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$ 499,789	36 months	10/01/00	

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A. PROJECT SUMMARY

Simulation of physical phenomena on computers has joined theory and engineering experiment as the third method of scientific investigation. It is in fact the only feasible method for analyzing many types of practical and important phenomena. The maturation of parallel computing technology, and the Grid, now demands close collaboration among scientists, engineers and computer specialists, as computation and information systems (CIS) hardware and middleware become increasingly capable.

In distinction, scientific software, specifically computational mechanics simulation codes used to solve industrial-scale design problems, is evolving at a much slower pace. While being migrated to parallel computing, this evolutionary (not revolutionary) process is paced by adaptability and compatibility constraints intrinsic in legacy software design. These codes also possess a fixed set of numerical methodologies not readily alterable for research advances or to suit users' specific formulational nuances.

The hardware revolution versus software evolution confluence catalyzes the opportunity to create a unified, expansible *problem solving environment* addressable as a national resource on Internet, and broadly applicable to multi-disciplinary computational mechanics design simulations. Building on inhouse projects, transformation of this concept into an operable capability is the subject of this proposal.

The objective of this project is to *develop*, *validate* and *proliferate* on Internet a Parallel Interoperable Computational Mechanics Simulation System (PICMSS). In constructing PICMSS, the approach is to collate the *significant recent advances* in CIS, and in computational mechanics theory/practice, and to deploy the result *onto the desktops* of researchers *and* engineering practitioners via Internet.

PICMSS will uniquely facilitate rapid definitions, leading to *on-time* simulation of engineered systems involving complex non-linearly coupled fluid/thermal/solid mechanics aspects. PICMSS will as well be an extremely versatile toolkit to support *academic instruction* and *graduate research* in multi-disciplinary computational mechanics, with outreach enabled (and proven) within the Internet environment.

This project is organized to develop and deliver as a *national resource*:

- a modular parallel compute engine using, but not limited to, finite element (FE) implementations of weak forms to *rapidly* cast into computational syntax the physics, chemistry and mathematics description of diverse multi-disciplinary continuum mechanics problem statements, comprising
- an equation based graphical client user interface to encapsulate the FE computational theory via specification "in English" of the identified differential/algebraic equation system, leading to
- a middle server layer adapted to NetSolve, an Internet-based metacomputing environment, to steer and monitor the parallel computational state of the defined simulation, with
- enhancements to NetSolve to facilitate data exchange between the computing engine and users or secondary storage brokers during and after execution, and
- proliferation of the developed system nationwide via Internet, providing a
- uniquely organized, component-based computational platform for supporting large-scale validation of theoretical research/development advances in the computational sciences applicable to non-linearly coupled, multi-disciplinary problem statements in engineering and science.

Upon release of PICMSS, an open source Alliance will be established analogous to the NPARC Alliance in aerodynamics. In the Internet-based computational environment managed by this Alliance, the emergent user community will be encouraged to expand the physics model and numerical capabilities of PICMSS as a *national repository* for industrial and research applications (a truly significant opportunity). By design, PICMSS will serve as the platform for incorporating cutting-edge computational methods (academic research) and software (from DOE, NASA DOD laboratories). Thus, nationwide access to PICMSS creates the desired *truly open computing environment* for industrial-scale design problems.

TABLE OF CONTENTS

For font size and page formatting specifications, see GPG section II.C.

Section		Total No. of Pages in Section	Page No.* (Optional)*
Cover Sheet (NSF Form 1207) (Submit Page 2 with original proposal only)			
A	Project Summary (not to exceed 1 page)	1	
B	Table of Contents (NSF Form 1359)	1	
C	Project Description (plus Results from Prior NSF Support) (not to exceed 15 pages) **(Exceed only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)**	15	
D	References Cited	3	
E	Biographical Sketches (Not to exceed 2 pages each)	5	
F	Budget (NSF Form 1030, plus up to 3 pages of budget justification)	5	
G	Current and Pending Support (NSF Form 1239)	4	
H	Facilities, Equipment and Other Resources (NSF Form 1363)	1	
I	Special Information/Supplementary Documentation	0	
J	Appendix (List below.) **(Include only if allowed by a specific program announcement/ solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)**		

Appendix Items:

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

C. PROJECT DESCRIPTION

C.1 OBJECTIVE

The objective of the proposed project is to develop, advance and proliferate a Parallel Interoperable Computational Mechanics Simulation System (PICMSS). The common lament in the engineering computational mechanics community is the lack of adaptability in available software for effectively and efficiently attacking multi-disciplinary problems in engineering design. This project directs particularly pertinent resources to address this fundamental issue.

In constructing PICMSS, the goal is to collate the *significant recent advances* in the computation and information sciences (CIS) with those in computational mechanics theory/practice (CFD/CSM), hence to deploy the result into the hands of academics, researchers and engineering practitioners. The innovation is to better facilitate *rapid* conversion of theoretical and design musings into optimized design of engineered systems involving non-linearly coupled fluid/thermal/solid mechanics disciplines. PICMSS will as well excellently serve as a faculty toolkit to support academic instruction and graduate research in computational mechanics of continua, with operation/dissemination via Internet.

Upon establishing the first release of PICMSS, an association similar to the NPARC Alliance [1], the computational aerodynamics community supporting the WIND national CFD aerodynamics code, will be established. Under the proposed Internet-based computational environment, as managed by this consortium, the established user community will be encouraged to expand the physics models and numerical robustness of PICMSS as a *national repository*. PICMSS will as well serve as the collocation point for incorporating available CS computational methodologies and software, e.g., Parallel Multilevel Krylov Schwarz techniques [2-5] and the Aztec [6], PETSc [7], PSPASES [8], and SuperLU [9] numerical packages.

Pertinent legacy computational practice and formulations in computational fluid/thermal systems (CFD) and computational solid mechanics (CSM) will be adapted in generating the required multi-disciplinary capability. Extensibility to assimilate new and innovative algorithm constructions will be intrinsic to the design of PICMSS. Installation of PICMSS on the Internet metacomputing environment will be accomplished via the NetSolve system, [16], which will be enhanced and adapted to manage and monitor computational resources for the proposed PICMSS environment.

The specific goal of the proposed project is to develop and deliver as a national resource:

1. a modular parallel compute engine using, but not limited to, an arbitrary-grid finite element (FE) discrete implementation of a weak form to formulate the computational algorithm for the physics, chemistry and mathematics description of the problem statement at hand,
2. an equation-based graphical client user interface to encapsulate the established FE computational theory for the identified non-linear, partial differential equation system describing the multi-disciplinary problem to be simulated,
3. a middle server layer adapted to NetSolve to steer and monitor the computational state of the defined simulation, and
4. enhancements to NetSolve to facilitate data exchange between the compute engine and users or secondary storage brokers during and after execution, thus producing,
5. a uniquely organized, component-based computational platform for supporting large-scale validation of theoretical research advances in the computational sciences applicable to non-linearly coupled, multi-disciplinary problem statements in engineering and science.

The project will also have as a component the streamlining of the exchange of I/O and geometrical data with various production commercial grid generation and visualization packages. In its completion, PICMSS will uniquely support validation of research advances in the computational sciences as applicable to simulation of large scale, multi-disciplinary practical engineered-systems designs.

C.2 INTRODUCTION

Simulation of physical phenomena on computers has joined experiment and theory as the third method of scientific and engineering investigation. It is in fact the only feasible method for analyzing many different types of critically important phenomena, e.g., geological time scale evolution, options for clean/efficient combustion, quenching/heat treating, optimized ventilation design, etc.

The need to address such problems involves the collaborative work of academics, scientists, engineers, and computer specialists. With the rapid infusion of the parallel computing technology in recent years, the opportunity to create a unified problem-solving environment in computational mechanics to attack large-scale problems on a production basis has emerged [10,11].

To meet the challenge, many issues have to be thought through and resolved. Foremost, an interoperable software infrastructure has to be designed which deals with issues like physics encapsulation, I/O streaming, heterogeneity, security, etc. A year ago, a group of engineering, academics, computational and software scientists, mathematicians, and engineering mechanics specialists at the University of Tennessee started a collaborative in-house research project on this topic. The charter was to address the theoretical, algorithmic, and numerical implementation issues necessary to assess the potential for success of a Parallel Interoperable Computational Mechanics Simulation System (PICMSS) operating on Internet.

Project initiation was catalyzed by donation to UT CFD Lab of a predecessor PSE prototype (*AKCESS*.*, from prior SBIR-funded activities of the proposed project PI, [12,13]) coupled with graduate academic research on parallel CFD computing housed within Engineering Science, Computer Science and the Joint Institute for Computational Sciences (JICS) at UT. From graduate instruction in CFD, the prototype confirmed that such a user-instructed system, based on FE weak form computational theory, can be readily adapted by faculty and graduate students as a research and teaching tool. It was also envisioned how it could become an extensible platform to be utilized by industrial practitioners to design and prototype engineering processes and products, in the spirit of the NPARC Alliance in aerodynamics CFD.

The internal project's initial focus was in non-aerodynamics CFD simulation, i.e., incompressible fluid-thermal-mass transfer systems analysis, but has since expanded to encompass thermal-solid mechanics simulation, as the interest/need grows within the manufacturing community, e.g., the American Society for Metals (ASM), [14,15]. This in-house effort has now developed an implicit finite element multi-dimensional CFD/CSM software platform (*aPSE*) capable of admitting diverse CFD/CSM formulations, as well as closure models for physics phenomena, as required by the specific user.

A client-server model is now being designed to provide the interface support required by the user with a metacomputing engine. The core of the front-end interface consists of an equation editor that admits expressing conservation law forms of diverse type, leading via intrinsic conversion to a finite element weak form construction to a computable statement. A server will then connect the front-end to the computing engine using NetSolve [16] as the computing resources broker. This proposed project has emerged as observations by the in-house participants have identified the opportunity to deliver an interoperable computational mechanics simulation system, which is not just engineer-orientated but rich in mathematical context, expandable to assimilate resources available in the Grid community.

C.3 BACKGROUND

The seeds of today's components of applied computational simulation were sown during the 1960s NASA moon project. The space race resulted in the computer revolution that impacts every aspect of scientific discovery nowadays. With the emergence of parallel computing and Internet, the dimension of computational simulation once again leaps to a new era, as exemplified by, "… the new paradigm of parallel, distributed, collaborative, *immersive* computing is emerging," [17].

The combination of proliferation of distributed computing and advances in network technology has led to yet a new class of networked virtual supercomputing termed *metacomputing*, [18]. The dynamics and availability of such an immersional computational resource poses new challenges to developers of system software and tools adapted to these emerging technologies. Together with the idea of metacomputing comes the call for the "Problem Solving Environment (PSE)," [10,11]. Several software platform projects, e.g. Globus, [19], Legend, [20], NetSolve, [16], *aPSE*, etc, are under development to address and integrate the treatment of functioning applications and virtual network communication.

C.3.1 Limitations of traditional commercial software

In distinction to hardware and networking, the scientific software environment, specifically computational mechanics simulation codes used to solve industrial design problems, is evolving at a much slower pace. Although most of these software products, e.g., ABACUS, PATRAN, NASTRAN, FLUENT, CFX, . . . , are being migrated to parallel computing, this evolutionary (not revolutionary) process is limited by adaptability and compatibility limitations intrinsic in their legacy software design involving millions of lines of code.

These limitations lead to upgrade versions that are constrained and non-portable. These packages also come with a set of fixed methodologies and control parameters not readily alterable to suit the users' specific formulation nuances, e.g., closure models, non-standard boundary conditions. This inexorably leads to a proliferation of special-purpose modifications requiring vendor support. It was indeed this issue, i.e., existence of a hundred or more "buggered" versions of the original NPARC code (derived from the NASA Ames ARC3D CFD code), that lead to the NPARC Alliance aerodynamics WIND code.

The NPARC Alliance is a partnership among the NASA Glenn Research Center, the Arnold Engineering Development Center, commercial aerospace companies and academia. It exemplifies a successful management model with aim to, "Develop, validate and support an integrated, general purpose, computational flow simulator for the U.S. aerospace community," [1]. As the NPARC Alliance continues to thrive, with introduction of the new parallel code, the need for a similar effort in the more generic multi-disciplinary CFD/CSM arena continues to grow, which has been particularly foreseen by the UT in-house project team for this proposed NSF project.

C.3.2 Software platforms with modular control

Object-oriented design for computational codes is catching up with the developer community. The ability to attack different aspects of the same class of problems under the encapsulation of an object reflects the new trend in design criteria in software development. A few commercial software platforms, e.g., FASTFLO by NAG, [21], and DIFFPACK by the University of Oslo, [22], as well as the *aPSE* successor to *AKCESS*.* at UT CFD Lab, [cfdlab.engr.utk.edu/codes], have demonstrated the ability to develop such a capability.

FASTFLO offers a Matlab-type programming interface to manipulate/solve specific input formulations for differential equation systems. It is limited to running on a serial machine at this point. DIFFPACK also provides an object oriented approach for solving algorithmic construction of differential equations.

Similar research efforts using object oriented programming philosophy can be found in similar projects at University of Texas, [23], Purdue University, [24], and at UNICAMP in Brazil, [25].

There also exist within DOE programs the restructuring of in-house software platforms to take advantage of available computing resources on the network through computational middleware such as GLOBUS and NetSolve. It is thus quite apparent that a uniquely timely opportunity exists to integrate software technology, applied engineering, and simulation mathematics, as reflected in this proposed project, to develop an interoperable parallel modular Internet-distributed computational continuum mechanics national resource.

C.4 SCOPE OF THE PROJECT

Imagine that engineers in industry as well as academic researchers will be enabled to

- remotely describe their problem to a genuine *production* simulation environment from their own PC,
- submit their computational tasks to a pool of collaborative machines located anywhere in the country,
- monitor their computational tasks interactively, and then,
- examine their final results locally from remotely available graphics utilities, hence
- provide the heretofore unavailable capability to test computational theory and practice in an efficient, parallel, production Grid computing environment.

This is exactly the environment the to-be-developed PICMSS system will provide. To deliver such capabilities, this NSF project will integrate innovative software design, and cutting-edge computational mechanics theory with CS packages with proven methodologies. The simulation system will be assembled using six levels of abstraction:

1. construction of a JAVA graphical user interface (GUI) uniquely tailored to the implementation of problem frameworks in language constructions familiar to engineers and researchers,
2. conversion of this differential/closure differential/constitutive equation system into computational form using either state-of-the-art numerics or the most recent research advances,
3. creation of backend server interface to control and distribute computing information to sought-out processing units,
4. expansion of the computational engine to admit diverse classes of problem statements,
5. induction of PICMSS to NetSolve for metacomputing, and
6. exposition of output data with monitoring and control during execution.

Figure 1 graphs schematically the essential units of the PICMSS system. The translation from GUI differential equation system to computational form will be based on, but not limited to, a finite element unstructured discrete implementation of a weak form. An equation editor similar in form to the equation editor in Microsoft Word [26] will be developed, via JAVA, enabling users to express their problem statements, constituted of non-linearly coupled partial differential, algebraic and algebraic-differential equations in "mathematical English," i.e., the vector calculus found in engineering texts. The GUI will naturally admit any selected formulation of a fluid/thermal/solid problem statement, as constructed by a user, and will contain utilities to verify a well-posed statement regarding boundary and initial conditions.

Geometrical (domain definition, discretization, etc.) inputs and initial/boundary conditions will be admitted to PICMSS as external files created at the client site using their favorite meshing package. The encapsulated information will pass through a JAVA server deamon to manage and schedule resources on which the computational engine will act. The computational kernel of PICMSS can be located independently on the pool of local machines, or can be put under the control of NetSolve for global access. Output is piped to designated resources for local retrieval or remote examination.

C4.1. Front-end JAVA client interface

The *Front-End Client Interface* will allow users to define, formulate and monitor their problems. It will be written in Java and be portable to Windows and Unix/Linux environments. The two key files coming from the interface are the job control and input data files. The job control file will define the formulation and the sequence of its execution, i.e., Newton or quasi-Newton constructs. The data input file encapsulates all geometric and physical data. The interface will appear as a set of pull down modular units as follows.

- *Parametric Input Unit*. This unit let users define the physical model and other numerical parameters. The users may supply input by files, URLs, FTP addresses, or pick and choose within the input panel. The current prototype implementation of the Parametric Input Unit allows addition of new sets of parameters by editing the client's configuration file. The resulting information provided by a user is encapsulated into the input and control files that can be saved, opened, or passed to the server layer.
- *An Equation Builder Toolkit*. The equation editor enables users to formulate their problem statement by choosing among appropriate vector-differential operators and operands needed to express the given equations. As stated, it will appear similar to the Microsoft Equation Writer with pull down operator and operand symbols. An equation parser converts the drawn formula into the textual file that can be reused by the user.
- *Job Submission Unit*. This unit will handle requests for resources by the user. Once the problem is formulated, and the job submission information provided, the job is submitted to the server layer, which authorizes resources and initiates computation.
- *Job Monitor*. This component provides a uniform mechanism for obtaining real-time information about the status of the executing job. The mechanism of posting and receiving information will be implemented via communication with the Status Information module, of the server layer, using the Java RMI framework. The client posts the request for a particular job to the server that sends back checkpoint or status information from a local scheduler or the NetSolve server.

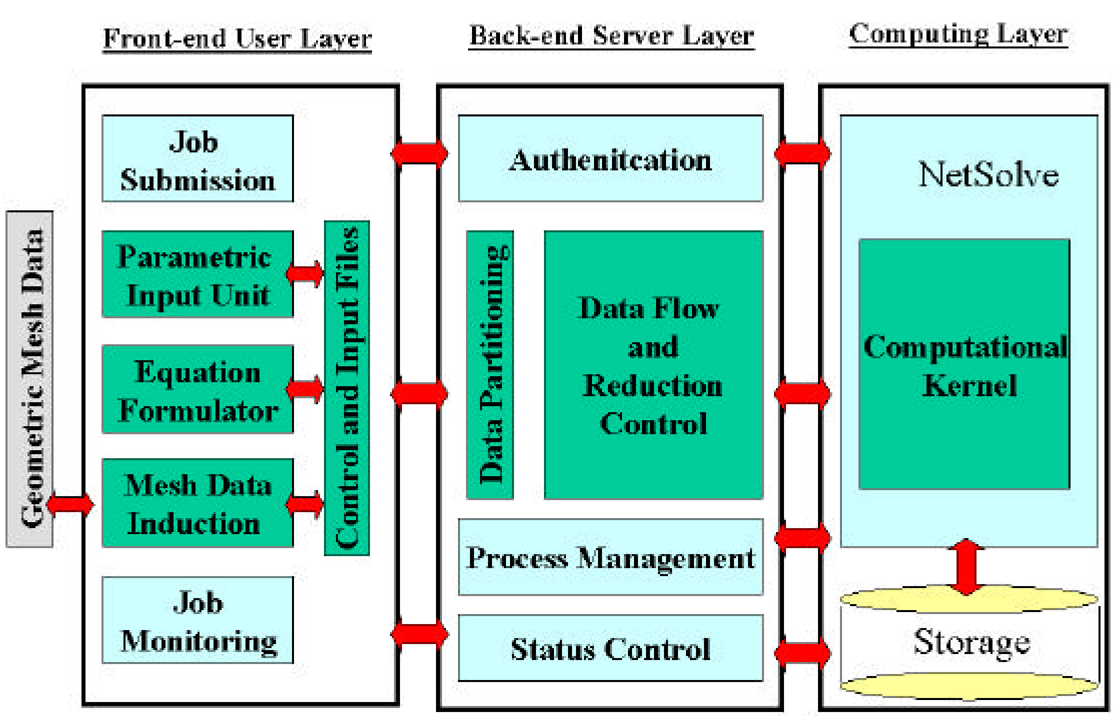

Figure 1. Schematic units of PICMSS

- *Data Induction Unit.* Input/output data management is crucial to the effectiveness of a software platform. Two input files are used to activate the computational kernel. The first one is a control file that lists the sequence of tasks to be executed as designated by a user. The other is an input data file consisting of geometric data and physical and numerical parameters needed to process the computation. Many input data file standards exist. PICMSS will initially use the PLOT3D format. Conversion to neutral file or other standardized formats will be provided. Although mesh generation is one of the most important units in computational mechanics simulation, it is nevertheless reinventing the wheel to develop a new mesh generator for PICMSS. Many viable mesh generation software packages exist, hence. Geometric mesh data obtained from representative packages will become incorporated via the Data Induction Interface. Specifically, PICMSS will interface data formats associated with commercial mesh generation packages (the common approach with legacy CFD codes). In addition, representative meshings supporting validation purposes will be available to users from an archival data storage library. Partitioning of the input file for parallel computation will be achieved via the METIS [27] data partitioning package called in the server layer.

C.4.2 Problem statement translation into computational syntax

This project seeks to generate a user-definable *component-based software platform* specifically designed to operate in the *high performance computing and communications* (HPCC) Internet environment. Such a system must admit a range of numerics theory implementations, as a fundamental capability, as well as problem statement adaptability.

Following recent advances in computational theory, the PICMSS approach to numerics theory expression generalization will employ discrete implementations of a weak form for partial differential equation (PDE) systems [28-30]. The weak form is a collection of theory-rich concepts and techniques that clearly delineate ingredients to constructing a *near-optimal* approximate solution process for the initial-boundary value problem statements omnipresent in computational continuum mechanics. This theory, refined over the past several decades by the mathematics community [31], with contributions from engineering academia [32-35], is thereby fully amenable to the required generalized construction.

Prior to imposition of any specific temporal-spatial discretization, if chosen (can be non-discretized (spectral) as well), a weak form requires one to:

- identify a functional support of the sought approximate solution, which involves selecting a set of functions (the trial space) spanning the physical and temporal domains.

- upon substitution of this approximation into the given partial differential equation system, require the associated approximation error to be orthogonal, in the sense of distributions, to another (initially arbitrary) set of functions (the test space).

- selecting a specific trail and test space, establish an error estimate in suitable norms, hence bound the error by options available within the selected approximation and the given information (called data).

- complete the theoretical performance estimate utilizing available methodology to assess accuracy, consistency, stability and convergence (rate) issues

Historically, finite difference/finite volume (FD/FV) methods have been used for "solving" the PDE systems for fluid/thermal simulation, called "CFD," while finite element (FE) implementation of an energy principle is the choice for structural systems. The weak form theoretical foundation very clearly identifies these apparently *major* distinctions as no more than a differentiable test function space [31, 28], providing the opportunity to use calculus rather than difference algebra for forming the identified integrals, both in concert with use of a spatial discretization.

The weak form is an integral form devoid of a discretization. However, once a weak form algorithm is implemented using a trial space that exhibits *compact support*, a spatial sub-division process called *discretization* is required. Only data interpolation distinctions exist among FD, FV and FE discrete methods for linear spatial derivatives in 1-dimension. However, in multiple-dimensions with non-linearity, truly *significant distinctions* result, since the differentiable test space (FE) construction facilitates *calculus* to accurately form all (non-linear) integral expressions. In contrast, FD methods rely on uni-directional Taylor series in developing a "scheme," while FV methodology employs the same discrete FD forms for averaged (without calculus) evaluation of effluxes over closed surface integrals.

A substantial archival literature exists on theoretical analyses and comparative performance estimates/validations for the range of FD, FV and FE algorithms for fluid-thermal systems regarding consistency, stability, accuracy (order of) and spectral distributions of artificial stability mechanisms, c.f., [35,36,37]. These and current studies [38] clearly delineate the construction aspects that improve performance fidelity, and each has been clearly and unequivocally established as partial differential forms fully amenable to weak form construction. Thereby, the weak form is the proposed theoretical generalization statement framework for PICMSS. Of course, the structural mechanics FE formulations are a direct interpretation, hence the multi-disciplinary requirement is met.

A truly valuable instruction distinction accrues to use of calculus in weak form implementation. Specifically, in compact support (FE) form, *all* resultant algorithm components are universally expressed as a matrix statement, with *all* formation processes on a *master element* domain. The element statement matrix rank equals the degrees-of-freedom (DOF) for the state variable on the master element, i.e., the product of geometric nodes/element and the number of unknowns in the parent PDE system. For all such terms, the discrete weak form construction identifies that only six types of operations are involved, which directly enables the discussed object-oriented graphical user interface (GUI) instruction environment. The six data-type element-level operations resultant from weak form FE discretization, i.e., compact support trial space and differentiable test space, are:

$$\begin{aligned} WF_e = &\text{(global constant) (avg. element data)}_e \text{ \{distributed element data\}}_e\text{\{metric data arrays\}}_e \\ &\text{[element master (hyper-)matrix] \{unknown or data\}}_e \end{aligned}$$

Here, subscript "e" denotes that the data depends on the specific FE cell, ( ) denotes a scalar, { } contains an array and [ ] signifies a matrix (that becomes a hypermatrix for non-linear phenomena). Every term in any discretized simulation weak form exhibits character therein expressed, hence the GUI connection to computational form is analytical and direct.

This observation led to formation of the previously cited PSE prototype *AKCESS*.* computational mechanics platform. This system currently supports the Internet-enabled collaborative research environment for the Global Basins Research Network [39]. Upon donation to UT CFD Lab, this prototype has been upgraded to the *aPSE* platform, now used regularly in support of academic graduate instruction and research in CFD computational mechanics [cfdlab.engr.utk.edu/internet/CFD/aPSE]. Therein, FE (and comparative FV) discretized weak form algorithm instructions are *word-processed* into a "template," which with "hooks" imprints every nuance in a completely user-definable mode.

In this project, the rather detailed mechanical aspects of forming the template will be replaced by the GUI. Complete versatility accrues to the process, as each individual specifically writes the "source code." The modeler knows exactly what is running, since the instructions are "in English." The operational status of *aPSE* at UT CFD Lab is proof positive of the soundness of this approach to an entirely new level of software versatility/reliability for widely diverse engineering analysis applications fully amenable to distributed parallelization of the resultant operations..

C4.3 Backend JAVA Server Layer

The back-end Java server will provide basic services for security, resource location, resource management, status monitoring, and data movement as required for high performance computing in distributive environments. The communication mechanism between the server and service providers, NetSolve, is based on a request protocol to be implemented. The following set of components constitutes the back-end Java server.

- *Authentication:* provides the basic mechanisms for authentication, authorization, and encryption. Any client's request first reaches the authentication mechanism. If access is granted, the request is processed to pass to NetSolve. Otherwise, the appropriate error message generated by the Security Service is passed to the client via the server.
- *Resource Allocation and Process Management:* provides mechanisms for passing information about application resource requirements to NetSolve's Resource Management Service for scheduling and initiation of computation on allocated resources. This process includes different tasks such as identifying resources, setting up executables, and passing arguments and files. If a task fails, the appropriate message is sent to the server that passes it to the client. Otherwise, the process creation

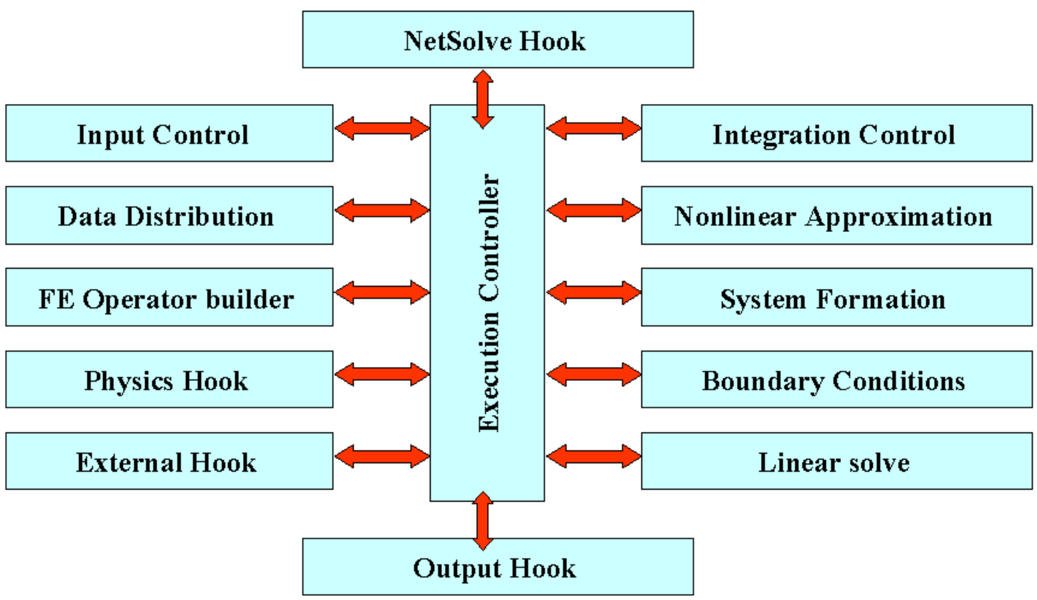

Figure 2. Schematic of the Computation Kernel

is acknowledged and the server notifies the client.

- *Status Control:* designed to provide basic mechanisms for monitoring the status of a submitted job. Each submission is registered with NetSolve's Monitoring Service which creates a log file. This file contains information regarding the status of registered job, which is used to implement various fault detection or fault recovery mechanisms, e.g., network or computer failure, abnormal process execution, or problem convergence failure.

- *Data Flow Control:* responsible for remote access to pertinent data storage such as files on FTP servers, HTTP servers, database servers, or any host on the Internet. This component is implemented by integrating the NetSolve Data Management Service designed to provide high-speed remote access to the complex, heterogeneous, and distributed GRID environment.

C4.4 Computational Kernel. The computational kernel takes the input file and executes the sequence of tasks defined in the control file. It is built on modular differential and integral operators acting on operands (problem state variable). A schematic of the computational kernel is shown in Figure 2. As stated, the finite element discrete weak form implementation is the method of choice.. The encapsulation of mesh construction and assembly procedures increases the modularity and portability of the method to attack problems of different nature and formulations. It is also inherently parallel.

The "solving" of partial differential equations generally involves a time integration scheme, a Newton or quasi-Newton strategy for nonlinear corrections, and a linear solver for a matrix statement of large scale. The use of Krylov iterative methods is primarily coupled with preconditioners to improve convergence as the problem size increases. Although incomplete factorization preconditioners (ILU) have been quite effective in many applications, they are difficult to scale. For problems that include multi-million degrees of freedom, Multilevel Krylov-Schwarz (domain decomposition) methods can offer efficient yet fast numerical solutions for system of equations, and numerous variations have been proposed and examined [5, 40-42].

For the most part, all of these methods approximate the original problem on a hierarchy of grids. The solutions on the coarse grids are used to accelerate convergence on the fine grids. Adapting the general framework of efficient multilevel schemes to the computational kernel will be a focus of the project. Petsc [7], from ANL, and Aztec [6] from SNL both offer a wide variety of preconditioners and Krylov solvers that will be used. Petsc is a suite of data structures and routines to solve a system, and only the pertinent portion of its functionality need be incorporated. Aztec is restricted to a parallel iterative library to solve linear systems of equations. For some problems, or problem components, a direct solver may still be needed. For treatment of SPD matrices, PSPASES [8], a SPD parallel direct sparse solver from University of Minnesota will be incorporated for this. SuperLU [9], a parallel sparse direct solver, will be used for general matrices.

C4.5 NETSOLVE and Metacomputing

To insure that PICMSS is well integrated into the Computational Grid movement that is now emerging [18], it will utilize NetSolve [43], which has emerged as a leading software environment for building grid-enabled PSEs [44-46]. NetSolve (www.cs.utk.edu/netsolve/) is a software environment for networked computing that transforms disparate computers and software libraries into a unified, easy-to-access computational service. It aggregates the hardware and software resources of any number of computers that are loosely connected across a network and offers up their combined power through familiar client interfaces such as MATLAB, Mathematica, or library calls in C, FORTRAN or Java. NetSolve makes a potentially massive pool of distributed resources easily accessible to the ordinary user of Computational Grids in general, and PICMSS in particular, ultimately aspire to serve.

NetSolve will play the role of providing all of the backend services to PICMSS. The system envisioned is a three-tiered. At the interface level, PICMSS will provide a user-friendly graphical interface that the end user will use to access the PICMSS system. Beneath this layer will be the PICMSS server that will do some intermediary processing and interface with the NetSolve system in order to access NetSolve's computational servers. This will, for instance, enable PICMSS to access distributed computational resources on the Grid so that, as opposed to only having local resources at its disposal, it can use the network to access high-end workstations, super computers, and clusters of workstations from low-end hosts. NetSolve will use its load-balancing policies and scheduling to allocate resources in an efficient and reliable manner and manage these processes and provide fault-tolerance (using a restart protocol) should one of these processes fail. NetSolve's client authentication mode will also be used to grant access to end-users with such access privileges. NetSolve servers will maintain Access Control Lists (ACL) that will describe who has access to these services.

The NetSolve package includes a suite of software for a variety of clients and servers, along with simple forms of inter-server and intra-server fault-tolerance and load balancing. It has been ported to every major UNIX platform. Windows 95/NT versions of the client (C, Fortran, MATLAB, and Java) are available and a server version is being developed. The NetSolve team has integrated many key numerical and scientific libraries into NetSolve computational servers, e.g. ARPACK, FitPack [47], ItPack [48], MinPack [49], FFTPACK [50], LAPACK [51], BLAS [52,53] and QMR [54], ScaLAPACK [55]. The ease with which NetSolve can assimilate additional server resources will allow PICMSS servers to be incorporated for distributed access via NetSolve's other client interfaces.

The interoperability and integration of NetSolve with other grid-based software systems is ongoing and well developed, and this be important in maximizing the ability of PICMSS leverage Grid resources. NetSolve already provides an interface to *Condor* [56-58] and *Ninf* [59], and a client proxies that support the utilization of *Globus* [19] and *Legion* [20] resources are now in prototype and being tested. This continuing work with NetSolve will insure that PICMSS can access the widest array of computational resources and facilitate its use other components (e.g. directory services) from these systems.

In addition to the work of integrating PICMSS and NetSolve, this project will directly support two extensions to the NetSolve system that are needed by PICMSS users, hence will become valuable to the rest of the NetSolve community as well:

- Status Information —NetSolve is being enhanced with new features that will allow a client to have more control over the servicing of a request that it has submitted. Specifically, a process monitoring facility will be added. This will allow clients to query NetSolve servers for information and "current data" as it is computing. These preliminary queries will allow the user of NetSolve and PICMSS to access the current state of affairs before a service is completed. They will therefore be able to determine if execution is progressing in a satisfactory manner. After querying the status of the request, the next step will be to allow the user to change input parameters and "steer" the computation towards a better result than was achieved by the previous parameters. This benefits the end-user by saving time and effort, hence creates a better execution of a problem without having to wait for completion of the first run.
- Data Flow Control — In order to manage distributed state, mechanisms for the staging of data for the NetSolve servers will be implemented. This will entail NetSolve servers getting (and putting) data from (to) some secondary storage locations -- other than the host of the originating request. The newly developed *Internet Backplane Protocol* (*IBP*) [60] (www.cs.utk.edu/~plank/IBP/) or some other protocol, like http or ftp, can be used to facilitate this service.

The NetSolve team is participating closely with the new Grid Forum (www.gridforum.org), which is working to develop common approaches to common needs and problems (e.g. directory services, security and access control, accounting, user support, etc.) for the entire Grid community. This participation will insure that PICMSS will be able stay current on all these fronts.

C4.6 Monitoring and Data Exposition

Abilities to monitor and perform data reduction in the middle of an extensive computation are important to users doing any large scale numerical simulations. But this creates another level of difficulties for a semi-black box resource scheduler such as NetSolve. To achieve this capacity, NetSolve will be enhanced to pipe out data to secondary storage devices registered to NetSolve. In the Grid Computing environment, output data may be scattered among resources in different locations. The capacity to retrieve such data and deliver to the designed location, as indicated by the remote user, will be embedded into NetSolve. Such enhancement will eventually increase the capability and adaptability of NetSolve to be an efficient and viable Grid Computing resources dealer.

Gigabytes of output typical result from large-scale scientific numerical simulations. However, only a portion of these data need be examined or visualized for process control. Conversely, full data sets are generally required to restart a simulation in the typical design processes. As such data may be dispersed among the Computational Grid, it is unwise to let it occupy those shared devices for a long time. Secondary storage devices are created to store temporary files for remote users for a fixed period of time. Users can then choose to examine the data remotely, resubmit for restart simulation, or retrieve it entirely. Conversion of output data to specific format will be provided remotely, for supporting local graphics review capabilities.

C.5 RESEARCH AND INDUSTRIAL APPLICATIONS

This project will develop and verify PICMSS for diverse applications in computational continuum mechanics in both academic research and industrial production environments. Over the past decade, the UT Engineering Science graduate program, in concert with CFD Lab, has become involved in a diversity of problem statements. The associated process of analyses provides firm confirmation of the need for such a system. This section briefly describes research projects and applications to which PICMSS will become immediately available. Names and organizations of collaborating institutions to this project in the specific category are noted.

C.5.1 CFD algorithm research (Profs. Baker, Iannelli, UT ES, and K.L. Wong, JICS)

The UT Engineering Science graduate program in FE CFD has averaged about one MSc and one PhD degree per year over that past decade. Principal focus to date has been on establishing thorough, directly comparative analytical assessments of FE/FV performance issues for model problems. The superiority of FE weak form constructions for modified conservation laws is fully established, [35,37]. Validation for extension to genuine (turbulent flow) three-dimensional problems demands a PSE, as student-generated codes at this level are inefficient and unreliable. The current research of Kolesnikov [61,37] will employ *aPSE* for two-dimensional validation studies, but the next students' research must address 3-dimensions, hence parallel computing. The PICMSS system fully represents *the* system required to enable this advance is theory confirmation, hence reduction to efficient production capability in minimal time.

C.5.2 Multiphase flow simulation (Prof. Y. Tao, Tennessee State Univ., and K.L. Wong, JICS)

The TSU project requires development of a simulation model for multi-phase flow with phase change in 3-dimensional unsteady convective solidification and melting of dispersed or packed solid particles. Flow among phase change particles (packed or dispersed) is a phenomenon occurring in many engineered systems and processes such as melting and alloying operations, vitrification, porous metal manufacturing, food processing and environmental processes. Process control or monitoring requires, (a) advanced sensors. and (b) real-time models to interpret the sensor data for control decisions. In concert with UT ES and JICS, a 3-dimensional FE numerical model is being designed to replace an under-performing FD model. The goal is to predict convective melting and solidification, for a range of particle sizes, temperatures and flows, via a microscopic (particle level) differential equation formulation as formulated at TSU Dr. Yong Tao. PI. Introduction of the developed model into PICMSS will be an application benchmark, with results computation on a parallel PC Linux cluster to be compared to those obtained in the NetSolve environment when PICMSS is stabilized.

C.5.3 Reliability of structural analyses (Profs. K. Chou, C. Pionke, UT CE and ES)

The acceptance and use of probability-based load resistance factor designs has increased worldwide. Currently, the concept focuses solely on design of individual components or members, even though the reliability of an entire system is generally recognized as different from that of individual components. The reason for this is that structural system reliability assessment techniques require a tremendous amount of computational effort. Conversely, methods that are computationally less intensive are characterized by relatively large margins of inaccuracy. For this current UT research project, an incremental energy optimization method is developed to determine a single failure path for a structural system of reasonable complexity. The approach is a combination of optimization (linear programming), a fundamental energy principle (a FE variational statement), and advanced computing technology (both in processing and hardware development). If this goal is achieved, structural engineers could economically, hence regularly, implement reliability analysis into the design process. The resultant FE computational algorithm will develop a parallel processing implementation within the framework of PICMSS.

C.5.4 Fire Simulation (Drs. D. Icove, D. Wong, TVA, UT ES)

Applications of progressively more complex CFD technologies to fire and smoke modeling have been underway for decades, with the US leadership role at NIST. However, truly rigorous, organized and formal studies of benchmark cases in the discipline of fire simulation are still limited. Dr. David Icove, US TVA Fire Police leads a TVA project in forensic analyses of fire events, which over the past decade has established the required database. This availability of PICMSS will advance the PhD work of Wong [62], for an algorithm construction to produce practically detailed validation cases for the fire research community. The approach will address sensitivity issues comparing perceptively formulated engineering models with Navier-Stokes systems with closure models. The nominal simulation period is 15 minutes, as the fire is either under control (by a fire suppression system) or out of control, whence further simulation serves no purpose in LS-FP design. Important state conditions, e.g., velocity, temperature profiles, at strategic locations where sprinkler and detectors are located; and the amount of smoke produced based on the rate of heat release, enclosure geometry, HVAC effects and number of openings, can be determined.

C.5.5 Large scale industrial ventilation analyses (Profs. Baker, Winowich, UT ES, ME)

The UT CFD Lab has installed the NPARC Alliance national resource code on the UT CS Sun Ultra II parallel workstation environment (PVM), and applied it to prediction of industrial scale ventilation flowfields for assessing atmospheric transport of pathogens. The Alliance code, designed for aerodynamics, i.e., significant Mach number, is not characteristic of a ventilation environment. A contractual project has demonstrated a 5 million node solution for a complete chlor-alkali mercury cell building with football-field size footprint more than 100 interior geometrical objects requiring meshing definition. The zero-Mach FE algorithm of Williams, [34], the premier *aPSE* formulation slated for PICMSS, represents the preferred construction, enabling parallel performance validation for application to truly large-scale flowfield analyses addressing environmental transport issues.

C5.6 Materials, quenching, heat treating (Profs. Baker, Frankel, UT ES, ME, Dr. G. Totten, ASM)

In the recent few years, the American Society for Metals (ASM) under guidance of Dr. Totten is seeking development of computational fluid/thermal/structural analysis techniques for application to materials processing in manufacturing. Prof. Baker (PI) has participated widely in interest generation via short courses, titular articles and technical paper presentations at national and international symposia organized by ASM (cfdlab.engr.utk.edu/publications). A dialogue is established within ASM to seek out methods for establishing a collaborative environment for this development via an ASM sustaining membership concept. The materials tempering industry is not at all exposed to use of computational techniques, hence the establishment of PICMSS via NetSolve on Internet presents a truly unique approach to penetrating this extremely important manufacturing sector. The technical problem class is fully coupled fluid-thermal-structural interaction with complex phase change thermodynamics, crystal growth and all forms of convective/radiative heat transfer. Creation of PICMSS thereby represents a truly unique vehicle to penetrate this extremely important industrial sector.

C.6 ACADEMIC IMPACT

The roots of Internet implementation of a "Problem Solving Environment (PSE)" lie of course in the academic sector, [10,11]. The creation of PICMSS as the genuine implementation portends absolutely fundamental impact on development and delivery of advanced. technical content courses in computational mechanics for continuum systems. UT ES has initiated a leading role in penetrating graduate education at-a-distance by offering synchronous, video-streamed lecture/practice courses in modern computational mechanics supported by (fledgling) PSE environments (Matlab, aPSE), c.f., cfdlab.engr.utk.edu/Internet. Fundamentally, this initiative addresses the absolutely critical issue of CIS technology spin-off into the professional industrial sector constituting the heart of the US manufacturing engineering economy. Creation and Internet dissemination of PICMSS will impact realization of this advance in the most efficient and effective way.

C.6.1 Internet based graduate level education, outreach

The UT ES graduate degree program in computational mechanics analysis enjoys a sound track record in degree production and archival publications (cfdlab.engr.utk.edu). The decade of the 90s is termed the *Information Age* in recognition of the fundamental impact that computer/Internet technology is having on communicating information at the speed of light worldwide. Full impact of the associated Computational and Information Sciences (CIS) on technical education is yet to occur, but is becoming better appreciated by academic institutions. Charp [63] states, "Teaching paradigms of the past are inadequate. Students are interacting with their peers and experts around the world . . . (The) Four "pillars" identified as critical to . . . teaching and learning . . . (are) *hardware, connectivity, digital content and professional development*."

Simulation of physical phenomena on computers, i.e., *advanced applied computational simulation* (A^2CS), has today joined engineering experiment and theory as the third method of scientific investigation.. The education need *clearly exists*, and it will be of truly major impact on engineering technology utilization in the US, hence worldwide. PICMSS will be fundamental to, [64], ". . . the new paradigm of parallel, distributed, collaborative, immersive computing is emerging." Impacting research in engineering education, the UT ES *vision is outreach to the global* technical practice community via a specifically-designed MSc degree curriculum in *industrial* A^2CS employing state-of-the-art real-time, video-streamed lectures utilizing available HPCC resources. Any professional with the interest need only log into the UT developed website to "tune in," (cfdlab.engr.utk.edu/Internet).

Critical proof of concept, hence viability, exists via Internet delivery of the first graduate level ES course "*Finite Elements for the Engineering Sciences*" in the fall 1998 and 1999 semesters. Remote students at LSU in Baton Rouge took it for credit, while local industry engineers took the courses (audit or credit) at their company office (or at home!). The course content was *identical* to the historical lecture room presentation, but with the significant addition of computational laboratories enabled via the embedded, remotely-addressable PSEs. The innovative pioneering development was design and construction of the *fully functional website* [65] to support the curricular delivery on today's Internet. The resident archived lecture series also directly serves professional training, certification and PE training satisfaction requirements on an *anytime basis*, as the replacement to attendance at remote short courses. This spring semester, three students are "taking" the archived course, following exactly the "regular" schedule regarding assignments and computer labs, with contact among themselves and the "instructor" via networked email. Further, the follow-on CFD graduate course is now presented in the similar manner, with *aPSE* providing the networked PSE environment. Indeed, a *new paradigm* is upon academia using CIS and *innovation in education research*.

C.6.2 Proliferation of the platform, outreach, HBCU involvement (Dr. C. Halloy, JICS)

The UT Joint Institute for Computational Science (JICS), under the direction of Dr. Christian Halloy, has been committed to encouraging and facilitating the utilization of High Performance Computing (HPC) resources for academic and scientific research since 1991. In particular, JICS has actively pursued an outreach program to Historically Black Colleges and Universities (HBCU) through its NSF-funded MetaCenter Regional Alliance (MRA) grant first awarded in 1995. Thereby, the staff of JICS has worked closely with faculty members and students of Alabama A & M University, Fayetteville State University, Fisk University, Meharry Medical College, Southern University, Spelman College, and Tennessee State University (TSU) in advocate HPC utilization at their institutions. Project collaborations among UT and HBCU partners involve such research areas as neural networks, parallel algorithm development, PC cluster computing, and modeling and simulation of fluid/thermal/solid phenomena. Most significantly, for this project, affiliated researchers at Tennessee State University will be actively involved, with the early release of PICMSS installed at TSU on a network of PCs for development and testing as soon as it is available.

Proliferation of PICMSS will start with the partner HBCUs of the MRA program, hence will expand to other institutions. An outstanding candidate is Kettering University (formerly GMI), in Troy, MI, where an ES PhD in CFD (S. Roy, UT '95) has now joined the ME faculty. The ME department has 1400 undergraduates, all involved in co-op education. This represents a significant contact base within industry, hence the unique opportunity to interface their fledgling graduate program with elements of the A^2CS graduate curriculum employing PICMSS.

With UT CFD Lab and JICS as the focal points for the academic, educational and research foci of this project, the infrastructure is fully in place to efficiently organize and direct outreach to the academic and industrial sectors. We look forward to this challenge.

C.7 PROJECT ORGANIZATION, STAFFING AND CONTENT

This NSF project will be conducted as a fully collaborative activity involving researchers in computer science, fluid/thermal systems, materials/structural mechanics, mathematics and system programming. Assistance from the development teams of PETSc and Aztec will also be sought. The following table summarizes project organization and collaboration contributors.

Personnel (Institution)	Function	Area of Expertise, Specialties
A. J. Baker (ES, UT)	P.I.	FE theory, CFD, turbulence
C. Halloy (JICS, UT)	Co. PI	HPC, Computational Physics & Chemistry
K. Wong (JICS, UT)	Co. PI	HPC, CFD, Numerical Linear Algebra
J. Dongarra (CS,UTK, ORNL)	Collaborator	Numerical Library, Software Tools, NetSolve
K. Chou (CE, UT)	Collaborator	Structure, Reliability Analysis
D. Icove (TVA)	Collaborator	Fire Engineering and modeling
C. Pionke (ES, UT)	Collaborator	Solid Mechanics, Finite Element, CSM
X. Feng (Math, UT)	Collaborator	Domain Decomposition, Multigrid, FE
Y. Tao (ME, TSU)	Collaborator	Two Phase Flow, fluid mechanics
D. Wong (UT ES)	Collaborator	Fire Analysis, CFD
S. Roy (UT ES , Ket. U))	Collaborator	Manufacturing, Acoustics, CFD

Delivery of the fully integrated PICMSS platform involves completion of five main tasks.

1. A JAVA front-end graphical user interface to define formulation of the analysis problem
2. A JAVA middle server interface to manage the status of computation
3. A computational kernel to solve the problem
4. An enhancement module to NetSolve to facilitate exchange of data
5. Proliferation of the developed system to the user community

These tasks will be completed in this three year project, with progress measured by several categorically important milestones. The time-table for milestone/task completions is the following:

Task	Milestone	Existing	Year 1	Year 2	Year 3
1	Input Panel, Job submission Panel	X	X		
	Equation Builder		X		
	Monitoring of execution		X	X	
	Version release			X	X
2	Resource management		X	X	
	Data I/O Control		X	X	
	Job Status Control			X	
	Version release			X	X
3	Limited CFD Computing Unit	X			
	Full CFD Kernel		X	X	
	CSM Kernel		X	X	X
	Fluid/Solid Interaction capability			X	X
	Multi-level Schemes			X	X
	Practical Applications Simulations			X	X
4	NetSolve	X			
	Interface to NetSolve		X		
	Job Monitoring			X	X
	I/O Enhancement				X
	Full Integration				X
5	Alliance Initiation			X	
	Alliance Integration				X

C.8 PRIOR WORK AND FUTURE EXPANSION

JICS has successfully established an outreach program to HBCUs through its NSF-funded MetaCenter Regional Alliance (MRA) grant ["A MetaCenter Regional Alliance for Computational Science Collaborations with HBCUs", NSF ASC-9523470] awarded in 1995. Seven HBCU partners are currently actively collaborating with JICS as part of this project. Additional activities under the MRA grant have included: 2 two-week summer workshops with 27 participants, 2 one-day colloquia with 10 hourly lectures involving 7 institutions and 67 participants, 7 collaborative research projects, 6 grant proposals with 4 awards, 2 high performance PC cluster laboratories configured at HBCUs, initiation of 2 undergraduate HPC courses, and 8 student assistantships at HBCUs. The UTK MRA program continues its effort to foster and promote collaborative academic and research activities in the area of HPC with its partner HBCUs.

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45. Gannon, D. and A.Grimshaw, *Object-based Approaches*, in *The Grid: Blueprint for a New Computing Infrastructure*, I. Foster and C. Kesselman, Editors. 1998, MorganKaufman Publishers: San Francisco, CA. p. 205-236.

46. Casanova, H., *et al.*, *Application-Specific Tools*, in *The Grid: Blueprint for a New Computing Infrastructure*, I. Foster and C. Kesselman, Editors. 1998, MorganKaufman Publishers: San Francisco, CA. p. 159-180.
47. Cline, A., *Scalar- and Planar-Valued Curve Fitting Using Splines Under Tension*. Communications of the ACM, 1974. 17: p. 218-220.
48. Young, D., et al., Itpack2c: a FORTRAN package for solving large sparse linear systems by adaptive accelerated iterative methods, 1996, University of Texas at Austin/Boeing Computer Services Company.
49. Moré, J., B. Garbow, and K. Hillstrom, *Minpack : Documentation file*, 1998.
50. Swarztrauber, P., *FFTPACK : Documentation file*, . 1998.
51. Anderson, E., *et al.*, *LAPACK Users' Guide, Second Edition*. 1995, Philadelphia, PA: SIAM.
52. Duff, I., *et al.*, *A set of 3 basic linear algebra subprograms.* ACM Trans. Math. Software, 1990(16): p. 1-17.
53. Dongarra, J., et al., An Extended Set of Fortran Basic Linear Algebra Subprograms. ACM Transactions on Mathematical Software, 1988. 14: p. 1-32.
54. Freund, R.W. and N.M. Nachtigal, QMR*: A quasi-minimal residual method for non-Hermitian linear systems.* Numer. Math., 1991. 60: p. 315-339.
55. Blackford, L.S., *et al.*, *ScaLAPACK Users' Guide*. 1997, Philadelphia, PA: Society for Industrial and Applied Mathematics.
56. Litzkow, M.J., M. Livny, and M.W. Mutka, *Condor - a hunter of idle workstations*, in Proc. of 8th International Conference on Distributed Computing Systems. 1988p. 104-111.
57. Litzkow, M. and M. Livny, *Experience with the condor distributed batch system*., in Proc. IEEE Workshop on Experimental Distributed Systems. 1990: Huntsville, AL.
58. Pruyne, J. and M. Livny, *A worldwide flock of condors : Load sharing among workstation clusters*. Journal on Future Generations of Computer Systems, 1996. 12.
59. Sekiguchi, S., et al. *Ninf : Network based Information Library for Globally High Performance Computing.* in Proc. of Parallel Object-Oriented Methods and Applications (POOMA). 1996. Santa Fe, NM.
60. Beck, M., *et al.*, *Logistical Quality of Service in NetSolve.* Computers and Communications, 1999 - To appear. Special Issue on Network-based Parallel and Distributed Computing.
61. Kolesnikov, A.and Baker, A. J., *Efficient Implementation of High Order Methods for the Advection-Diffusion Equation, Comp. Mtd. App. Mech. & Engr.*, in press, 2000.
62. Wong, D., Fire Modeling:*Application of a Finite Element CFD Method to Three Dimensional Fire Simulation Based on Buoyant Viscous Flow with Thermal Radiation,* PhD dissertation, University of Tennessee, Knoxville, 1995.
63. Charp, S., *Improving Teacher Preparation for the Use of Technology,* T.H.E. Journal, April, 1999.
64. Reilly, R. A., *Providing Quality Professional Development via the Internet,* T.H.E. Journal, April, 1999.
65. *Finite Elements for the Engineering Sciences*, video-streamed Internet graduate course, University of Tennessee, @ cfdlab.engr.utk.edu/internet.

A. J. Baker, Ph.D., P.E.

Professor, Engineering Science, and Director, CFD Laboratory, Dept. Mechanical and Aerospace Engineering & Engineering Science, 316A Perkins Hall, Knoxville, TN 37996-2030.
tel.:865 974 7674, fax.865.974.6372, e-mail: ajbaker@cfdlab.engr.utk.edu

Education

Ph.D. Engineering Science - St. U. New York/Buffalo, NY, 1970
Dissertation: "Diagnostics in Magnetically Balanced Cross-Flow Arcs"

M.Sc. Engineering Science - St. U. New York/Buffalo, NY, 1968
Thesis: "Temperature Determinations in Cross-Flow Arcs"

AREAS OF EXPERTISE

Computational mechanics, weak form constructions, finite element/finite volume, fluid mechanics/ heat transfer, turbulence closure models, atmospheric transport.

SYNERGISM ASPECTS

Three decades experience in CFD research, computer codes, computer systems, most recently problem solving environments in parallel constructs. Major professor for a dozen each PhD dissertations and MSc theses in last dozen years. Innovative development of Internet environments for graduate course outreach using video streaming in real-time.

RELEVANT PUBLICATIONS (max 5 in category)

Archival journals (61 articless, 1975-1999)

1. Kolesnikov, A. & A.J. Baker, "Efficient Implementation of High Order Methods for the Advection-Diffusion Equation," *Comp. Mtd. App. Mech. & Engr.*, to appear, 2000.
2. Baker, A.J., D.J. Chaffin, J. Iannelli & S. Roy, "Finite Elements for CFD - How Does the Theory Compare?," *Int. J. Num. Mtds. Fluids,* V. 31, p. 345-358, 1999.
3. Roy, S. & A.J. Baker, "A Non-linear Sub-Grid Embedded Finite Element Basis for Steady Monotone CFD Solutions - Part II: Benchmark Navier-Stokes Solutions," *J. Num. Heat Transfer, Part B. Fundamentals,* V. 33, p. 1-32, 1998.
4. Williams, P.T. & A.J. Baker, "Numerical Simulations of Laminar Flow over a 3D Backward-Facing Step," *Int. J. Num. Mtd. Fluids,* V. 24, p.1-25, 1997.
5. Baker, A.J., R.M. Kelso, E. B. Gordon, S. Roy & E. G. Schaub, "Computational Fluid Dynamics: a Two-Edged Sword," *ASHRAE Journal*, V. 39, No. 8 , p. 51-58, 1997.

Books: (2 textbooks, 1 courseware text, 9 monograph chapters, 1975-1998)

1. "*Finite Elements for the Engineering Sciences,"* Internet courseware for online graduate course http://cfdlab.engr.utk.edu, University of Tennessee, Knoxville TN., 1999.
2. "The Finite Element Method for Numerical Solution of the Equations of Fluid Mechanics," Ch. 28 in R.W. Johnson (ed), *The Handbook of Fluid Dynamics,* 98 pages, CRC Press, FL, 1998.

Conferences and Proceedings (127 contributions, 1970-2000)

1. Baker, A.J., A. Kolesnikov, M.B. Taylor & J.A. Orzechowski "Stabilized High-Order Finite Element CFD Methods Based on Modified Conservation Law Forms", in E. Onate, et al (ed), *Proc.* ECCOMAS 2000, *European Congress on Computational Methods in Applied Sciences & Engineering* , Barcelona, Spain, September, 2000.
2. Wong, K.L. & A.J. Baker, "A Modular Finite Element Parallel Fluid Applications Simulator," Proc. IMECE99, ASME *Int. Mech. Engr. Congress & Exposition*, 1999.

3. Baker, A.J., M. Taylor, N. Winowich and M. Heller, "Prediction of the Distribution of Indoor Air Quality and Comfort in Aircraft Cabins," ASTM *Symposium on Air Quality and Comfort in Airliner Cabins*,, ASTM SP 1393, Conshohocken, PA, 1999.

4. Baker, A.J., Z. Chambers & M.B. Taylor, "Finite Element Analysis for the Engineering Sciences: a Web-based Video-Streamed Education Environment at a Distance," *Proc., ASEE Annual Conference*, 1999.

5. Kolesnikov, A. & A.J, Baker, "Efficient Implementation of High Order Methods for the Advection-Diffusion Equation," *Proc., 3rd ASME/JSME Joint Fluids Engr. Conf.*, 1998.

MEMBERSHIPS

Associate Fellow, Amer. Inst. Aero. & Astro. (AIAA)
Member, New York Academy of Sciences (NYAS),
American Society Engineering Education (ASEE),
American Academy of Mechanics (AAM),
Amer. Soc. Heat, Refrig, Air Cond. Engr (ASHRAE)
Licensed Professional Engineer, New York and Tennessee
Editorial Board Member of five technical journals
Listed in *Who's Who in Science & Technology*

RECENT RESEARCH GRANTS AND CONTRACTS

U.S. Army (TARDEC), "The NAC CFD Collaboratory Concept," 3/98-3/99, $50K.
Olin Corporation, "CFD Prediction of Ventilation Flowfields in a Chlor-Alkali Cell Building," 1/98-2/99, $77K.
Oak Ridge Nat. Lab (ORNL), "Validation of CFD for the HFIR Cold Source," 10/99-6/00, $58K
Square D Corp., "CFD Modeling of Coupled Arc-Gas Circuit Breakers," 10/99-4/00, $21K.

HONORS

B. Otto and Kathleen Wheeley Award for *Excellence in Technology Transfer*, UT, 1993
Faculty Development Award, Engineering Science & Mechanics, UT, 1991
Chancellor's Research Scholar designation, UT, 1987

LIST OF COLLABORATORS

P.D. Manhardt, J.A. Orzechowski, Computational Mechanics Corp., Knoxville, TN.
Prof. J. T. Oden, University of Texas
Prof. S. Y. Wang, University of Mississippi
Prof. M. Kawahara, Chuo University, Tokyo, Japan

LIST OF GRADUATE STUDENTS

PhD: M.B. Taylor, A. Kolesnikov, K. Kilpatrick, J.M. Barton, M. Grubert, D. Berkey
MSc: A. Mitra, M. Yambert, S. Erickson, R. Williams.

TOTAL NUMBER OF GRADUATE STUDENTS ADVISED - 27

LIST OF GRADUATE ADVISORS - Prof. D. M. Benenson, Prof. I. H. Shames

Christian P. J. Halloy

Director, Joint Institute for Computational Science
Executive Director, Division of Scientific/Research Computing
University of Tennessee, Knoxville, TN 37996-1508
Phone: (865) 974-3907, Email: challoy@utk.edu

Education

- Ph.D. in Physical-Chemistry (Docteur de Specialite), Institut National Polytechnique de Lorraine (INPL), France, 1983 (with *la plus haute distinction)*
- M.S. in Computer Science, University of Tennessee, Knoxville (UTK), 1991
- M.S. in Physics (Licenciado en Fisica), Universidad Nacional de Tucuman (UNT), Argentina, 1977
- B.S. in Physics, UNT, Argentina, 1975

Areas of Expertise and synergism aspects

High performance scientific computing, parallel programming, optimization techniques, computational physics, computational chemistry, numerical methods, instructional development, research and educational outreach interaction with minority institutions

Teaching and Research Positions

- Executive Director, Division of Scientific/Research Computing, July 2000 - present
- Director, Joint Institute for Computational Science, May 1997 - present
- Associate Director of Research of the Innovative Computing Laboratory (Jack Dongarra's group), UTK (half-time) May 1996 - April 1997
- Adjunct Professor of Physics, Dept of Physics and Astronomy, UTK, March 1996 - present
- Assistant Director, Joint Institute for Computational Science, November 1992 - April 1997
- Adjunct Instructor for Intel's Scalable Systems Division, PARAGON, 1994 - 1996
- Director of the *Laboratorio Docente de Computacion* (Educational Laboratory of Computation) and Associate Professor of Physics at the UNT, 1988 - 1992 (on leave 1989 - 1992)
- Assistant Professor, Dept of Physics, UNT, 1981 - 1987

Professional Activities

Research works in the area of Dielectric Properties of Liquids, and Electric Relaxation of Emulsions. Thesis works, scientific meeting presentations, and publications (in *American Journal of Physics*, and the *Journal of Physics, D: Applied Physics* etc.), 1975 -- 1986. Interdisciplinary collaborations include:

Scientific computational programs developed for different research groups such as:

- Laboratory of Transductors, Dept. of Physics, UNT, 1978
- Theoretical Research in Physical-Mathematics, Dept. of Physics, UNT, 1979, 1981, 1985
- Laboratory of Ionospheric Studies, Dept. of Physics, UNT, 1980
- Numerical Taxonomy for the Dept. of Herpetology, School of Natural Sciences, UNT, 1979, 1981, 1984-1987
- Group of Research on Porous Media, ENSIC, Nancy, France, 1981
- Group of Automatic Treatment of Chemical Information, ENSIC, Nancy, France, 1982
- Graphic interfaces for Prof. Ken Stephenson, Dept. of Mathematics, UTK, 1990

Interdisciplinary research projects in high performance parallel computing with scientists from:

- UT-Hospital Medical Imaging Group, 1992
- UTK, Chemistry Department, Computational Chemistry, 1992-1995
- UTK, Physics Department, Computational Physics, 1992-ongoing
- UTK, Mechanical Engineering Dept, Computational Fluid Dynamics, 1992, 1993, 1996-ongoing
- UTK, Chemical Engineering Dept, Molecular Dynamics, 1992-1996, 1998-ongoing
- UTK, Mathematics Dept, and Mathematical Ecology Group, 1992-1994
- UTK, Dept of Geology, Geophysics, 1995-ongoing

developing and porting codes on computers such as a **CM-5** (32 nodes), an **MP-2** (4096 nodes), an **iPSC/860** (128 nodes), a **KSR1** (64 nodes), a **Paragon** (66 nodes), an **SP-2** (16, 48 and 512 nodes), **SGI Origin-2000** (32 nodes) and also using **PVM, MPI** and **HPF**.

Recent workshops (1993--2000)

- Instructor of more than 45 workshops on Parallel Processing on: the Thinking Machines CM-5, the MasPar MP-2, the Intel Paragon, the IBM SP-2, and the SGI Origin 2000, as well as PVM, MPI and Performance Techniques on these machines as well as on clusters of workstations and PCs.
- Selected by Intel's Scalable Systems' Division as one of the first three Adjunct Instructors to teach their "Paragon Programming Courses I and II," October 1994 (at WPAFB, Ohio), and April 1995 (at HKUST, Hong Kong).

Recent works

- "Neural Network Simulations on Massively Parallel Computers; Application in Chemical Physics," B. Sumpter, R. Guenther, C. Halloy, C. Getino, and D. Noid; International Neural Network Conference, June 1993, Barcelona, Spain.
- "Using Parallel Supercomputers to Calculate Surface Energy Distributions from Absorption Isotherm Data," by B. Stanley and C. Halloy; Scalable High Performance Computing Conference (SHPCC '94), May 1994, Knoxville, TN.
- "Using Parallel Supercomputers to Calculate Surface Energy Distributions," by Brett J. Stanley, Christian Halloy, and Georges Guiochon; *J. Chem. Inf. Comput. Sci.* 1995, v35, pp110-114.

Number of Graduate Committee Advisees:

PhD: 3: Amitabha Gosh, Geophysics, 1997; Asim Yarkhan, CS, expected Fall 2000; Korak Dasgupta, Geology, expected Fall 2000

MS: 9: Stephanie Wolf, CS, Spring 1996; Doug Hyatt, CS, Fall 1997; Chris Hastings, CS, Summer 1998; Nagiza Samatova, CS, Spring 1998; Venkatech Chidambarah, CS, Spring 1999; Erin Miller, TIEM, Summer 1999; Gerald Bowers, CS, Fall 1999; Hui Ji, CS, expected Fall 2000; Jay Koehler, CS, expected Fall 2000

Membership

- Member of the Dielectric Society of England 1982 - 1988
- Member of the Upsilon Pi Epsilon national computer science honor society, UTK chapter, 1994-present.

Kwai L. Wong

Research Scientist
104 South College
Joint Institute for Computational Science
University of Tennessee, Knoxville
Email : wong@cs.utk.edu, Phone: (865) 974-9488

Education

PhD, Engineering Science and Mechanics, University of Tennessee, 1995
MS, Mathematics, University of Tennessee, 1986
BS, Mechanical & Aerospace Engineering, University of Tennessee, 1982

Employment

Research Scientist – Joint Institute for Computational Science, University of Tennessee, January 98 – present
Adjunct Professor – Department of Mechanical and Aerospace Engineering and Engineering Science, University of Tennessee, September 97 – present
Postdoctoral Research Associate – Joint Institute for Computational Science, University of Tennessee, May 96 – December 97
Postdoctoral Fellow – Department of Mathematics, Chinese University of Hong Kong, October 95 – April 96

Relevant Publications

K. L. Wong and A. J. Baker, "A Parallel Embedded Finite Element Algorithm For 3-D Incompressible Flow in Velocity-Vorticity Form," Proc. First Asian CFD Conf., HKUST, 1995.
K. L. Wong, "3D CFD Benchmark Results on the 140-node Paragon," Proc. Intel Supercomputer Users Group Meeting, Knoxville, 1996.
K. L. Wong and A. J. Baker, "A Modular Finite Element Parallel Fluid Application Simulator," Proc. ASME Fluids Engineering Division, Feb-Vol. 250, 1999.
T. Kerr, C. D. Pionke, K. L. Wong, and K. C. Chou, "Space Frame Analysis Using Parallel Processing on PC's Operating Under the Linux Operating System," Proc. Canad. Soc. Civil Eng. Ann.Conf., 1999.

Professional Activities

Program Liaison - NSF grant, "A MetaCenter Regional Alliance for Computational Science Collaborations with Historically Black Colleges and Universities."
Research Scientist - Computational Fluid Dynamics Analysis of Ventilation Air Circulation in an Olin Chlor-Alkali Mercury Cell Plant, Validation of a CFD Prediction of Flowfield in the HFIR Cold Source
Workshop Instructors – Parallel Processing on the IBM SP2 and on Clusters of Workstations, Parallel Processing the SGI O2000, and Setting Up a PC Cluster for High Performance Computing.
Tutorial and lecture author – Parallel Computing Techniques to Maximize Your Megaflops (SC99), Parallel Computing for Undergraduate Education (http://www-jics.cs.utk.edu/PCUE)
Advisor - Parametric Study of Space Frame Analysis on a Cluster of PC's Using Parallel Processing (MS thesis of Mr. Travis Kerr - MAES Dept.), A Numerical Method for the Incompressible Navier-Stokes Equations with Application to Two-Phase Flow (MS thesis of Mr. Bo Chen, Math Dept.)

SUMMARY PROPOSAL BUDGET

YEAR 1

ORGANIZATION: **University of Tennessee Knoxville**				FOR NSF USE ONLY: PROPOSAL NO.	DURATION (months) Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Allen J Baker**				AWARD NO.		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)	
1. Allen J Baker - Professor	0.00	0.00	1.00	$ 9,951	$	
2. Christian P Halloy - Director, JICS	0.50	0.00	0.00	0		
3. Kwai Wong - Research Scientist	2.40	0.00	0.00	11,341		
4.						
5.						
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	0		
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)	2.90	0.00	1.00	21,292		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0		
2. (2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	12.00	0.00	0.00	46,000		
3. (1) GRADUATE STUDENTS				15,000		
4. (0) UNDERGRADUATE STUDENTS				0		
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0		
6. (0) OTHER				0		
TOTAL SALARIES AND WAGES (A + B)				82,292		
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				18,842		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				101,134		
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) Disk storage $ 1,000						
TOTAL EQUIPMENT				1,000		
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				5,000		
2. FOREIGN				0		
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 0 2. TRAVEL 0 3. SUBSISTENCE 0 4. OTHER 0						
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS				0		
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES				100		
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0		
3. CONSULTANT SERVICES				4,000		
4. COMPUTER SERVICES				0		
5. SUBAWARDS				0		
6. OTHER				4,244		
TOTAL OTHER DIRECT COSTS				8,344		
H. TOTAL DIRECT COSTS (A THROUGH G)				115,478		
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Facil. & Admin. (Rate: 43.0000, Base: 111234)						
TOTAL INDIRECT COSTS (F&A)				47,830		
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				163,308		
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				0		
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 163,308	$	
M. COST SHARING PROPOSED LEVEL $ 0	AGREED LEVEL IF DIFFERENT $					
PI / PD TYPED NAME & SIGNATURE* Allen J Baker	DATE			FOR NSF USE ONLY: INDIRECT COST RATE VERIFICATION		
ORG. REP. TYPED NAME & SIGNATURE*	DATE			Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET YEAR 2

ORGANIZATION			FOR NSF USE ONLY		
University of Tennessee Knoxville			PROPOSAL NO.	DURATION (months)	
				Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Allen J Baker			AWARD NO.		

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. Allen J Baker - Professor	0.00	0.00	1.00	$ 10,150	$
2. Christian P Halloy - Director, JICS	0.50	0.00	0.00	0	
3. Kwai Wong - Research Scientist	2.40	0.00	0.00	11,568	
4.					
5.					
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	0	
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)	2.90	0.00	1.00	21,718	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0	
2. (2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	12.00	0.00	0.00	46,920	
3. (1) GRADUATE STUDENTS				15,300	
4. (0) UNDERGRADUATE STUDENTS				0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0	
6. (0) OTHER				0	
TOTAL SALARIES AND WAGES (A + B)				83,938	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				19,219	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				103,157	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) Disk storage $ 1,020					
TOTAL EQUIPMENT				1,020	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				5,100	
2. FOREIGN				0	
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 0 2. TRAVEL 0 3. SUBSISTENCE 0 4. OTHER 0					
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS				0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				102	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0	
3. CONSULTANT SERVICES				4,080	
4. COMPUTER SERVICES				0	
5. SUBAWARDS				0	
6. OTHER				4,329	
TOTAL OTHER DIRECT COSTS				8,511	
H. TOTAL DIRECT COSTS (A THROUGH G)				117,788	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Facil. & Admin. (Rate: 43.0000, Base: 113459)					
TOTAL INDIRECT COSTS (F&A)				48,787	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				166,575	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 166,575	$
M. COST SHARING PROPOSED LEVEL $ 0	AGREED LEVEL IF DIFFERENT $				

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY		
Allen J Baker		INDIRECT COST RATE VERIFICATION		
ORG. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET

YEAR 3

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months)	
	Proposed	Granted
AWARD NO.		

ORGANIZATION
University of Tennessee Knoxville

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Allen J Baker

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. Allen J Baker - Professor	0.00	0.00	1.00	$ 10,353	$
2. Christian P Halloy - Director, JICS	0.50	0.00	0.00	0	
3. Kwai Wong - Research Scientist	2.40	0.00	0.00	11,799	
4.					
5.					
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	0	
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)	2.90	0.00	1.00	22,152	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0	
2. (2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	12.00	0.00	0.00	47,858	
3. (1) GRADUATE STUDENTS				15,606	
4. (0) UNDERGRADUATE STUDENTS				0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0	
6. (0) OTHER				0	
TOTAL SALARIES AND WAGES (A + B)				85,616	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				19,603	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				105,219	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) Disk storage $ 1,040					
TOTAL EQUIPMENT				1,040	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				5,202	
2. FOREIGN				0	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ 0					
2. TRAVEL 0					
3. SUBSISTENCE 0					
4. OTHER 0					
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS				0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				104	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0	
3. CONSULTANT SERVICES				4,162	
4. COMPUTER SERVICES				0	
5. SUBAWARDS				0	
6. OTHER				4,416	
TOTAL OTHER DIRECT COSTS				8,682	
H. TOTAL DIRECT COSTS (A THROUGH G)				120,143	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) Facil. & Admin. (Rate: 43.0000, Base: 115727)					
TOTAL INDIRECT COSTS (F&A)				49,762	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				169,905	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 169,905	$

M. COST SHARING PROPOSED LEVEL $ 0 — AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY		
Allen J Baker		INDIRECT COST RATE VERIFICATION		
ORG. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET — Cumulative

ORGANIZATION **University of Tennessee Knoxville**	**FOR NSF USE ONLY** PROPOSAL NO.	DURATION (months) Proposed	Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR **Allen J Baker**	AWARD NO.		

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. Allen J Baker - Professor	0.00	0.00	3.00	$ 30,454	$
2. Christian P Halloy - Director, JICS	1.50	0.00	0.00	0	
3. Kwai Wong - Research Scientist	7.20	0.00	0.00	34,708	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	0	
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)	8.70	0.00	3.00	65,162	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0	
2. (6) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	36.00	0.00	0.00	140,778	
3. (3) GRADUATE STUDENTS				45,906	
4. (0) UNDERGRADUATE STUDENTS				0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0	
6. (0) OTHER				0	
TOTAL SALARIES AND WAGES (A + B)				251,846	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				57,664	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				309,510	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) $ 3,060					
TOTAL EQUIPMENT				3,060	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				15,302	
2. FOREIGN				0	
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 0 2. TRAVEL 0 3. SUBSISTENCE 0 4. OTHER 0					
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS				0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				306	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0	
3. CONSULTANT SERVICES				12,242	
4. COMPUTER SERVICES				0	
5. SUBAWARDS				0	
6. OTHER				12,989	
TOTAL OTHER DIRECT COSTS				25,537	
H. TOTAL DIRECT COSTS (A THROUGH G)				353,409	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				146,380	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				499,789	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 499,789	$

M. COST SHARING PROPOSED LEVEL $ 0	AGREED LEVEL IF DIFFERENT $			
PI / PD TYPED NAME & SIGNATURE* **Allen J Baker**	DATE	**FOR NSF USE ONLY** INDIRECT COST RATE VERIFICATION		
ORG. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked	Date Of Rate Sheet	Initials - ORG

Budget Justification Page

These budgets assume a 2% cost of living and salary increase in each year.

Other Personnel: Two half-time research associates will work on this project.

Travel: Funding is requested to support 3-4 trips each year for the PI and Co-PIs to participate in related conferences, workshops or other meetings.

Consultant Services: Dr. Yong X. Tao, Tennessee State University, will be supported via a consultant fee for his work on this project.

Other: Graduate student(s) working on this project will receive additional support for tuition and fees, as appropriate.

College of Engineering and Technology
Tennessee State University
3500 John A. Merritt Blvd.
Nashville, TN 37209-1561

Mechanical Engineering Department

Yong X. Tao, Ph.D.
Associate Professor
(615)963-5390
Fax: (615)963-5496
E-mail: taoy@harpo.tnstate.edu

February 11, 2000

Dr. Kwai Wong, Ph.D.
Joint Institute of Computer Science
University of Tennessee
104 South College
Knoxville, TN 37996-1508

Dear Dr. Wong,

I will be happy to collaborate with the Joint Institute of Computer Science under the research proposal submitted to NSF.

I plan to work closely with you on problems arising in development and implementation of a two- phase flow with phase change model. The work is to be focused specifically on the interface subroutine development that can be incorporated into the PICMSS platform. This also requires us to establish the PICMSS platform at Tennessee State University for related research purpose. Finally, I will commit to expand the use of PICMSS platform in research and teaching at TSU.

Our collaboration has started since a number of years ago, and will continue to lead more interesting research results as well as educational training in the field of computational fluid mechanics.

Sincerely yours,

Yong X. Tao, Ph.D.
Associate Professor
Mechanical Engineering

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Allen Baker**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **A Parallel Interoperable Computational Mechanics Simulation System**

Source of Support: **National Science Foundation**

Total Award Amount: $ **499,789** Total Award Period Covered: **10/01/00 - 09/30/03**

Location of Project: **University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **0.00** Acad: **0.00** Sumr: **1.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Validation of a Computational Fluid Dynamics Prediction of the Flowfield in the HFIR Cold Source**

Source of Support: **Lockheed Martin Energy Research Corporation**

Total Award Amount: $ **57,925** Total Award Period Covered: **11/01/99 - 07/31/00**

Location of Project: **University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **0.00** Acad: **0.00** Sumr: **0.50**

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **An Internet-delivered Engineering Master of Science Curriculum in Advanced Applied Computational Simulation**

Source of Support: **National Science Foundation**

Total Award Amount: $ **462,080** Total Award Period Covered: **08/01/00 - 07/31/03**

Location of Project: **The University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **0.00** Acad: **1.00** Sumr: **1.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

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*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Christian Halloy**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Computational Science Collaborations with Historically Black Colleges and Universities**

Source of Support: **Lockheed Martin Energy Research Corporation**

Total Award Amount: $ **87,000** Total Award Period Covered: **08/11/99 - 07/31/00**

Location of Project: **Oak Ridge National Laboratory**

Person-Months Per Year Committed to the Project. Cal: **2.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **A Parallel Interoperable Computational Mechanics Simulation System**

Source of Support: **National Science Foundation**

Total Award Amount: $ **499,789** Total Award Period Covered: **09/01/00 - 08/31/03**

Location of Project: **University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **0.50** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☒ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **ITR-ACS: The Tennessee Soft Computing Initiative**

Source of Support: **National Science Foundation**

Total Award Amount: $ **500,000** Total Award Period Covered: **09/01/00 - 08/31/03**

Location of Project: **The University of Memphis**

Person-Months Per Year Committed to the Project. Cal: **1.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Energy Based Optimization of the Critical Path for Structural System Reliability Using Parallel Processing**

Source of Support: **National Science Foundation**

Total Award Amount: $ **240,942** Total Award Period Covered: **10/01/00 - 09/30/03**

Location of Project: **The University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **0.50** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Kwai Wong**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **IBM's Shared University Research Program (IBM SP2)**

Source of Support: **International Business Machine Corporation**

Total Award Amount: $ **1,760,000** Total Award Period Covered: **11/15/96 - 11/14/01**

Location of Project: **University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **0.50** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **A Parallel Interoperable Computational Mechanics Simulation System**

Source of Support: **National Science Foundation**

Total Award Amount: $ **499,789** Total Award Period Covered: **10/01/00 - 09/30/03**

Location of Project: **University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **2.40** Acad: **0.00** Sumr: **0.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Validation of a Computational Fluid Dynamics Prediction of the Flowfield in the HFIR Cold Source**

Source of Support: **Lockheed Martin Energy Research Corporation**

Total Award Amount: $ **47,925** Total Award Period Covered: **11/01/99 - 02/28/00**

Location of Project: **University of Tennessee, Knoxville**

Person-Months Per Year Committed to the Project. Cal: **1.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Energy Based Optimization of the Critical Path for Structural System Reliability Analysis Using Parallel Processing**

Source of Support: **National Science Foundation**

Total Award Amount: $ **240,942** Total Award Period Covered: **10/01/00 - 09/30/03**

Location of Project: **The University of Tennessee**

Person-Months Per Year Committed to the Project. Cal: **1.50** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

FACILITIES, EQUIPMENT & OTHER RESOURCES

FACILITIES: Identify the facilities to be used at each performance site listed and, as appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Use "Other" to describe the facilities at any other performance sites listed and at sites for field studies. USE additional pages as necessary.

Laboratory: **Cetus Lab: 31 SUN Ultra1 Model 140, 100Mbps Ethernet, 7.75GB memory, 65GB disk. Gemini Cluster: 12 SUN Ultra2 Model 2170 with ATM connection, 3GB memory, 25GB disk. These labs are at UTK and are available for this project.**

Clinical: **None.**

Animal: **None.**

Computer: **TORC PC Cluster: 16 Dual 300MHz Pentium proc connected with GB switches and 100Mbps Ethernet Switch, total of 4GB memory. Galaxy PC Cluster: Four 400MHz Pentium proc with 1GB memory connected with 100MBPS Ethernet Switch. Both clusters are at UTK and are available for this project.**

Office: **Office space for the PI and Co-PIs are provided by the Department of Mechanical and Aerospace Engineering Science and the Joint Institute for Computational Science and are located at UTK.**

Other: **4000 SU Hr startup grant allows access to the SGI Origin 2000 at NCSA for this project.**

MAJOR EQUIPMENT: List the most important items available for this project and, as appropriate identifying the location and pertinent capabilities of each.

IBM SP2: 34-node 48 proc machine connnected by 150MB/s High Perf. Switch. Nodes are: two 8-way SMP high nodes with 1GB memory and 8GB disk; 24 120MHz thin nodes with 256MB memory and 2.2 GB disk; 8 160MHz thin nodes with 256MB memory and 2.2GB disk. Overall performance of 20 GFlops and total memory of 10 GBytes.
The SP2 is located at UTK and is available for this project.

OTHER RESOURCES: Provide any information describing the other resources available for the project. Identify support services such as consultant, secretarial, machine shop, and electronics shop, and the extent to which they will be available for the project. Include an explanation of any consortium/contractual arrangements with other organizations.

UTK Division of Information Infrastructure provides system administration for the IBM SP2. UTK Computer Science Department provides system administration for all other machines listed above.