ERDC MSRC/PET TR/01-03

Programming Environment and Training (PET) Core Support and Focused Efforts

for the period

27 March 2001 through 30 September 2001

U.S. Army Engineer Research and Development Center (ERDC)

Major Shared Resource Center (MSRC)

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PET Core Support and Focused Efforts

27 March 2001 through 30 September 2001

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Section 1: INTRODUCTION

1.1 Background

The Programming Environment and Training (PET) program began at the U.S. Army Engineer Research and Development Center (ERDC) Major Shared Resource Center (MSRC) in March 1996. The contract provided for an initial three-year program with a two-year renewal option. The option was exercised and the current PET program would be scheduled to end on 26 March 2001. PET had a successful program review in March 2000, and as a result the HPCMP made the decision to request proposals for the continuation on PET beginning on 1 October 2001. In order to provide continuous funding of the university team and support to the users of the ERDC MSRC, between the end of the existing PET contract and the start of the new contract, the ERDC MSRC has provided funding for core support and focused efforts for the period between 27 March 2001 and 30 September 2001.

Efforts supported by the ERDC MSRC PET program cover the primary Computational Technology Areas (CTAs) supported by the MSRC and other specialty areas, including Scientific Visualization (SciVis), Scalable Parallel Programming (SPP) Tools, support for Historically Black Colleges and Universities (HBCUs) and Minority Institutions (MIs), and Training and Collaboration/Communication (C/C). The primary CTAs supported at ERDC MSRC are Computational Fluid Dynamics (CFD), Computational Structural Mechanics (CSM), Environmental Quality Modeling and Simulation (EQM), Climate/Weather/Ocean Modeling and Simulation (CWO), and Forces Modeling and Simulation/C4I (FMS).

The academic partners associated with ERDC MSRC PET include: Engineering Research Center (ERC) at Mississippi State University (Lead university); Jackson State University (HBCU/MI Lead); National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign; University of Tennessee, Knoxville; Florida State University; Clark Atlanta University (HBCU); Ohio Supercomputer Center; Ohio State University; University of Texas at Arlington; Texas Institute for Computational and Applied Mathematics (TICAM) at the University of Texas at Austin; Texas A&M University – Kingsville (MI).

1.2 Core Support

"Core Support" refers to that portion of PET that captures the minimum funding required for full-time, on-site positions and university leads. Significant lead time and funding assurance are required prior to university hiring commitments, so there must be some level of assurance that annual funding will be maintained at each university throughout the program. This, of course, does not preclude corrective action based on non-performance. PET activities at ERDC MSRC within Core Support include, but are not limited to:

- Providing High Performance Computing (HPC) training courses for MSRC users
- Providing a continual base of academic involvement in PET
- Ensuring greater freedom in the scope of university efforts
- Providing for longer duration academic efforts
- User outreach based on constant CTA utilization monitoring, Department of Defense (DoD) HPC User Group Conference participation, and one-on-one user assistance as required
- Providing updated inputs to PET web pages
- Regular reporting of activities/progress for each PET area

1.3 Focused Efforts

Additional PET resources are allocated for "Focused Efforts." Focused Efforts are projects derived from PET team interactions with MSRC users. Proposals for Focused Efforts are submitted by the university partners and approved by the PET leadership and ERDC MSRC. Focused Effort proposals are evaluated according to the following guidelines:

- Relation of proposed activity to national defense or national security.
- Relevance of proposed activity to ongoing Common HPC Software Support Initiative (CHSSI) projects.
- Extent to which the proposed effort complements MSRC hardware acquisition strategy.
- Relevance of proposed activity to ongoing DoD Challenge Projects.
- Exploitation of the Defense Research and Engineering Network (DREN).
- Extent to which the proposed effort improves the effective utilization of HPC resources through:
  - Visualization and data interpretation,
  - Code performance enhancements,
  - Multi-architecture portability, etc.
- Extent to which the proposed effort enhances the capability to use MSRC systems through:
  - Training and graduate courses,
  - HBCU/MI activities,
  - Collaborative environments, etc.

Obviously, every Focused Effort cannot meet all of these criteria. These criteria are used to judge the importance of the proposed work with respect to the HPCMP mission. Focused Efforts are managed according to the following rules:

- Authority to Proceed (ATP) is based on informal proposals submitted to the PET Director and the review/concurrence of PET leadership and the government.
- Projects must have MSRC user advocacy and participation, if at all possible.
- Projects should have specific start and end dates, schedules, work products, budgets, and periodic progress reviews (every 3 months).
- Each effort is managed on a project-by-project basis and funding will be allocated on this basis.
- Final technical reports are due at the end of the contract year.

Detailed descriptions of the approved Core Support and Focused Efforts for this contract period are provided in Section 2.

Section 2: ERDC MSRC PET EFFORTS

2.1 Core Support Descriptions

The following Core Support efforts were approved for the contract period from 27 March 2001 through 30 September 2001:

Florida State University

- Communication/Collaboration (C/C), Off-site
- Training, Off-site

Jackson State University

- HPC Support to HBCU/MIs, Off-site

Mississippi State University

- Academic Lead, Off-site
- Computational Fluid Dynamics (CFD), On-site and Off-site
- Computational Structural Mechanics (CSM), On-site

Ohio State University

- Climate/Weather/Ocean Modeling and Simulation (CWO), On-site and Off-site

University of Texas at Austin

- Computational Structural Mechanics (CSM), Off-site
- Environmental Quality Modeling and Simulation (EQM), On-site and Off-site

PET EFFORTS FOR 27 MARCH 2001 THROUGH 30 SEPTEMBER 2001

1. **Core Support Area:** Communication/Collaboration (C/C)

2. **Organization:** Florida State University

3. **Lead:** Prof. Geoffrey Fox

4. **E-Mail:** gcf@cs.fsu.edu

5. **Telephone:** (850) 644-4587

6. **Fax:** (850) 644-0098

7. **Statement of Work:**

   Florida State will provide a core level of effort to support technology transfer, user outreach, training, and assessment of tools and technologies to facilitate communication and collaboration among the PET team and users of the ERDC MSRC. Technologies of interest include, but are not limited to, both synchronous and asynchronous collaboration over the Internet and use of databases to manage large volumes of information, especially when coupled with web servers to facilitate access to the information.

   Florida State will maintain frequent contact with ERDC MSRC Webmaster, database administrators, and other on-site personnel to insure that C/C resources provide the maximum utility to the PET/user community. Florida State will also maintain regular contact with PET team members to assess needs. Florida State will select and attend focused conferences and other meetings that have high payoff and direct application for team and user interaction and technology transfer.

   Past experience will be used (where TangoInteractive only had limited acceptance outside training) to design a requirements analysis covering training, computer users and MSRC staff. Preliminary reports will be presented at midyear and used to design some experimental deployment efforts in the last half of the year.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as appropriate)
   - Contribute materials pertaining to collaboration and communication technologies to the ERDC MSRC PET C/C web site (on-going)
   - Report on selected collaboration tools and their possible roles within the ERDC MSRC and PET organizations
   - Selected experimental deployment of identified collaboration tools
   - Deliver a training course on Computing Portals and the Grid Computing Environment
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentation for PET Final Review

1. **Core Support Area:** Training

2. **Organization:** Florida State University

3. **Lead:** Prof. Geoffrey Fox

4. **E-Mail:** gcf@cs.fsu.edu

5. **Telephone:** (850) 644-4587

6. **Fax:** (850) 644-0098

7. **Statement of Work:**

Florida State will provide a core level of effort to support technology transfer, user outreach, and long-range leadership on issues of technology, tools, and techniques related to PET training and educational needs. Technologies of interest include, but are not limited to, synchronous and asynchronous web/Internet-based distance education tools and electronic repositories of training materials.

Florida State will work closely with the on-site training team at the ERDC MSRC to understand the needs and use of training technology at the MSRC in the context of the changing technology base. This requirement analysis will be complemented by a survey of current and emerging tools, which will be classified in terms of the concept of a "collaborative portal" which will underlie research efforts at Florida State and capture the lessons from the PET and other efforts funded over the last few years. Tools and standards will be recommended that will enable authoring of training material that can best be re-used as the underlying technology base shifts. Some key tools will be selected and supported for user experimentation and evaluation during the contract period.

Florida State will continue to select and attend focused conferences and other meetings that have high payoff and contribute directly to providing leadership on training technology issues. This effort is expected to position the MSRC to make innovative use of emerging training technology and standards and continue its leadership position in year 6 and beyond.

8. **Deliverables:**

- Trip reports for conferences and user contacts
- Contribute materials pertaining to education and training technologies to the ERDC MRSC PET Training web site (on-going)
- Involvement in PET Program-Wide Training Group meetings and activities
- Report evaluating training and education tools linked to both the MSRC user and HBCU pipeline requirements
- Contribution to PET Annual Report

- Written progress report in June 2001
- Presentations for PET Final Review

PET EFFORTS FOR 27 MARCH 2001 THROUGH 30 SEPTEMBER 2001

1. **Core Support Area:** HPC Support for HBCU/MIs

2. **Organization:** Jackson State University

3. **Lead:** Prof. Willie G. Brown

4. **E-Mail:** wbrown@jsums.edu

5. **Telephone:** (662) 979-4300

6. **Fax:** (662) 979-4301

7. **Statement of Work:**

   Jackson State University (JSU) will continue to provide a core level of effort to support student-training activities at JSU. This will include HBCU/MI web page maintenance and updating, maintaining the HBCU/MI capabilities database, participation in users group meetings, visits to ERDC MSRC and conduct of the Summer Institute. Summer Institute activities include student recruitment, student room, board, and stipends, presenter/instructor scheduling and coordination, and course materials and supplies.

   JSU will collaborate with the ERDC MSRC and FSU on applications of the Access Grid in distance education.

8. **Deliverables:**

   - HBCU/MI Web Pages
   - HPC Summer Institute
   - Reports on HBCU/MI Activities
   - Attendance and participation in PET meetings, conferences, workshops, colloquia, etc.
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review

1. **Core Support Area:** Academic Lead

2. **Organization:** Mississippi State University

3. **Lead:** Prof. Joe Thompson

4. **E-Mail:** joe@erc.msstate.edu

5. **Telephone:** (662) 325-7299

6. **Fax:** (662) 325-7692

7. **Statement of Work:**

   Mississippi State University (MSU) ERC will continue to provide a core level of effort to support the academic leadership of the PET program at ERDC MSRC. Responsibilities include, but are not limited to, participation in the Academic Executive Committee (ExComm) for PET across the four MSRC's; maintaining knowledge of current status of all Focused Efforts ongoing at the participating university partners; review and recommendations for funding of PET Focused Efforts and participation in planning and execution of PET meetings (Final Review, workshops, DoD Users Meeting, etc.), as appropriate. The PET Academic Lead will select and attend conferences and other meetings that have high payoff and direct application for the PET Program.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Preparation of the PET Year 5 Annual Report

1. **Core Support Area:** Computational Fluid Dynamics (CFD)

2. **Organization:** Mississippi State University

3. **Lead:** Prof. Bharat Soni

4. **E-Mail:** bsoni@erc.msstate.edu

5. **Telephone:** (662) 325-2647

6. **Fax:** (662) 325-7692

7. **Statement of Work:**

   Mississippi State University (MSU) ERC will continue to provide a core level of effort to support the CFD on-site position for the PET program at ERDC MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training and assessment of targeted codes and algorithms in CFD. Targeted codes include, but are not limited to, the CFD Common High Performance Computing Software Support Initiatives (CHSSI) codes. Technology of interest includes, but is not limited to, grid generation codes, parallelization of CFD algorithms, numerical solvers, management and interpretation of large data sets, and adaptive and meshless techniques. MSU will maintain frequent contact with the DoD CTA Lead for CFD. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Contributions to PET website for CFD (as appropriate)
   - Support for JSU HPC Summer Institute
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review
   - On-Site CFD Lead at the ERDC MSRC
   - At least one technical report by on-site lead

1. **Core Support Area:** Computational Structural Mechanics (CSM)

2. **Organization:** Mississippi State University

3. **Lead:** Prof. Joe Thompson

4. **E-Mail:** joe@erc.msstate.edu

5. **Telephone:** (662) 325-7299

6. **Fax:** (662) 325-7692

7. **Statement of Work:**

   Mississippi State University (MSU) ERC will continue to provide a core level of effort to support the CSM on-site position for the PET program at ERDC MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training and assessment of targeted codes, and algorithms in CSM. Targeted codes include, but are not limited to, EPIC, CTH, DYNA3D, and NASTRAN. Technology of interest includes, but is not limited to, grid generation codes, management and interpretation of large (terascale) data sets, and adaptive and meshless techniques. MSU will maintain frequent contact with the DoD CTA Lead for CSM to understand the priorities and ongoing CHSSI activities. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Contributions to PET website for CSM (as appropriate)
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review
   - On-Site CSM Lead at the ERDC MSRC
   - At least one technical report by on-site lead

1. **Core Support Area:** Climate/Weather/Ocean Modeling and Simulation (CWO)

2. **Organization:** Ohio State University

3. **Leads:** Prof. Keith W. Bedford, Prof. Ponnuswamy Sadayappan

4. **E-Mail:** bedford.1@osu.edu, sadayappan.1@osu.edu

5. **Telephone:** (614) 292-7338, (614) 292-0053

6. **Fax:** (614) 292-3780

7. **Statement of Work:**

   Ohio State University (OSU) will continue to provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CWO. Targeted codes include, but are not limited to, WAM, CH3D, SWAN, SED, FBM, MM5, and COSED. Technologies of interest include, but are not limited to, application of circulation and wave models to sea condition prediction; and coupling of wave, sediment, and circulation models. OSU will maintain frequent contact with the DoD CTA Lead for CWO to understand the priorities and ongoing CHSSI activities, as well as with the local CWO representative at ERDC MSRC. User outreach will also consist of presentations at the DoD HPC Users Group Conference. OSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Monthly updates of CWO material on ERDC PET web site
   - Presentation at DoD HPC Users Group Conference
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review
   - On-Site CWO Lead at the ERDC MSRC
   - At least one technical report by on-site lead

PET EFFORTS FOR 27 MARCH 2001 THROUGH 30 SEPTEMBER 2001

1. **Core Support Area:** Computational Structural Mechanics (CSM)
2. **Organization:** University of Texas at Austin
3. **Lead:** Prof. Tinsley Oden
4. **E-Mail:** oden@ticam.utexas.edu
5. **Telephone:** (512) 471-3312
6. **Fax:** (512) 471-8694
7. **Statement of Work:**

   TICAM will continue to provide a core level of effort to support technology transfer, user outreach, and training. Technology of interest includes, but is not limited to, adaptive mesh and grid algorithms and tools, management of large CSM data sets, and parallelization/coupling of key CSM codes. TICAM will maintain regular contact with the ERDC MSRC PET On-site Lead for CSM to facilitate technology transfer, user outreach, and relevance to current MSRC issues. Related codes include CTH, EPIC, and DYNA3D. During the contract period, TICAM will make site visits to ERDC MSRC to work with the DoD users and on-site personnel for CSM.

   TICAM will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, TICAM will submit, in advance, a "statement of benefits" to PET that allows the PET management to determine whether ERDC MSRC PET funding should be used to cover the cost of that meeting.

8. **Deliverables:**

   - One or more papers or poster sessions will be submitted for presentation at the DoD HPC Users Group Conference
   - Trip reports for conferences and user contacts (as conducted)
   - Contributions to CSM portion of ERDC PET website
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review

1. **Core Support Area:** Environmental Quality Modeling and Simulation (EQM)

2. **Organization:** University of Texas at Austin

3. **Lead:** Prof. Mary Wheeler

4. **E-Mail:** mfw@ticam.utexas.edu

5. **Telephone:** (512) 475-8625

6. **Fax:** (512) 471-8694

7. **Statement of Work:**

   In this project, The University of Texas at Austin (UT-Austin) will support research and an on-site person in the EQM area. Technology transfer will occur through the on-site EQM personnel, the EQM web page, EQM success stories, activity reporting, and user training. UT-Austin personnel will accomplish user outreach through frequent visits to user sites and contacts with users. UT-Austin personnel will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Trip report for DoD HPC Users Group Conference and other conferences attended
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review
   - On-Site EQM Lead at the ERDC MSRC
   - At least one technical report by on-site lead

2.2 Focused Effort Descriptions

The following Focused Efforts have been approved for contract period from 27 March 2001 through 30 September 2001:

Clark Atlanta University

- Development of Web-based Training Material on ERDC MSRC HPC Systems (Student Internship)
- Parallel Simulation of Wave Break and Waves Interacting with Vessels in Motion

Florida State University

- Modular Collaborative Environment
- Collaborative Portals for Training and Computational Science

University of Illinois at Urbana-Champaign

- Standard File Format for Large Data Problems and Visualization
- Visualization for EQM

Mississippi State University

- Grid Assembly Enhancements for Chimera Technology
- Java Based CFD Training
- Library of Interpolation and Approximation Modules (INLiB **)**
- Web Portal Infrastructure to Support Land Management System

Ohio Supercomputer Center

- HPC Training Courses

Ohio State University

- Enhancement, Evaluation, and Application of a Coupled Wave-Current-Sediment Model for Nearshore and Tributary Plume Predictions

Syracuse University

- Delivering SPEEDES Based HPC Simulations over WebHLA to ERDC MSRC and/or Joint Simulation System (JSIMS) Users

University of Tennessee, Knoxville

- Parallel IO
- Metacomputing Support for the SARA3D Structural Technology Acoustics Application

University of Texas at Austin

- AMR and CTH Capability and Algorithm Enhancements
- Adaptive Mesh Technology, Mesh Improvement and Algorithms for Hypervelocity Impact and Penetration Analyses
- Discontinuous Galerkin Finite Elements and Adaptive Grids for DoD Problems
- Algorithms for Error and Feature Indication in Interpolation and Approximation
- Improved Parallel Performance for Environmental Quality Models
- A Full 2-D Parallel Implementation of CH3D-Z
- Interpolation and Projection Between Arbitrary Space/Time Grids
- Reactive Transport Schemes for Water Quality Modeling on Unstructured Grids

Texas A&M University – Kingsville

- Parallel FEMWATER Visualization
- Parallel FEMWATER Data Management

1. **Focused Effort Title:** Development of Web-based Training Material on ERDC MSRC HPC Systems (Student Internship)

2. **Organization:** Clark Atlanta University

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Name:** Prof. Kofi Bota

5. **E-Mail:** kbota@cau.edu

6. **Telephone:** (404) 880-6996

7. **Fax:** (404) 880-6880

8. **Statement of Work:**

   Clark Atlanta University will provide a student to work on -site at ERDC MSRC during the months of June, July, and August 2001. The student will assist in the development of ERDC MSRC web pages to provide users information on the ERDC MSRC HPC computer systems. For example, this could include information on using PBS, compiling and executing programs, migrating data, and resources (hardware and software) available on the various systems.

   Assumption: All equipment, material, and information will be supplied by ERDC MSRC.

9. **Deliverables:**

   - Web pages for ERDC MSRC Webmaster
   - Presentation and Final Report

1. **Focused Effort Title:** Parallel Simulation of Wave Break and Waves Interacting with Vessels in Motion

2. **Organization:** Clark Atlanta University

3. **Thematic Areas:** Scalable Computing Migration, HPC Performance Metrics/Tools

4. **PI Name:** Prof. Shahrouz Aliabadi

5. **E-Mail:** aliabadi@cau.edu

6. **Telephone:** (404) 880-6433

7. **Fax:** (404) 880-6880

8. **Statement of Work:**

This is the continuation of the year 5 project Clark Atlanta proposed. During the extension period, continuing efforts will be focused on "Parallel Simulation of Wave Break and Waves Interacting with Vessels in Motion".

During the past several years, Clark Atlanta has developed highly scalable parallel finite element flow solvers for simulation of multi-fluid flow applications. These solvers are based on the Navier–Stokes equations for multiple incompressible fluids mixing with each other. Stabilized finite element formulations are used for the discretization of the governing equations. The non-linear systems of equations resulting from the finite element discretizations are solved using sophisticated vector -based iterative solvers. As a result, minimal memory is required to solve applications with 10 to 100 million unknowns. The parallel implementation of the solver assumes that the finite element mesh is totally unstructured. This greatly broadens the application of the solver to problems with complex geometries discretized with automatic mesh generators. The parallel implementation is also based on MPI, which makes the solver portable to any supercomputer platform. Currently we are running our solver on the Cray T3E, IBM SP2, and SGI Power Challenge. Recently, the accuracy of this flow solver has been verified in 3D applications.

In the continuation of this project, we will focus on simulations of 3D waves. So far, the simulations have been carried out only for 2D domains. We will also investigate wave impacts on coastal structures. To verify the accuracy of our flow solver, we will compute flow around a test ship with available experimental data. This project will be conducted through extensive collaborations and discussions with Drs. Charlie Berger and Jane Smith from the ERDC Coastal and Hydraulics Laboratory (CHL).

9. **Deliverables:**

- Simulation of wave formation and wave breaking problems in 2D and 3D

- Verifying the accuracy of the flow solver
- Web-based visualization to study the computed results
- Presenting the results in conferences or workshops
- Trip reports
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Modular Collaborative Environment

2. **Organization:** Florida State University

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Name:** Prof. Geoffrey Fox

5. **E-Mail:** gcf@cs.fsu.edu

6. **Telephone:** (850) 644-4587

7. **Fax:** (850) 644-0098

8. **Statement of Work:**

Florida State University (FSU) will support and help design the Access Grid development at Jackson State University (JSU) and ERDC MSRC. FSU will also give access to low end desk top audio systems - today the systems from HearMe and Lipstream are viewed as best but there are rapid developments in the VOIP (Voice over IP) field which could change this evaluation.

The goal is to be in a position to offer a graduate level computational science course to the ERDC Graduate Institute and JSU in the fall of 2001. FSU will aim at deployment by June 2001, allowing testing over summer for use by August 2001. FSU is starting Access Grid planning now and expect that this schedule is easily achievable. FSU will integrate this audio-video with best practice collaborative training environment - currently these are WebeX, Centra, and Placeware, but this area is very volatile as well. This choice will be made around April 2001 after consultation with ERDC MSRC and JSU. In all this work, ongoing support issues will be addressed.

9. **Deliverables:**

- Access Grid and HearMe or equivalent audio-video conferencing deployment at ERDC MSRC, FSU and JSU, June 2001
- Integration with best available training platform, June 2001
- Final tested and supportable system, August 2001
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentation for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Collaborative Portals for Training and Computational Science

2. **Organization:** Florida State University

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Name:** Prof. Geoffrey Fox

5. **E-Mail:** gcf@cs.fsu.edu

6. **Telephone:** (850) 644-4587

7. **Fax:** (850) 644-0098

8. **Statement of Work:**

This focused effort completes the work of the year 5 effort of this name. Florida State University (FSU) intends to finish the new collaborative infrastructure in June 2 001, which has been designed to exploit commercial infrastructure as much as possible. The current focused effort develops the infrastructure for both training and computing portals.

FSU will take the new Advanced Distributed Learning (ADL) / Instructi onal Management System (IMS) standards and build the necessary distributed object standards (XML specifications) that support DoD PET needs and are consistent with these community standards. The extensions, which are allowed by ADL/IMS, will support two ke y features. Firstly, the extensions will support the specific type (PowerPoint/Web) and content (CTA's, HPC technology etc.) used in PET training material. Secondly, the specification to support collaborative delivery will be enhanced. This is a serious omission in current standards and is connected with their incomplete client-server architecture. As explained in Prof. Fox's ERDC MSRC talk in September 2000, one should use a three tier model. Hopefully this will help DoD HPCMO work more closely with DoD ADL and together help advance their common goals of modular web-based training

FSU will integrate the Object standards developed in Gateway with those in Globus and in the hierarchical style of IMS, and develop a demonstration involving Globus, Gateway, and the same XML standards used in IMS. This allows collaborative computing to be implemented with the same infrastructure as training and general collaboration functions. This system will be built on top of the Gateway portal, which is being modified to h ave the same infrastructure as the training portal. This involves using Java Message Service (JMS) as its core. This should show how one can access distributed computers from the same web interface and support collaborative consulting at a distance.

9. **Deliverables:**

- ADL SCORM/IMS Extended Specification for DoD PET Training, June 2001

- Integration of Gateway Portal with Globus, July 2001
- Integration of Globus based Gateway Portal with IMS standards based collaborative infrastructure, September 2001
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentation for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Standard File Format for Large Data Problems and Visualization

2. **Organization:** University of Illinois at Urbana-Champaign, NCSA

3. **Thematic Areas:** Management and Interpretations of Large Data Sets, SciVis for Very Large Problems

4. **PI Names:** Dr. Polly Baker, Dr. Mike Folk

5. **Email:** baker@ncsa.uiuc.edu, mfolk@ncsa.uiuc.edu

6. **Telephone:** (217) 244-1997, (217) 244-0647

7. **Fax:** (217) 244-2909, (217) 244-1987

8. **Statement of Work:**

   This is a continuation of an existing effort, supplemented with new work to support scalable computing migration objectives. The existing effort is a collaboration between NCSA and Ronald Heath of the ERDC Coastal and Hydraulics Lab to investigate the use of NCSA's HDF5 file format to address the need for efficient access and storage of data generated and used by the CH3D surface water modeling code. NCSA proposes to continue this work by (a) porting the HDF5 Fortran API to the Windows Visual Fortran environment, which is a preferred for some CH3D applications, and (b) continuing to support Mr. Heath and other ERDC investigators who are using HDF5.

9. **Deliverables:**

   - An HDF5 library for Visual Fortran on Windows NT in June 2001
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentation for the PET Final Review
   - Final Technical Report

1. **Focused Effort Title:** Visualization for EQM

2. **Organization:** University of Illinois at Urbana-Champaign, NCSA

3. **Thematic Areas:** Management and Interpretations of Large Data Sets, SciVis for Very Large Problems

4. **PI Names:** Dr. Polly Baker, Dr. Alan Shih

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8. **Statement of Work:**

This initiative will continue to support Dr. Carl Cerco's team in using those visualization tools developed through past Focused Efforts, especially in their efforts to visualize the results of long-running scenarios. In Year 5, the capability to include observed data collected from the field during recent decades was added.

In this extension, the visualization techniques available for making comparisons between the collected data and the simulation output will be enhanced. Particular attention will be paid to making these newer capabilities easy to use and robust, such that the tools can serve Dr. Cerco's team well into the future.

In this extension, NCSA will also experiment with ways to include GIS data into the tool so that observed data and/or simulation output can be displayed within the appropriate geographical context. This will provide the user a more comprehensible spatial context. The way to provide a tool for such integrated visualization , which will allow the user to visualize a combination of observed data, benthic organism data (if available from user), simulated model output, and GIS data will be explored.

9. **Deliverables:**

- Assistance in use of current tools
- Prototype to integrate visualization of observed data, benthic organism data (if available from user), simulated model output, and GIS data
- Contribution to PET Annual Report
- Presentation for the PET Final Review
- Written progress report in June 2001
- Final Technical Report

1. **Focused Effort Title:** Grid Assembly Enhancements for Chimera Technology

2. **Organization:** Mississippi State University, ERC

3. **Thematic Areas:** HPC Training and DoD User Productivity,
HPC Performance Metrics/Tools

4. **PI Name:** Prof. Bharat Soni

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8. **Statement of Work:**

Under the current effort, the grid assembly process is being studied, analyzed and improved with a focus on large-scale applications. In particular, Mississippi State University (MSU) is concentrating on the data structures for grid assembly including polygonal mapping (PM) trees, Cartesian inverse maps, and Meakin's X-rays. MSU is analyzing the strengths and weaknesses of the hole cutting and stencil searching al gorithms used in different grid assembly codes including the opportunities offered for parallel execution. Techniques for visualizing the appropriate data structures are being developed. This will improve the processes of debugging grid assembly problems and developing grid assembly algorithms. The enhancements and improvements made in this development are to be validated using the BEGGAR and OVERFLOW-D codes.

Under this extension, the grid assembly algorithms in BEGGAR will be extended to assemble overset structured grids based on node centers rather than cell centers. The grid communication information will also be made available in the standard PEGSUS data file formats. Some software restructuring will be performed to make the BEGGAR grid assembly process more accessible as a stand-alone utility or for inclusion in other packages such as OVERFLOW-D. This will be the first step towards making the BEGGAR grid assembly algorithms ready for inclusion in the CTK library.

9. **Deliverables:**

- Validation and demonstration of the new capabilities to assembly overset structured grids based on node centers and to run other flow solvers using the standard PEGSUS files created by BEGGAR
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Java Based CFD Training

2. **Organization:** Mississippi State University, ERC

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Name:** Prof. Bharat Soni

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8. **Statement of Work:**

   Mississippi State University (MSU) proposes to enhance a Web based CFD training and demonstration tool for students and non-CFD users. This enhancement will facilitate parallel execution of CFD codes and incorporate test problems for students to execute and exercise various "what if" scenarios. The student will be able to exercise various numerical schemes, boundary conditions (BCs) and macros for geometry and grid information . The students will also be able to exercise "what if" scenarios with respect to grid, BCs and flow parameters. Students will also be able to understand and grasp the usefulness of parallel processing and performance gains as a result of parallel computing .

9. **Deliverables:**

   - An enhanced Web based parallel CFD demonstration and training tool with interactive grid, BCs and flow parameter set-up and visualization
   - On-line test problem execution with self evaluation system
   - A training tool demonstration at JSU
   - Contribution to PET Annual Report
   - Written progress report in June 2001
   - Presentations for PET Final Review
   - Final Technical Report

1. **Focused Effort Title:** Library of Interpolation and Approximation Modules (INLiB **)**

2. **Organization:** Mississippi State University, ERC

3. **Thematic Areas:** HPC Training and DoD User Productivity

4. **PI Name:** Prof. Bharat Soni

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8. **Statement of Work:**

The enhancement of the INLiB – Interpolation, approximation and grid manipulation toolkit is proposed. This library will be enhanced to contain various key functionalities associated with numerical simulations for CFD, CSM, CWO and other CTAs. The toolkit modules will be accessible from FORTRAN, C, and C++ applications via APIs. For example, the following additional modules will be included:

1. GUI based software to validate INLiB functionalities
2. Enhanced feature detection module
3. Enhanced interpolation/approximation of solution characteristics addressing conservative properties
4. Improved error indicator module
5. Grid quality assessment module with additional and improved quality measures

9. **Deliverables:**

- Enhanced software package containing INLiB and associated documentation
- GUI based validation and demonstration of INLiB for DoD applications
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Web Portal Infrastructure to Support Land Management System

2. **Organization:** Mississippi State University, ERC

3. **Thematic Areas:** HPC Training and DoD User Productivity

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8. **Statement of Work:**

This project is a follow-on effort to provide the middle-tier support for building CTA-specific Web Portals that provide seamless access to MSRC resources through a familiar and ubiquitous interface of a Web Browser. The Web Portal allows the user to define his or her own problem-solving environment, which is accessible anytime from anywhere (given an internet access). Using the portal, the user can access all data he or she needs, submit jobs on remote computational servers, and analyze the results through a visual interface that hides complexity of the back-end systems. The initial focus of this effort is to support remote job submission and monitoring in a secure environment of the ERDC MSRC, and to investigate the possibility of integrating the middle-tier components between the Distributed Marine Environment Forecast System (DMEFS) and LMS systems, as well as interoperability between the LMS front-end and the middle-tier.

This projects builds on the earlier experience building a Web-based prototype of LMS, the Gateway project supported by the Aeronautical Systems Center (ASC) MSRC, and it leverages the DMEFS project - a multi-million dollar effort sponsored through the Naval Oceanographic Office (NAVO) MSRC. The synergy between DMEFS and this proposed project makes the realization of the project possible in this short 6 month period. The system implements a multi-tier architecture. The client-tier comprises two elements: a generic Web browser (Microsoft Internet Explorer or Netscape Navigator, in both cases version 4.0 or later), and a mini "personal" server running on the same machine as the web browser. The personal server listens to https requests from the browser and converts them into CORBA requests. The requests are then forwarded to the middle-tier servers through a secure kerberized channel. MSU uses a commercial implementation of CORBA ORB from Object Oriented Concepts, Inc, (Orbacus), with security services coming from Adiron Inc. (ORBasec). The middle-tier ORB delegates processing of the requests to a J2EE server of Sun Microsystems. The J2EE server integrates a Web server (https), servlet and Java Server Pages (JSP) engine, and Enterprise JavaBeans (EJB) container. The JSP technology is used to provide front-end contents displayed by the browser, while EJB

components serve as proxies of the back-end services (job submission and monitoring, resource brokers, file systems, and so forth). The middle-tier server (https, JSP and EJB processing) is being developed within the DMEFS project. The scope of this project is to replace the currently used https protocol for communications between the client and middle-tier by the secure CORBA. This is to be achieved by the development of the client-side personal server described above. As a result, the system will provide support for seamless access to MSRC resources (including job submission and monitoring at both ERDC and NAVO) through a secure kerberized channel. The personal server can be also used to access local resources, for example, to launch desktop applications such as WMS). In addition, MSU will develop interfaces that will allow integration of a CTA specific front end (such as LMS) with these middle-tier components.

9. Deliverables:

- A client-server system that allows for remote job submission and monitoring at ERDC MSRC.
- Plan for integration of the middle-tier components between LMS and DMEFS environments.
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** HPC Training Courses

2. **Organization:** Ohio Supercomputer Center

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Names:** Dr. Richard Pritchard, Ms. Leslie Southern

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8. **Statement of Work:**

Ohio Supercomputer Center (OSC) will provide quality training by experienced instructors for the DoD HPC Community. OSC has provided heterogeneous high -performance computing facilities and services to a statewide community for over 11 years and more recently a broader national community through the DoD Modernization Program and the National Computational Science Alliance. Training offerings are developed and designed specifically for the HPC user community. Instructors are both experienced HPC specialists and experienced users and are not economically bound to any one vendor or vendor product.

OSC proposes the following training offerings for the ERDC MSRC Extension:

- **Advanced UNIX**
  Length: 2 day
  Approximate Date: TBD
  Description: This customized course will cover advanced UNIX topics that are of particular interest and applicability to the audience. Topics available for selection by the participants include:

  - Comparison of the features and strengths of the various UNIX s hells available
  - UNIX environmental variables
  - Advanced UNIX text processing
  - The make utility for large program maintenance
  - Using the awk and perl programming languages
  - Introduction to UNIX system-level commands

- **Multilevel Parallel Programming**
  Length: 2 day
  Approximate Date: TBD

Description: This course is intended as an introduction to multilevel parallel programming, a style of parallel programming in which both message passing techniques (such as MPI) and shared memory techniques (such as OpenMP or pthreads) are used. This allows high performance codes to best take advantage of the distributed/shared memory architectures of modern parallel supercomputers, such as SGI Origins, IBM SP3s, and clusters of commodity SMP systems. Users will learn how to apply multilevel parallel programming techniques to problems of interest, how to optimize these techniques for different architectures, and how to avoid potential problems. Topics covered include:

- Introduction to distributed/shared memory architectures
- Overview of message passing techniques
- Overview of shared memory techniques
- Mixing message passing and shared memory
- Optimization techniques
- Examples

OSC will provide course announcements and electronic copies of training materials for each course prior to each course date. All courses are available in Microsoft PowerPoint and a combination of HTML and JPEG files. The web pages are designed to move sequentially through course materials and contain embedded links in the table of contents and section indices. This provides the student the flexibility to jump to particular sections of interest.

9. Deliverables:

- Delivery of training courses on-site at the ERDC MSRC
- Provide training material in advance for each class taught

1. **Focused Effort Title:** Enhancement, Evaluation, and Application of a Coupled Wave - Current-Sediment Model for Nearshore and Tributary Plume Predictions

2. **Organization:** Ohio State University

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Keith W. Bedford, Prof. Ponnuswamy Sadayappan

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8. **Statement of Work:**

This Focused Effort provides continuation for the ongo ing development, deployment, and evaluation of the COupled MArine Prediction System (COMAPS). COMAPS is comprised of coupled, parallel-processing, numerical models that together generate hydrodynamic, wind-wave, and sediment tranport predictions. Accurate, timely predictions of this kind are vital for the planning of many military operations. Circulation, water elevation, and wave height predictions are important in the planning of fleet navigation, amphibious landing, and search and rescue missions. Sediment tranport predictions are valuable for the planning of dredging operations, and also aid the interpretation of sonar response in submarine tracking activities. COMAPS includes the WAM wind-wave model, the CH3D-SED circulation and sediment transport model, and the WCBL combined wave-current bottom boundary layer model.

A portion of the PET year 5 funding for this Focused Effort provides for the deployment of COMAPS in support of the Dredging Operations and Environmental Research (DOER) program. DOER is a major research initiative of the U.S. Army Corps of Engineers (USACE); the program is designed to benefit the USACE Operation and Maintenance Navigation Program. COMAPS is being used in connection with a particular DOER work unit which involves the tracking of dredged material placed in a mound close to the ERDC Field Research Facility at Duck, NC. The aim of the work unit is the improvement of ERDC scientists' ability to predict the movement of mound material, leading to better planning and management of dredging operations.

Dr. Joe Gailani (ERDC CHL) will carry out high-resolution, near-field numerical modeling of mound evolution for the DOER work unit described above. Simulations will be done using the Long Term FATE of dredged material (LTFATE) model. This code predicts local hydrodynamics, wave shoaling, erosion, and deposition. Notably, LTFATE includes a

layered bed model which will account for the effects of mound consolidation on erosion rates. Benefit would be gained from a coupled deployment li nking COMAPS and LTFATE. This strategy would aid both models: LTFATE would be provided with spatially and temporally varied boundary conditions, while COMAPS would receive high -resolution mound erosion source terms which account for consolidation effects. The CH3D-SED model used in COMAPS does not account for consolidation.

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9. Deliverables:

- Presentation for PET Final Review
- Written progress report in June 2001
- Final Technical Report
- Contribution to PET Annual Report
- Coupling of COMAPS and LTFATE (4/2001 – 6/2001)
- Hindcast of DOER field experiment (7/2001)
- Analysis of DOER hindcast (8/2001)
- Tuning of COMAPS based on DOER hindcast (9/2001)

1. **Focused Effort Title:** Delivering SPEEDES Based HPC Simulations over WebHLA to ERDC MSRC and/or Joint Simulation System (JSIMS) Users

2. **Organization:** Syracuse University

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

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8. **Statement of Work:**

This project is an extension and a natural completion of the currently ongoing (from 27 Sept 2000 to 26 March 2001) Year 5 PET FMS effort on "Synchronous P arallel Environment for Emulation and Distributed Event Simulation (SPEEDES) Installation and Training at ERDC MSRC", conducted by Syracuse University. SPEEDES is a general purpose object - oriented (C++ based) parallel/distributed event driven simulation framework. The system is under development/completion by FMS Common HPC Software Support Initiative (CHSSI) projects at the Space and Naval Warfare Systems Command (SPAWAR). Other SPEEDES sponsors and customers include Wargame2000, JMASS and JSIMS. In response to the interest in SPEEDES, expressed recently by ERDC MSRC, Syracuse University will install the system on the Origin 3000 platforms at ERDC MSRC and will deliver entry level SPEEDES training to the ERDC MSRC users within the current focused effort.

In the proposed extension/completion project: Syracuse University will do the following: a) install the WebHLA environment at ERDC MSRC; b) integrate it with SPEEDES installation; c) select or prototype and port a trial SPEEDES based HPC simulation to such integrated WebHLA+SPEEDES simulation and delivery environment; and d) deliver a trial simulation to the interested DoD users using this framework. Syracuse University will work with ERDC MSRC users, FMS CHSSI, and JSIMS communities to identify the most adequate trial simulation. More specifically, Syracuse University will explore the following three possible avenues: a) a JSIMS specific simulation module that uses SPEEDES, explores HPC facilities at ERDC MSRC, and cooperates via WebHLA with other remo te JSIMS federates, b) an internal simulation of relevance for ERDC MSRC users that uses WebHLA to integrate the SPEEDES HPC module with other federates of relevance such as ModSAF, etc., and c) an advanced training simulation demo, based on selected Wargame2000 or JSIMS federates, that uses WebHLA to link SPEEDES trainees with trainers and with the SPEEDES federate within an interactive, collaborative hands -on

training session. The most promising avenue will be selected and implemented in the proposed project.

9. Deliverables:

- WebHLA installation at ERDC MSRC
- Integration of WebHLA with SPEEDES that facilitates Web delivery of HLA compliant SPEEDES based HPC simulations
- Porting, integrating or prototyping a trial SPEEDES based HPC simulation, demonstrated and delivered via WebHLA to interested DoD users (ERDC, JSIMS, or both) at the end of the project
- Presentation for the PET Final Review
- Written progress report in June 2001
- Final Technical Report
- Contribution to PET Annual Report

1. **Focused Effort Title:** Parallel IO

2. **Organization:** University of Tennessee, Knoxville

3. **Thematic Areas:** HPC Training and DoD User Productivity, Management and Interpretation of Large Data Sets

4. **PI Name:** Dr. David Cronk

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8. **Statement of Work:**

This project is a continuation of the existing University of Tennessee, Knoxville (UTK) Parallel IO focused effort that has the following three main objectives:

1. To evaluate and performance test the vendor P arallel IO subsystems installed on the EDRC MSRC platforms, as they would be utilized by current system users (i.e. high level API access from MPI 2).
2. To educate users on the benefits of using such Parallel IO systems.
3. To demonstrate benefits to users by t uning an existing DoD Challenge application, which is currently "IO bound," and by assisting with use of MPI 2 Parallel IO in the EQM CE-QUAL-ICM code.

Evaluation done this far of vendor Parallel IO subsystems on ERDC MSRC machines indicates further perfo rmance benefits could be gained by installing extensions for shared file pointers on the Cray T3E and SGI Origin 3000 and by upgrading to the vendor's full MPI-2 IO implementation on the IBM SP3 (cobalt). UTK will work with vendors and ERDC MSRC systems staff to help ensure that the best possible Parallel IO subsystems are installed and performing well.

Initial Parallel IO implementation will have been completed by March 2001 for the Contaminant Dispersion model challenge code and the CE -QUAL-ICM code. Continuation of the project will allow further tuning of these codes and incorporation of parallel IO into additional EQM codes.

The HDF5 data format and IO library is designed to support Parallel IO. NCSA is working with users of CH3D to incorporate HD F5 support. Continuation of UTKs Parallel IO project will allow UTK to collaborate with NCSA on implementing parallel IO support for HDF5 on ERDC MSRC machines, thus improving scalability and efficiency of access to data by CH3D.

As a part of this effort, UTK will offer a training course on advanced techniques in MPI programming.

9. Deliverables:

- Presentation for the PET Final Review
- Written progress report in June 2001
- Final Technical Report
- Contribution to PET Annual Report
- Updates to benchmark results for ERDC MSRC Parallel IO subsystems
- Collaboration with EQM code developers on use of MPI-2 Parallel IO
- Collaboration with NCSA on use of Parallel IO with HDF5
- Advanced MPI course offered on-site at ERDC MSRC

1. **Focused Effort Title**: Metacomputing Support for the SARA3D Structural Technology Acoustics Application

2. **Organization**: University of Tennessee, Knoxville

3. **Thematic Areas**: Scalable Computing Migration, Management and Interpretation of Large Data Sets

4. **PI Name:** Dr. Shirley V. Moore

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8. **Statement of Work**:

This project is a continuation of the existing Year 5 UTK focused effort on using the NetSolve MATLAB interface to provide access to MSRC HPC platforms for users of the SARA3D structural acoustics code. NetSolve is a client/server system that provides access to HPC hardware and software from familiar desktop environments, using a variety of client interfaces, including Fortran, C, and Java programming interfaces, and MATLAB and Mathematica interactive interfaces. Initially NetSolve has been used to allow the computationally intensive portions of the MATLAB-based post-processing for SARA3D to be carried out on ERDC HPC machines, while allowing users to run their MATLAB programs as usual from their desktop machines. Invocation of the computationally intensive routines is being implemented by remote procedure calls to versions of these routines installed on a NetSolve server. This approach will allow interactive use of HPC resources to improve real-time response for the post-processing and visualization of large-scale SARA3D output data.

Thus continuing this project will further improve scalability of SARA3D, enabling new computations, such as the inverse acoustic intensity problem, as well as generalize the approach to other applications.

9. **Deliverables:**

- Implementation of SARA3D computational and additional post-processing routines on NetSolve server, with parallelism provided using task farming
- Incorporation of NetSolve parallel solvers into SARA3D code
- Contribution to PET Annual Report
- Presentation for the PET Final Review
- Written progress report in June 2001
- Final Technical Report

1. **Focused Effort Title:** AMR and CTH Capability and Algorithm Enhancements

2. **Organization:** University of Texas at Austin

3. **Thematic Area:** Scalable Computing Migration

4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden

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8. **Statement of Work:**

The focus of this part of the work is enhancement of the capabilities of DoD codes such as CTH to meet some of the needs expressed by DoD users. TICAM has been expanding the CTH software framework to include adaptive mesh refinement (AMR). TICAM is also working with software developers at Sandia on parallel aspects of the study. The present component of the work deals with problems related to application programming interfaces to support the following: (1) improved capabilities to handle rigid obstacles of arbitrary shape in CTH; and (2) improved extraction of pressure -field data for interfacing with other DoD application codes (for example, DYNA). A second part of the work concerns the development of improved algorithms and, particularly, improved time integration procedures. This is a major stumbling block to efficient simulation: as the cells deform in Lagrangian calculations or are repeatedly refined in the Eulerian simulations the timestep is adversely affected. TICAM plans to study this problem and develop strategies for resolving or ameliorating it. This work will be conducted in the latter part of the contract period and, depending on the outcome, could become a major focused effort in the following year. The testbed will be utilized for some of these studies to expedite development and testing of ideas.

9. **Deliverables:**

- Contributions to PET CSM web page on capability enhancements, algorithms, test problems, and performance results
- Conference papers and journal articles detailing results of the project, expanded capabilities, new algorithm development, analysis, performance, and application studies
- Software for enhancements with supporting technical documentation in testbed
- Visit to Vicksburg and briefing to ERDC MSRC on research progress
- Contribution to PET Annual Report
- Written progress reports in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Adaptive Mesh Technology, Mesh Improvement and Algorithms for Hypervelocity Impact and Penetration Analyses

2. **Organization:** University of Texas at Austin

3. **Thematic Area:** Scalable Computing Migration

4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden

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8. **Statement of Work:**

TICAM will continue the present work to promote and develop unstructured grid approaches and adaptive mesh refinement methods for CSM codes used by DoD researchers in hypervelocity impact and penetration analyses. Both Eulerian and Lagrangian approaches and their derivatives (ALE codes) are impacted by this research effort. In support of this need, TICAM is developing local mesh refinement strategies for these analysis codes and investigating data structure issues related to implementation of various refinement strategies. The DoD codes CTH and EPIC are the primary test codes for this work. The work will be continued in the extension period and will also focus on several issues of immediate interest to the gridding and finite element analysis needs of the Structures Lab users at ERDC. Current work on local error indicators of residual types will be continued with emphasis on implementation and testing within the frameworks of the designated test codes. The work on the Lagrangian analysis codes involves deforming grids and an assessment of shape quality of the elements as the solution and grid evolve. The framework of the Eulerian computational testbed, which was commenced in last years funding, has recently been completed and tests with error indicators for "basic physics," including shock layers, will be carried out. The performance of different indicators and comparison tests with known analytic solutions are to be done to verify/test the indicators and will be completed during the proposed period. This can be used to enable rapid evaluation of indicators and algorithms for very large codes such as CTH. An extensive series of benchmark tests and comparison studies using different error indicators, which include shape quality indicators, have been initiated and will be completed during the proposed period. An important task in this part of the focused effort concerns mesh aspect ratio degeneracy and the effect on solution quality and algorithm efficiency. Finally, TICAM will expand work on mesh partitioning studies for parallel processing using domain decomposition on unstructured grids with TICAM and Sandia code modules to investigate dynamic partitioning. This work will include statistical studies of partitionings for representative adaptive grids.

9. Deliverables:

- Presentations at DoD HPC Users Group Conference
- PET technical reports and journal articles detailing results of th e project, testbed software, mesh quality strategies, new algorithms developed, error indicator/adaptivity analysis and partitioning studies
- Support for implementation of selected adaption methods in DoD codes
- Testbed software delivery and demonstration
- Briefing to ERDC MSRC on progress for all Focused Efforts
- Contribution to PET Annual Report
- Written progress reports in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Discontinuous Galerkin Finite Elements and Adaptive Grids for DoD Problems

2. **Organization:** University of Texas at Austin

3. **Thematic Areas:** Scalable Computing Migration, HPC Performance Metrics/Tools

4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden

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8. **Statement of Work:**

   The purpose of this project is to promote and develop new advanced computational techniques that have potential for technology trans fer to DoD Applications codes. The focus of this effort will continue the development, analysis, testing, and implementation of new Discontinuous Galerkin (DG) techniques for finite element simulations. Such methods are of growing interest for certain fini te element applications in the research community. The methods appear particularly appealing for transient simulations of applications with shock - like structures and similar hyperbolic or near-hyperbolic problems of interest to DoD users. (In the DG schemes the continuity requirements across the interfaces between elements are enforced only weakly in the variational formulation rather than in the basis itself. This implies that the degrees of freedom can be local to the element and allows for local conservation and other properties to be enforced strongly at the element level, with easier migration to higher degree elements. Stability and other properties may also be improved relative to other more conventional formulations.) These ideas are being investigat ed within the framework of unstructured grid approaches and adaptive grid technology that could enhance the accuracy and performance of CSM codes used by DoD researchers for damaged structures analysis. TICAM proposes to continue these investigations. As a part of this effort, preliminary comparisons will be made of a DG finite element simulation with traditional integration procedures (such as finite -volume Eulerian used in CTH) in a 2D blast test problem. TICAM will also continue ongoing work dealing with solution algorithms for these DG schemes, and investigate compatibility with existing data structures in current DoD analysis codes.

9. **Deliverables:**

   - Contributions to the PET CSM web page on DG methods, adaptive algorithms, test problems, error analysis, etc.
   - Conference and journal articles detailing results of the project, new methodology, algorithm development, performance results, and error indicator/adaptivity analysis

- Software and testing for CSM testbed with supporting technical documentation
- Briefing of ERDC MSRC on progress for all Focused Efforts
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Algorithms for Error and Feature Indication in Interpolation and Approximation

2. **Organization:** University of Texas at Austin

3. **Thematic Area:** Scalable Computing Migration

4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden

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7. **Fax:** (512) 232-3357, (512) 471-8694

8. **Statement of Work:**

The CSM TICAM members will continue ongoing collaborative work on algorithms and software for error or feature indicators that can be used in conjunction with the interpolation library (INLiB) routines provided by Dr. Bharat Soni, MSU. The TICAM CSM team members will also continue work on h,p and hp approaches and error indicators suitable for these classes of approximation. The h adaptive approaches will be applied in numerical tests on the "Testbed" software being developed in support of TICAMs other focussed effort activity. The CSM TICAM group will also work on software for projections between different grids including constrained projections for interfaces in multi physics applications involving different CSM codes. The deliverables are a technical description of the interpolation bases, the approximation properties, the related algorithms, and implementation together with supporting software modules. Dr. Carey will collaborate with Dr. Soni to review progress.

9. **Deliverables:**

- Contribution to PET Annual Reports
- Presentations for PET Final Review
- Written progress report in June 2001
- Final Technical Report
- Contributions to PET CSM web page on capability enhancements , algorithms, test problems, and performance results
- PET technical reports, conference papers and journal articles detailing results of the project, expanded capabilities, new algorithm development, analysis, performance, and application studies
- Software for INLiB package with supporting technical documentation
- Coordination with MSU researchers

1. **Focused Effort Title:** Improved Parallel Performance for Environmental Quality Models

2. **Organization:** University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Dr. Victor Parr

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8. **Statement of Work:**

The goal of this focused effort is to migrate the MPI parallel version of CE-QUAL-ICM from the prototype stage to a full production code that can solve problems much larger than the current Chesapeake Bay model.

To accomplish this goal, the prototype code will be extended in the following ways:

1. The prototype MPI Parallel I/O version of CE-QUAL-ICM will be tuned for optimal performance.
2. TICAM will port the code to each of the ERDC platforms. The current version of the code was only ported to the Cray T3E, because of unavaillability of the MPI-2 library on other ERDC platforms.
3. The MPI Parallel I/O mechanism will be extended to critical input files, which impact runtime performance or are time-consuming for the CE-QUAL-ICM pre-processor to localize. Likely candidates are the hydrodynamics datasets, which in the past on Chesapeake Bay EPA studies have been 10 GBytes, and the source load files, which have been larger than 50 MBytes. There are two benefits to this extension. One is reduced I/O wait time, the second is that the job will require half the disk space.

9. **Deliverables:**

- Benchmark the MPI Parallel I/O version of CE-QUAL-ICM against the original version for a 1 year run of a Chesapeake Bay scenario on Cray T3E, SGI Origin, and IBM SP to determine the success of this approach for production work (30 September 2001).
- Presentations for PET Annual Review
- Contribution to PET Annual Report
- Written progress report in June 2001
- Final Technical Report

1. **Focused Effort Title:** A Full 2D Parallel Implementation of CH3D-Z

2. **Organization:** University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Prof. Clint Dawson

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8. **Statement of Work:**

The CH3D-Z code is a widely used EQM hydrodynamics flow simulator, and is of high priority for efficient parallel migration. TICAM replaced the ADI solver in the CH3D-Z code and is implementing a full 2D domain decomposition parallelization. The approach that is taken is very similar to what has been used to successfully parallelize CE-QUAL-ICM and ADCIRC; i.e., a pre-processor is written that partitions the data among the processors, MPI calls are added to the code itself for message-passing, and a post-processor is used to gather the local information into global output files. A preliminary version of the parallel code will be completed by March 2001 and tested on the Chesapeake Bay-Delaware Bay data set provided by ERDC. TICAM proposes to fully test and debug this code, optimize the message-passing, and implement parallel I/O within the code. The code will also be ported to all parallel platforms at the ERDC MSRC. As many versions of CH3D-Z exist for different data sets, TICAM will collaborate with ERDC personnel to create a unified, parallel version of CH3D-Z without any “hardwired” sections of code.

TICAMs parallelization technique is also of use for other versions of CH3D, including CH3D-SED and CH3D-COSED. As a first step towards parallelization of these codes, TICAM will work with ERDC personnel in replacing the ADI solution method in CH3D-SED with a conjugate-gradient based algorithm.

9. **Deliverables:**

- Testing, debugging and optimizing parallel CH3D-Z completed (30 June 2001)
- Unified version of CH3D-Z (30 Sept. 2001)
- ADI solver replaced in CH3D-SED (30 Sept. 2001)
- Presentations for PET Final Review
- Contribution to PET Annual Report
- Written progress report in June 2001
- Final Technical Report

1. **Focused Effort Title:** Interpolation and Projection Between Arbitrary Space/Time Grids

2. **Organization:** University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity,
Scalable Computing Migration

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8. **Statement of Work:**

This project concerns the development of methodology and software for interpolating and/or projecting quantities from one finite element grid to another. The particular EQM applications of interest include the coupling of hydrodynamic and environmental water quality models and the coupling of groundwater flow and transport codes.

In these EQM applications, the flow and transport are often solved separately using different numerical methods and grids due to differences in time and length scales involved. For example, the hydrodynamics flow grid usually needs to incorporate high resolution near land boundaries and should extend into the ocean to avoid spurious boundary effects. The transport code may only simulate transport over a small portion of the flow domain and may use much coarser resolution. Therefore, for efficient coupling of flow and transport codes, it is critical to be able to take velocities and elevations from an arbitrary space/time flow domain and interpolate or project them onto an arbitrary transport grid. Moreover, this must be done generally at every transport time step. Th us, this operation can be very costly if not implemented efficiently.

This project is a follow-on to TICAMs recent work on projection methods. Once velocities and elevations have been interpolated, they need to be further projected so as to satisfy the underlying conservation principles. TICAM has developed a prototype software package, UTPROJ, that computes conservative velocity fields on a given prismatic or tetrahedral grid. The code has been interfaced with TABS -MDS for the purpose of testing the algorithms, and at the moment, the grid provided by TABS -MDS is being used. By the end of this contract year, TICAM will demonstrate coupling of TABS -MDS and CE-QUAL-ICM, through the use of the interpolation software INLIB from MSU, and UTPROJ. TICAM proposes to fully test, debug, and validate the coupled hydrodynamics flow and transport code for a number of data sets provided by ERDC and develop this code into a scalable, parallel production code suitable for large data sets. TICAM will continue work in developing parallel preconditioners for the elliptic solve in UTPROJ, as these are critical in

developing a scalable code.

To demonstrate coupling for groundwater problems, TICAM will also couple FEMWATER, a groundwater flow code developed at ERDC, and M T3D, a groundwater transport code, using UTPROJ.

9. Deliverables:

- Testing and validation of TABS-MDS/UTPROJ/CE-QUAL-ICM completed (31 July 2001)
- Improved preconditioners implemented and parallel scaling studies completed (30 September 2001)
- Preliminary coupling between FEMWATER and MT3D completed (30 September 2001)
- Journal paper on projection methodology (30 September 2001)
- Presentations for PET Final Review
- Contribution to PET Annual Report
- Written progress report in June 2001
- Final Technical Report

1. **Focused Effort Title:** Reactive Transport Schemes for Water Quality Modeling on Unstructured Grids

2. **Organization:** University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Prof. Clint Dawson

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8. **Statement of Work:**

ERDC has a substantial on-going effort in water quality modeling, through such codes as CE-QUAL-ICM and CE-QUAL-ICM/Toxi. These codes contain very sophisticated aquatic chemistry, but use somewhat dated numerical methods for modeling advection, diffusion, and reactions, and rely on the use of logically rectangular elements. TI CAM is investigating conservative, higher-order accurate methods for advection and diffusion, suitable for any type of elements. The methodology is based on the so -called discontinuous Galerkin (DG) methods, which have been developed by Wheeler, Dawson, a nd their collaborators over the past few years. These methods are locally conservative, can be defined on any type of element (in fact the elements can be non-conforming), and allow for higher-order accuracy. The methods are especially useful for so-called h-p adaptivity, where one varies both the size of the element and the degree of the approximating polynomial. TICAM is currently implementing the methodology within the current structure of the (parallel) CE -QUAL-ICM code, for comparison with the exist ing algorithms. ERDC will also be provided with a prototype three-dimensional advection-diffusion code on unstructured grids based on the DG methodology by the end of this fiscal year.

TICAM proposes to add the capability to handle multiple components and chemical reactions to the prototype, unstructured code for the purposes of simulating realistic water quality scenarios. TICAM will then perform a suite of tests in collaboration with ERDC personnel to assess the efficiency and accuracy of the code. In addition, TICAM proposes to carry out extensive testing of the two -point advection scheme that is currently being implemented in CE-QUAL-ICM.

9. **Deliverables:**

- Report on two-point advection scheme for CE-QUAL-ICM (15 August 2001)
- Multiple components and chemical reactions added to code (15 July 2001)

- Testing of code completed (30 September 2001)
- Journal paper on discontinuous Galerkin methods for water quality modeling (30 September 2001)
- Presentations for PET Final Review
- Contribution to PET Annual report
- Written progress report in June 2001
- Final Technical Report

1. **Focused Effort Title:** Parallel FEMWATER Visualization

2. **Organization:** Texas A&M University-Kingsville

3. **Thematic Area:** SciVis for Very Large Problems

4. **PI Name:** Prof. Thomas Lee McGehee

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8. **Statement of Work:**

Texas A&M University-Kingsville professors will teach the new aspects of surface water flow and canal flow that is coupled to FEMWATER groundwate r flow and transport to our graduate students. This will include the development of GMS file formats of FEMWATER 123. The graduate student will develop a reader that will convert the geometry and output files to Ensight Gold files. The next stage of re search will take the team into visualizing FEMWATER 123 datasets in Ensight Gold to develop flip -books and a video on the South Florida Project. This will require most of the students' summer time to develop several trial videos. Copies of the flipbooks and video will be sent to the Groundwater Modeling Technical Support Center for review and approval near the end of the summer. After the completion of the video presentation task, the graduate student will expand the Ensights FEMWATER tutorial to include the new visualizations learned during these applications. The team will try to determine the best use of the model for FEMWATER 123 visualization and include these operations in the tutorial. The team is preparing a publication on the use of the FEMWATER to Ensight Gold readers for use with high performance computers and all platform applications in groundwater modeling.

Dr. Thomas McGehee will travel to ERDC this summer to work with Dr. Jeffery Holland, Dave Richards, and Barbara Donnell, and the re search group with the Groundwater Technical Support Center. Dave Richards will assign the workstation, research projects, and research office space for the visit. Research project assignments include a close examination of the geologic characterization r eports, developing a strategy to model the hydrogeologic phenomena, development of computational detail around surface hydraulic sources/sinks into a two-dimensional mesh, creation of surface and boundary layer TINs, generation of the three -dimensional mesh, assignment of hydrogeologic properties and material types, assignment of boundary conditions, sending and compiling an executable on the supercomputers, running the programs, and examining the results. At each stage in the modeling effort a close exami nation of the work will be performed. At critical phases in the research, the project work will be presented to the research team. A final report will be submitted which will detail all accomplishments of this research.

9. Deliverables:

- FEMWATER 123 flipbooks and video fly-through.
- FEMWATER tutorial to prepare images, flipbooks, and film loops in Ensight Gold 6.2.
- Publication of the Ensight readers to the groundwater community.
- Presentation of this publication and results in a booth at SC2001 (DoD booth).
- FEMWATER models constructed on one or more of the above projects.
- Generation of groundwater modeling mini-projects for graduate students from lessons learned at these sites.
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

1. **Focused Effort Title:** Parallel FEMWATER Data Management

2. **Organization:** Texas A&M University-Kingsville

3. **Thematic Area:** Management and Interpretation of Large Data Sets

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8. **Statement of Work:**

Texas A&M University-Kingsville will continue to ask for support for the two graduate students. Both have agreed to work on the EQM goals and objectives for this project as part of their master's thesis. Texas A&M University-Kingsville will maintain the GIS data reduction ListServ and moderate discussion.

The team will work with ERDC MSRC to put the HDF5/GMS and the ArcIMS/FEMWATER tutorials on-line and develop appropriate Internet courses. Texas A&M University - Kingsville will continue their research on HDF5 (NSCA), GIS adaptation, and data visualization and reduction. The team at Texas A&M University-Kingsville will work closely with Mike Folk at University of Illinois, Champagne-Urbana and others at ERDC MSRC, who have interest in the project, making use of the data reduction ListServ (http://databasereduc.listbot.com) to facilitate interaction among the interested parties.

These students will be expected to produce reports each month on their project and post these to our ListServ. A working copy of the draft report comparing the two models will be in progress during this project period. Texas A&M University-Kingsville will provide EQM and the PET program access to these electronic reports to follow the progress of these projects.

9. **Deliverables:**

- An on-line version of the tutorials for HDF5/FEMWATER and ArcIMS/FEMWATER
- An accompanying Internet course for the above mentioned tutorials
- A general paper regarding data visualization and reduction from a supercomputer and GIS will be published in an appropriate journal or refereed publication.
- Contribution to PET Annual Report
- Written progress report in June 2001
- Presentations for PET Final Review
- Final Technical Report

Section 3: CONTACT INFORMATION

3.1 Academic Points of Contact

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- CSM Lead - Prof. Tinsley Oden (TICAM, University ofTexas at Austin)
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- SciVis Lead – Dr. Kent Eschenberg (Alpha Data)
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- Training Coordinator – Ms. Kelly Lanier (Mevatec)
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3.3 Related Web Addresses

ERDC Home Page: http://www.erdc.usace.army.mil/

ERDC MSRC Home Page: http://www.wes.hpc.mil/

ERDC MSRC Technical Reports: http://www.wes.hpc.mil/pet/tech_reports/available.htm

ERDC MSRC PET Training Schedule: http://www.wes.hpc.mil/training/training.htm

DoD HPCMP Home Page: http://www.hpcmo.hpc.mil/

DoD HPCMP PET Executive Committee: http://www.crpc.rice.edu/DODmod/index.html