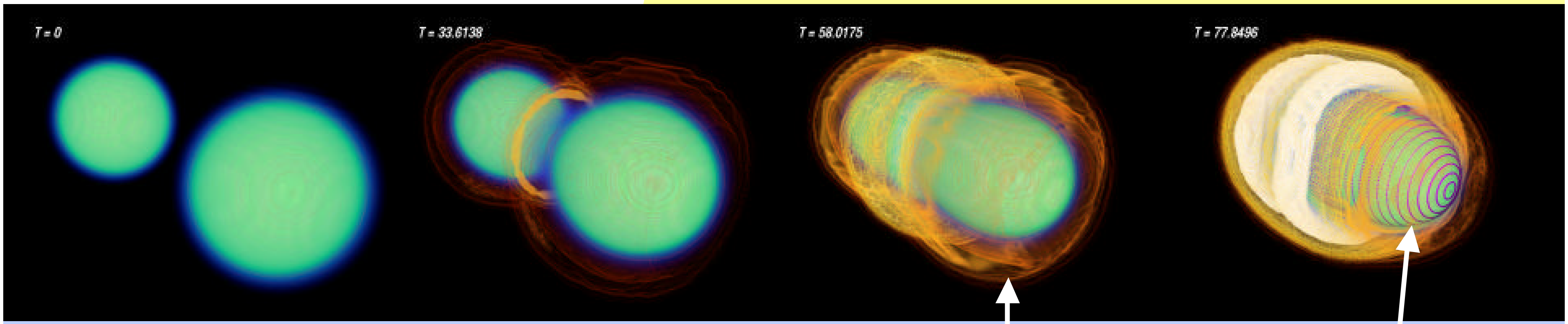
Relativistic Astrophysics and Gravitational Wave Astronomy

Paul Saylor, University of Illinois
http://wugrav.wustl.edu/Relativ/nsgc.html

Goal: *Combine fluid dynamics and General Relativity to investigate the merger of two neutron stars, a process that encompasses many aspects of relativistic astrophysics.*

For the first time, Neutron Star mergers are being simulated using Einstein's theory of General Relativity

Calculations using the fully relativistic model of gravity, as opposed to previous calculations using the post-Newtonian approximation, **reveal that a Black Hole can result from such a merger.**



In this calculation, two Neutron Stars, each having 1.4 solar mass, collide head-on and merge to form a Black Hole.

Visualization by: Werner Benger and the NCSA/Potsdam/Wash.U/ZIB visualization team
Simulation by: Mark Miller and the Washington University/Albert Einstein Institute neutron star team, the NASA Neutron Star Grand Challenge Collaboration.

Shock waves of heated gas generated by the collision.

The *Horizon* - inside this surface, the pull of gravity is so strong that even light collapses.

Results produced by GR3D, a 3-D General Relativity code coupling the Einstein Equations and relativistic hydrodynamic equations

- Computation carried out on a 160x160x160 grid run for 3000 time steps.
- Run at 25 Gigaflop/s sustained for 30 hours (totaling 100 trillion floating point operations) on 512 processors of the ESS Cray T3E at GSFC.
- GR3D couples multidisciplinary codes using the Cactus framework [http://cactus.aei-potsdam.mpg.de/index.html].

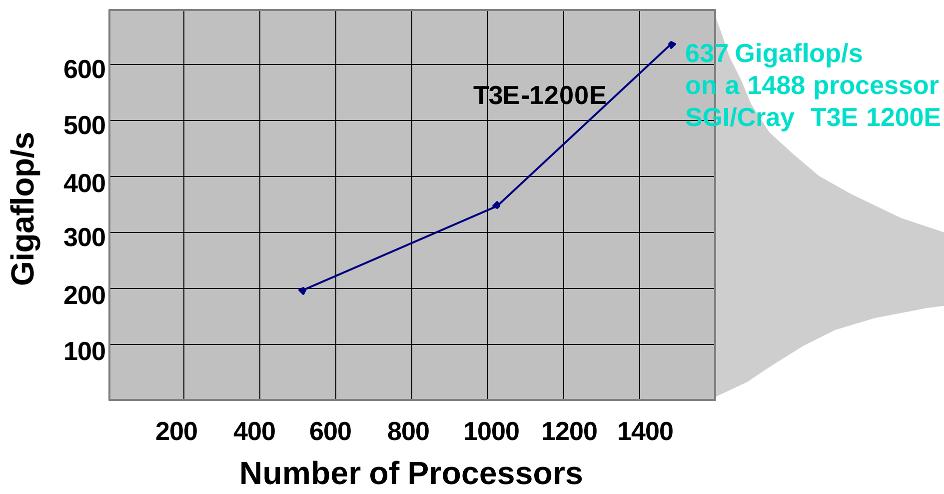
Future: extend simulations to compute signatures of gravity waves emitted by Neutron Star mergers to support gravitational wave observatories being built in the U.S. by the LIGO project and in Europe by the VIRGO and GEO projects.

Three-Dimensional Spherical Simulations of Earth's Core and Mantle Dynamics

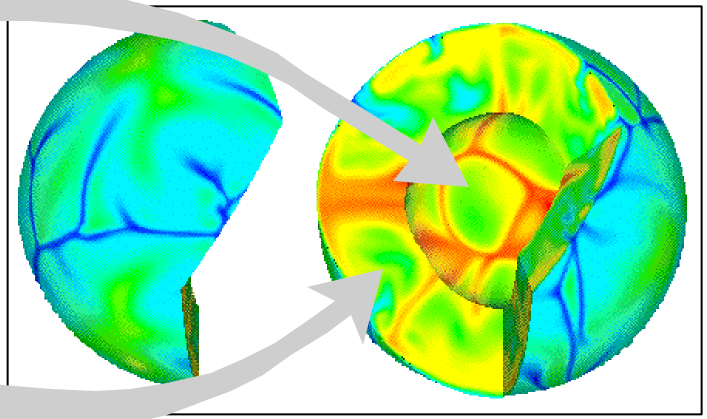
Earth and Space Science (ESS)
Round-2 Grand Challenge

Peter Olson, Johns Hopkins University, Principal Investigator
http://curie.eps.jhu.edu/nasa3/start.html

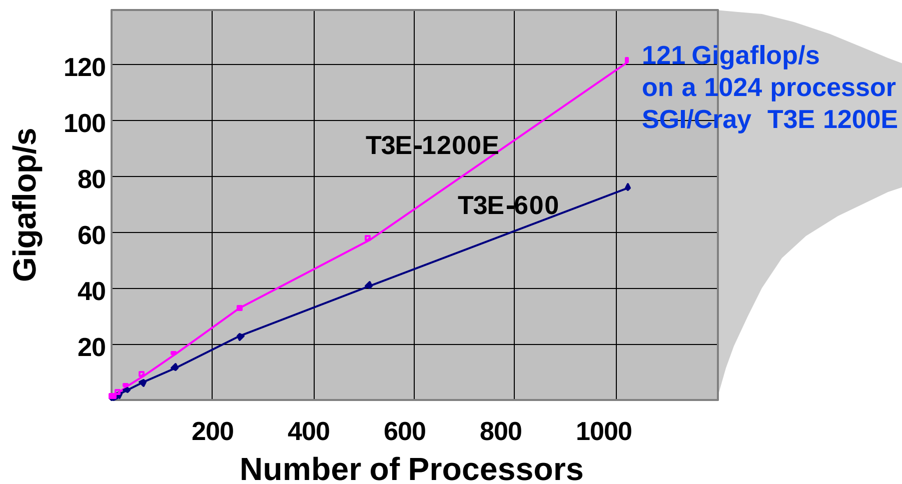
DYNAMO Performance



DYNAMO is a 3-D code for studying the Earth's magnetic dynamo which arises from the turbulent convective processes in the Earth's core. This code solves the full anelastic magnetohydrodynamic (MHD) equations in a spherical geometry using pseudospectral (spherical harmonic expansion) methods.



TERRA Performance



TERRA is a 3-D spherical finite element mantle dynamics code which treats the silicate material that comprises the Earth's mantle as a (non-linear) viscous fluid and solves the Navier-Stokes equations in 3-D spherical geometry for the motions that arise due to the temperature and density variations.

J.Fischer 990113

Ensemble Calculations for Seasonal Forecasting

Max Suarez/GSFC, NASA Seasonal to Interannual Prediction Project (NSIPP)
http://nsipp.gsfc.nasa.gov/

Goal: *Establish the degree to which clusters of PC's may reduce the cost of ensemble forecasting.*

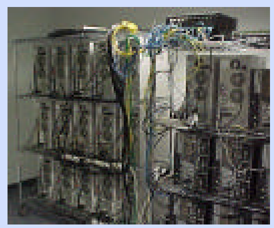
For the NSIPP atmospheric model, a cluster of commodity PC's provides performance similar to commercial products, but at significantly lower cost.

Computation of one simulated day using a 288x180x22 grid run on 32 processors of:

Cray T3E-600

Origin 2000

theHive (Linux cluster of PCs)



Requires:

Cray T3E-600	Origin 2000	theHive (Linux cluster of PCs)
20 minutes	10 minutes	29 minutes

The 32 processor Linux cluster cost $120K in mid 1999, making it roughly 3 times more cost effective than the Origin.

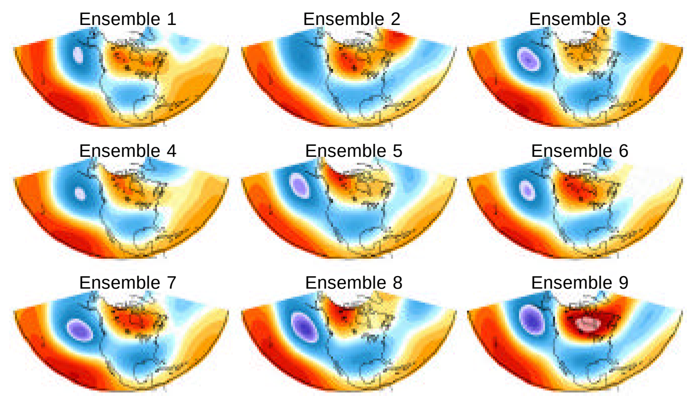
The PC cluster approach is now commercially offered. It allows the latest PC chips to be made available in the computing center for high end applications as soon as they are available to the public.

Creation of the Linux cluster: John Dorband/GSFC
Porting to the Linux cluster: Tom Clune/SGI
Porting to the Origin: Jim Abeles/SGI, Tom Clune/SGI
Timing on the T3E: Max Suarez/GSFC

Since ensemble members are independent they can be run in parallel. 18 runs, using 32 processors each, would efficiently utilize 576 processors. Such work can be done cost effectively on 18 small clusters, reserving large, tightly coupled supercomputers, such as the T3E, for tasks in which independent calculations cannot be so readily organized.

Results produced by NSIPP atmospheric model

Forecast anomalies of the upper level flow of the 1983 El Nino event.



The panels show nine realizations taken at random from an 18-member ensemble forecast. Anomalies over North America are very similar in all members. Over the North Atlantic, however, there is considerable random variability. Ensemble forecasts are required to distinguish between these situations.

The Beowulf Project *- the GSFC-centric time line*

http://beowulf.gsfc.nasa.gov/

1992
HPCC/ESS establishes requirement for a one Gigaflop/s workstation costing $50K or less.

1993
Beowulf Project formed at GSFC to achieve requirement using piles of commodity PCs and Linux.

1994
Don Becker is recruited to form technical core of team.

Beowulf I: Wiglaf
1994
16 - 100Mhz 486DX4
$40,000
50 MFlops sustained (PPM)
Dual 10Mhz Ethernet

1995
Beowulf II: Hrothgar
16 - 100Mhz Pentium
$40,000
150 Mflops sustained (PPM)
Dual 100Mhz hub-based Ethernet

Beowulf III: Ecgtheow
"T-Racks"
1997
60 - 200Mhz Pentium Pro
100Mhz Ethernet
1 Terrabyte disk
Goal: 1 Gigabyte/sec I/O

→ 128 - 200Mhz Pentium Pro
100Mhz switched Ethernet
72 port switch
1998

1997
Beowulf IV: theHIVE
128 - 200Mhz Pentium Pro
$210,000
7.5 Gflops sustained (PPM)
Five 16-port Ethernet switches

1998
72 port 100Mhz Ethernet switch
0.9 Tbytes disk
0.8 Gbyte/sec I/O

1999
Added 72 Pentium -3 Xeons

2000
Install Myrianet in theHive

1998
Real applications, First scientific result

1999
Aries climate code achieves 0.25 T3E performance on same number of theHive processors

Today

STORAGE

2000
Single vendor solution from SGI

2000
Large parallel file servers using Beowulf clusters

COMPUTATION

2000
Heterogeneous system consisting of selected different vendor PCs under a common software environment

2002
Some ESS Round-3 Investigator applications run on large Beowulf clusters (512-1024 processors)

1997
The NASA Beowulf-class Clustered Computing Workshop, the first NASA-wide meeting on PC cluster computing, held in Pasadena

1997
A Beowulf system wins the Gordon Bell Prize for cost/ performance

1999
Fourth Joint PC Clustered Computing Conference, sponsored by DOE and NASA, held in Pasadena

1999
How to Build a Beowulf book published by MIT Press

1999
Don Becker receives the 1999 Excellence in Programming Award, given annually by the Dr. Dobb's Journal, for development of Beowulf/Linux.

1999
Gordon Bell requests the 'first Beowulf' for exhibit in the computer museum at Moffett Field

J.Fischer 000106