High Level Descriptor-driven Integration of Prototyping, Communication, and Large Parallel Linear Solvers for Learning and for Simulation of Physical Systems

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Project Description

Introduction:

The development of scientific and engineering computational models involves discretization of the differential equtions, followed by evolution of the code and evaluation of results.

Each of these steps can involve very complicated procedures at the lowest, technical level. However, what the investigator wants to control is typically at a much higher, abstract level. For instance, repeated experiments may be run using different discretization prescriptions. The task of modifying such prescriptions at the level of manipulating matrices or loops is very tedious and error prone, and can be very profitably taken over by an automatic system driven by a high level language, enabling the scientist to concentrate on the fundamental features of the algorithm, rather than the details of the algorithm.. Similarly, study of graphical output is essentially the only way to understand even one-dimensional situations and becomes essential in multi-dimensional simulations. Automatic, interactive and collaborative graphical presentations thus can dramatically improve the ease (and speed) with which computational methods are tried, analysed, understood and, if necessary, modified.

In the current computational context, parallel approaches are required to achieve competitive performance. Thus, we require support for parallelization, for parallel I/O and for visualization of large parallel data sets, and we require large, parallel, *linear* solvers.

Precisely these same features are desirable in the teaching of computational techniques to a new generation of scientists. It certainly is important that students understand discretization schemes at the lowest level, and they can be taught. But it is important to provide to the student rapid, reliable access to prototyping tools that can describe the fundamental features of the desired code, without explicit low level writing, can handle parallellization and adaption, can efficiently run on todays parallel machines, and can be viewed responsively, and typically in a collaborative setting. The integrated environment here will be demonstrated in computational science classes taught at The University of Texas, and at Syracuse University, and will include collaborative instruction, initially in a research environment, eventually in a classroom setting, between the Center for Relativity, The Department odf Computer Science at The Universityof Texas, and at Syracuse University. .

The approach we propose here is to extend existing functional examples of these tools, to parallel systems and to multi-dimensional problems.

The existing systems include:

RNPL (Rapid Prototyping Numerical Language), which supports high level description of discretization methods, and handles many “housekeeping” features of the coding, and can genetate full update code if desired. [156]

DAGH (Distributed Adaptive Grid Heirarchy), which supports automatic parallelization, load balancing, and adaptivity. [8]

PLAPACK, a library supporting parallel solution of large linear systems and algebraic eigenvalue problems.[161]

SCIVIS, which is a collaborative visulization and data manipulation tool. [2] [4]

These tools will be developed and extended to handle development and analysis of large, parallel systems, and to provide responsive tools for direct and collaborative teaching of computational science concepts and techniques..

The acronym RNPL stands for *Rapid Numerical Prototyping Language*[156]. It is a language for expressing time-dependent systems of partial differential equations and the information necessary for solving them using finite-difference techniques. It has advantages over traditional programming languages such as C and FORTRAN because it only requires the user to enter the essential structure of the program while it fills in the details [156].

RNPL can produce complete working programs, or a "skeleton" that the user can complete. The programs include facilities for reading parameters from a file, interactive control over output times and functions, memory management, and state dumping for calculation interruption and restart. The compilable code generated by RNPL is (at the user's descretion) in C, C++, or FORTRAN.

Thus, RNPL provides the capability rapidly to generate C, C++, or FORTRAN code from high level specifications. The current implementation of RNPL introduces a number N of grid functions, $\phi^A[x^\mu] \quad A = 1 \cdots N; \quad \mu = 1, \quad \mu = 1, 2, \quad$ or $\mu = 1, 2, 3.$ on a Grid, G, labelled by i, j, k (or a superindex $I, I = 1$...(number of grid points)). The state of the system is then described by $u^\iota \iota = 1 \cdots N \times$(number of grid points).

Notice that we consider the temporal integration separately. We discuss a finite-difference evolution of the temporal dependences. The finite representation of the system (finite difference, finite element ...) discretizes the system into a matrix acting on the state vector.

Existing RNPL implimentation solves this system in the following way: The basic set of equations:

$f_\iota(u^\kappa) = 0$

is iterated:

$u^\kappa_{i+1} = u^\kappa_i - f_i(u^\kappa_i) / \left(\frac{\partial f_i}{\partial u^\kappa_i} \right.$

This iterative update succeeds in many contexts, but in some contexts (particularly with strong inhomogenieties in the domain) may not converge. The solution is to supply a general linear solver for the problem.

Our approach is to use PLAPACK, which we will extend here to large sparse parallel systems.

PLAPACK

Coding parallel algorithms is generally regarded as a formidable task. To make this task manageable in the arena of linear algebra algorithms, the Parallel Linear Algebra Package (PLAPACK) [161] is an infrastructure for coding such algorithms at a high level of abstraction. It is often believed that by raising the level of abstraction in this fashion, performance is sacrificed. Indeed there is a performance penalty, but by coding at a higher level of abstraction, more sophisticated algorithms can be implemented, which allows high levels of performance to be regained. This has been shown to be the case for the parallel solver package implemented using PLAPACK, which includes Cholesky, LU, and QR factorization based solvers for symmetric positive definite, general, and overdetermined systems of equations, respectively. Performance comparisons with other such packages, in particular ScaLAPACK, shows there is no real performance penalty when coding at this high level of abstraction.

In a dissertation by Tim Collins (Ph.D. in CS, UT-Austin, 1995, co-supervised by J.C. Browne and R. van de Geijn), hierarchical specification of matrices was shown to be a highly effective way of storing and manipulating large sparse linear systems arising from regular and irregular meshes

[160]. In that research, type information for submatrices in the hierarchy was also encoded and exploited, allowing for highly elegant and compact implementation of sparse iterative and direct linear solvers. In particular, type information allows a solver to take advantage of structure in subproblems. The hierarchical specification allows for pruning of the matrix where it has zero entries. In addition, it allows for natural detection of "supernodes" in sparse direct methods.

While PLAPACK was designed for *dense* linear systems, there are a number of reasons why PLAPACK is a natural candidate for integration with RNPL and DAGH, and systematic implementation of a hierarchical matrix infrastructure:

- The matrix distribution used by PLAPACK is *physically based* by which we mean that the distribution of the matrix is induced by the distribution of the physical domain for which the linear system is to be solved.

- Such domains are frequently partitioned hierarchically, e.g. in nested disection methods.

- It is uniquely appropriate for implementation of direct methods for solution of sparse linear systems since physically based matrix distribution implicitly specifies the distribution of dense interface matrices to distributed memory architectures.

- PLAPACK uses an object based programming paradigm, allowing hierarchical specification of matrices to be encoded using an elegant and simple interface.

- PLAPACK shares a common communication layer with DAGH, the Managed Message-Passing Infrastructured developed at UT-Austin by Carter Edwards [162].

- PLAPACK allows elegant and efficient implementation of the orthogonalization of vectors that define Krylov subspaces as occur in iterative solvers like conjugate gradient and GMRES.

DAGH

DAGH (which stands for Distributed Adaptive Grid Hierarchy) [?] was developed as a computational toolkit for the Binary Black Hole NSF Grand Challenge Project. It provides the framework to solve systems of partial differential equations using adaptive finite difference methods. The computations can be executed sequentially or in parallel according to the specification of the user. DAGH also provides a programming interface so that these computations can be performed by traditional Fortran 77 and Fortran 90 or C and C++ kernels.

Scivis

Scivis is a client-server data visualization and analysis system, which enables users to manipulate data from their scientific codes.[4] One of the major advantages of Scivis is that it is written in Java, so that it works on all computer platforms. Scivis uses a client-server model for data visualization. Users can send the data to the server anywhere sockets are supported so that the Scivis system can be used as a front end to other applications that originally produce the data sets. The application producing a data set can write the output data to a socket, which is connected to the Scivis server. Scivis then allows the user to analyze and visualize the data. The system is flexible and very responsive. The system allows vsualization rendering on remote fast servers, and only polygon lists are transported for the interactive visualization of 3D objects.

One of the key Scivis features is called *User-Definable-Filters (UDF)*. Filters are user definable actions, performed on data set(s) to create new data based on this action. (For instance a filter may take a derivative in space and/or time, of the original data, to create a new dataset.) The Scivis system contains Wizards to help enbale users design their own filters. Filters in Scivis can be created *on-the- fly* so that users can immediately apply these new filters to her/his dataset. Since the Scivis system is collaborative, it is possible to create a powerful platform where many different users can can evaluate the performance of collaboratively developed filters.

Another major feature of Scivis is that it is collaborative. Scivis currently uses it's own collboration system, but will eventually switch from using its own collaboration system, to one which takes advantage of the TANGO system.[139] Using TANGO, Scivis will become part of a very powerfull collaboration system which will allow it's users to take advantage of many of the tools already introduced into TANGO. For example, TANGO has many features such as shared web-browsers, whiteboards, audio-visual communications, etc. TANGO has been incorporated with Web Wisdom to allow for a new virtual University.[140] This has allowed NPAC to offer courses at university while teaching them from Syracuse University.

Since filters in Scivis are user-definable, Scivis users Serilization in Java to tranfer the algorithms to other collaborators, in case the collaborator does not have the filter being used during the collaboration. Using this collaborative framework, users can exchange their data and their own personalized filters. Users of the system collaboratively are identified as Masters, or Slaves. A Master can modify data, a Slave can only view data. Multiple Masters are allowed in a collaborative session.

Proposal:

Working collaboratively, and using the tools we are developing, Choptuik, van de Geijn, Matzner and Klasky will develop and extend the four components of this effort into a unified coherent development and pedagogical tool for large scale scientific computational development and for collaborative education and collaborative computational simulation.

Extensions include:

RNPL extension to include automatic solution of the generated equations by linearization and full solution of the equivalent linear-system (matrix) problem.

DAGH extension to inclusion of large linear system solvers such as PLAPACK, and PLAPACK extensions.

PLAPACK extensions to parallel algorithms for the solution of sparse systems of linear and nonlinear equations arising on structured and unstructured meshes, as well as for gridless methods, through extensions to PLAPACK that express sparse matrices as hierarchical matrices. This will include routines which recognize the sparsity structure of the matrices, and adapt the algorithm accordingly.

SCIVIS extension to large parallel dataset manipulation, and to user manipulation and visualization of extremely large parallel datasets.

INTEGRATION:

The components described above will be integrated into a coherent environment. RNPL will be extended to directly produce DAGH code, and will be modified to interface the sparse-solver development of PLAPACK. DAGH will be extended to incorporate large parallel solvers through PLAPACK. RNPL and SCIVIS will provide theuser interface element to the developer.

APPLICATIONS:

The environment as conceived will have broad applicability in the development of simulation codes. The 1D description currently in RNPL will be extended to full 2- and 3- dimensional support. Applications include: One- and two- dimensional simulations of the behavior of matter in strong gravitational fields, and in particular the appearance of critical phenomena in gravitational collapse, and simulations of 3-dimensional strong-field gravitating systems.

The topics described in this proposal address the KDI topics listed in the announcement:

Knowledge Networking: -focus on attaining new levels of knowledge integration, information flow, and interactivity among people, organizations, and communities. -enhance communication across disciplines, languages, and cultures -improve the processing and integration of knowledge from different sources, domains, and non-text media types -increase the effectiveness of teams, organizations, classrooms, or communities that work together across distances or over time -deepen understanding of the ethical, legal, and social implications of new developments in connectivity

In particular the research would focus on interactive and collaborative tools for rapid development and analysis of multi-dimensional structured adaptive PDE codes. This constitutes Knowledge Networking Foundational Research in: -Computational aspects of distributed intelligence: dynamic task allocation, interaction, coordination, process and organization representation, collective learning, consistency management, protocol, negotiation -Managing heterogeneity and interoperability in dimensions such as syntax, semantics, scale, and structure -Large-scale remote data acquisition, distributed data analysis, experiment and sensor control, and simulation; especially interactive and real-time aspects -Distributed knowledge: sharable ontologies, processes for distributed classification and taxonomy, collaborative knowledge construction, representation and filtering tools, digital libraries and repositories across disciplines and application domains, and translation of representations

In The New Computational Challenges, these topics contribute to: -Interplay Between Computations and Data

Matthew Choptuik and Richard A. Matzner

Binary Black Holes: Coalescence and Gravitational Radiation, ASC/PHY 9318152 (ARPA Supplemented)

1. Summary of Previous Results

The ASC/PHY 9318152 Grand Challenge Project was initiated in September 1993. Richard Matzner is the Principal Investigator and M. Choptuik is a coInvestigator on this grant. More than 100 publications have so far resulted from the Binary Black Hole Grand Challenge Alliance. (see: http://www.npac.syr.edu/projects/bh/) Three of the technical components to be extended here (RNPL, SCIVIS, and DAGH) were developed in the context of the Binary Black Hole Grand Challenge Alliance. Firther the research of that Grand Challenge presented and presents a suite of pedagogical and research applications for the integrated environment proposed here.

The purpose of the Alliance is to compute the interaction of black holes and the gravitational radiation produced. The Alliance developed a parallel adaptive structure to take advantage of the fast, large computers being promised. Computer science structures, such as data structures definitions, and interface definitions, to direct the construction of the "toolbox" (which has become the "problem solving environment") were immediately addressed. One feature was adaptive mesh refinement, which was immediately demonstrated in 1-d by Choptuik[22], and developed within the Alliance[23, 24].

Initial effort concentrated on High Performance Fortran, which is an extension of FORTRAN90[11]. The Alliance began with a collection of legacy codes, and these codes were successfully expressed in HPF (High Performance Computing)[11]. This work was carried out by computational scientists (especially Masso, Seidel , Cook, ...) and computer scientists (especially Haupt, ...). Further, the "toolkit" effort produced early results[25]. However, we were aware of the need to accommodate parallel computing, and immediately undertook efforts to do so.[26]. It became clear that the limitations of HPF inhibited easy implementation of adaptive parallel structures such as would become necessary in the Alliance codes. Thus, an effort was begun to develop DAGH (Distributed Adaptive Grid Hierarchy) which was written in C and built on an underlying structure called SDDA (Symmetric Distributed Data Array).

In early 1996 the HPF efforts were concluded, and concentration centered exclusively on DAGH development. DAGH consists of a C++ driver which handles parallelization (it uses space-filling curves to convert from the conceptually 3-d computational space to a linear layout of processors). It also handles adaptive refinement, given routines to define an error measure and threshold[27, 28, 29, 30, 31, 32]. It contains standard clustering routines, as well as injection and restriction routines, to communicate at the boundaries between different levels of refinement. In most applications as intricate as computational relativity, however, specially-tuned programs have to be supplied by the computational scientist. DAGH is written so that this C++ structure calls application science modules which can be written in C or in FORTRAN[8]. In the Alliance, the practice has been to write these codes in FORTRAN90. Codes are typically written in a unigrid context by the developer, following certain rules: no global variables, array bounds passed in at call, etc., that guarantee parallelizability, and with a FORTRAN90 driver which calls the various science modules. We have written a script which reads the F90 driver and constructs a DAGH driver to run the program in parallel (adaptive refinement is being debugged). This means that we have a fast and efficient development process which can be translated immediately into production-style DAGH code for large-scale development or production runs. DAGH has been adopted into other research applications[33, 34] and has been extended in other research directions[35]. Relativity, i.e. applications-science use of the computational resources, began with the set of legacy codes referred to above. A period of testing and evaluation ensued. A number of systems were studied: spherical systems, typically with scalar radiation to provide a dynamical field;[37, 38, 39] initial studies of axisymmetric vacuum collapse;[40] and collapse to black holes with matter sources[41]. Fully 3-dimensional data setting and initial computation was carried out by Matzner and Laguna in cosmology[42] using an ADM (g-dot, K-dot) code developed by Kurki -Suonio, and a similar code was used at NCSA[137].Additionally, we had expertise on 2+1-d characteristic codes, which allow integration all the way to radiative infinity[43]. Work soon began on a 3-dimensional characteristic code. A number of technical approaches were studied to expand the computational science resources available to the Alliance[44]. Some of these took the form of internal reports[46, 47, 48].

Validation of codes proceeded in the 1-d case in work by Evans and Coleman[49], who studied gravitational collapse of a radiation fluid, and found critical phenomena related to the Choptuik[50] effect. Development proceeded on broad paths with a number of test and example cases used to develop technique for the Einstein equations and for the important problem of radiation extraction[121, 51]. Critical Phenomena remain a topic of current interest, and code development, especially in the spherical case, has continued to touch on this problem[52, 53, 54, 55].

There are a number of ways that data can be set for multiple black hole configurations. Cook et al[56] had, prior to the initiation of the Alliance, shown computationally convergent methods of preparing data, based on the "classic" approach of using the York technique on conformally flat backgrounds. Cook extended this to a study of quasi-circular black hole orbits[57].

Early 2-dimensional black hole collision simulations were done using maximal lapse (a singularity-avoiding coordinate system)[58]. A number of these studies were carried out, and laid the groundwork for the considerably more demanding 3-d simulations: These included studies of distorted and rotating black holes,[59, 60, 61, 155] both vacuum and from collapse [121], and a thorough development of the dynamics of the collision[62, 63, 64]. These studies (based also on previous work by Shapiro and Teukolsky[41]) culminated in a thorough description of the surface of merging black holes, explicating many previously unclear aspects of the process[65]. A fuller exposition subsequently was given in[66, 67, 68].

An important aspect of computational physics is to compare with other (perhaps approximate) methods[130, 101, 100, 103, 102]. Perturbation theory of distorted black holes surely describes the late evolution of a black hole merger. A number of studies have been carried out predicting radiation in situations that can be treated by close (standard perturbative) or other approximate methods. For axisymmetric problems, these results are in often surprising agreement with computation[69, 70, 71, 72, 73]. See also work on perturbative fields on fixed backgrounds[102]. Three-dimensional black hole work has progressed with maximal slicing in 3-d[45, 114]. However, it became clear that an Eddington-Finkelstein adapted coordinate system is preferable because the representation of a single black hole is static in that case.

At present we have succeeded in long-term single black hole evolution for both nonrotating (Schwarschild) an drotating (Kerr) black holes. By imposing blending boundary conditions to analytically known solutions, we can in some situations run the code *forever*. Norms of changes of field variables across the grid decrease to, and remain at, machine round-off levels. [36] We are investigating the range of parameters that allows this result. We have also demonstrated a black hole moving across the grid for periods up to $60M$[74], and shorter times for moving spinning black holes [36]. Further, we have been able to demonstrate brief evolutiuons of interacting spinning black holes moving through the computational grid [36]. Apparent horizon "locking" and is necessary for better performance. This means that we will activelytrack the apparent horizon and fix coordinates to it. We have developed three separate approaches: expansion in spherical harmonics;[75, 76, 77, 78, 79] direct solution of the apparent horizon elliptic equation,[80] and curvature flow methods[81] to the tracking problem, and we are enabling horizon tracking for new runs.

Essential to simulations of gravitational waveforms is the ability to extract waves at infinity. We have developed a method based on matching to a perturbative outer module,[73, 82, 83] and a matching to characteristic evolution[84, 85, 86, 87, 89, 90, 91]. Various technical aspects of the matching approaches require computation or integration on the matching sphere, and these have been developed[92, 93, 94].

A substantial effort was made to rewrite the Einstein system in a way that more closely presented its hyperbolic nature. This work proceeded on two fronts. A scheme which is based on the Arnowitt-Deser-Misner formalism, but which introduces additional spatial variables, was introduced by Bona and Masso,[95] and developed substantially[96],[97, 98]. A new formulation, which deals with one higher time derivative of the metric, and demonstrated explicit hyperbolicity, was also developed[12, 99, 82, 104, 105, 106]. This latter formalism has had significant impact outside relativity, and has been studied in the context of more general field theory.

A number of more or less general reports have been given describing the Binary Black Hole Grand Challenge Alliance[107, 108, 109, 110, 111, 112, 113, 45] and other work supported/stimulated by the Alliance[44].

Cray Research used figures from Grand Challenge Alliance research on the cover of its 1997 University Research and Development Grant Report.

Human Resource Development

Our group has a large and growing number of graduate students who share our enthusiasm regarding the future of computational science. These students receive an outstanding grounding in computational physics, numerical analysis and systems-development skills, and a continued high level of graduate training is a primary goal of our overall research program. They contribute substantially to the research program.

A very large number of students and postdocs were involved in the Binary Black Hole Grand Challenge. Those from Texas supported by the Alliance or by other NSF funding to Matzner and Choptuik were: Matthew Choptuik (postdoc, now Associate professor of Physics), Robert Marsa (PhD 1995, now a post-doctoral fellow in the Center), Dale Choi (PhD expected 1997), Steven Liebling (PhD expected 1997), Randall Correll (PhD expected in 1999), Mark Dubal (postdoc), Tim Galavan (graduate student), Reid Guenther (PhD 1995), Eric Hirschman (postdoc), Paulo Holvorcem (postdoc), Mijan Huq (PhD 1996, now a postdoc in the Center), Scott Klasky (PhD 1994, now a postdoc at Syracuse), John LaChapelle (postdoc), Juan Lara (graduate student), Manish Parashar (postdoc), Premana Premadi (PhD 1996), Jonathan Thornburg (postdoc), Robin Tuluie (PhD 1993) David Neilsen (graduate student), Scott Hawley (graduate student) Chun Yen Wang (graduate student), Carmen Molina-Paris(graduate student), Jodie Martin (undergraduate student), Mike Hicks (undergraduate student), Johnathan Thornburg (postdoc).

Results of Prior Research Sponsored by NSF

Robert van de Geijn

Grant: CMS-9522964 Principle Investigators: Greg Rodin (PI), J.C. Browne (Co-PI), J. Tinsley Oden (Co-PI), Robert van de Geijn (Co-PI) Period: April 1, 1995 - March 31, 1998 Amount: $1,200,000 Title: Application of High Performance Computing to Micromechanical Characteristics of Composite Materials

This grant has supported 4 Ph.D. students (1 has completed his Ph.D., 1 will defend in Aug. 1998, and 2 will finish within the next two years), 1 MS student, and 3 post-doctoral students. In addition, the project supported a visiting scientist from the People's Republic of China.

The principal results obtained during the project are as follows:

Fast Boundary Element Methods: We have developed FLEMS, a 3-D boundary element code for rapid solution of many-particle problems in linear elasticity [163, 164] This code allows the integration of any boundary element method with any iterative strategy that includes a fast summation method. The present version includes the standard collocation boundary elemetn mehthod and a GMRES solver in which matrix-vector multiplication is performed with the fast multipole method. FLEMS is the first code of its kind for solving multiscale materials problems.

Fast Dislocation Dynamics Methods: Following theoretical ideas developed in connection with FLEMS, we have developed a similar approach and code for dislocation dynamics simulations [165, 164]. This code is being adapted by researchers at LLNL, ALCOA and in France.

Modeling Error Estimates: We have introduced and analyzed the concept of modeling errors. These errors are associated with replacing a fine-scale model with a coarse-scale model. Clearly this displacement procedure is central to multiscale problems. Main results have been published by Zohdi et al. [166] and Oden and Zohdi [167].

Domain Decomposition Methods: We have developed two complementatry domain decomposition methods for multiscale problems. The first method [166, 167]. is based on hierarchical partitioning of the domain. The second [168] allows one to represent complex microstructures as a combination of problems that involve individual miscrostructural features whose interactions are computed using a structured mesh.

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Facilities, Equipment and Other Resources

This is a proposal for computational research. In the past few years, the Center has become quite well-equipped with medium- and high-end graphics workstations. This equipment has been, and will continue to be, absolutely vital to the success of our research. Our current facilities include four Silicon Graphics (SGI) R10000 Impact machines with a total of nearly 1.5 Gbyte main memory and 32 Gbyte of disk storage, as well as two older SGI Crimson R4000 VGXT machines. Together, the six R10000/Crimson machines provide powerful platforms for scientific visualization, code development, and medium-scale production runs for the PIs, our postdocs, and (at most) two graduate students. We also have two entry-level SGI Indigo and two SGI Indy machines which are used heavily by graduate students, but which are rapidly approaching obsolescence and will soon need to be replaced. We have very good access to campus networks, and adequate access to national networks and national supercomputer centers.

Budget Justification

This proposal is to support work by Professor M. Choptuik, and Professor Richard A. Matzner, in computational research on the interaction of black holes. This work will be done in collaboration with colleagues at The University of Pittsburgh, and The Pennsylavania State University, and involves computational science support through the University of Syracuse. The budget principally supports one postdoc, who will be supervised by Matzner and Choptuik. It also modestly supports travel, publications, and very necessary communication to carry out this collaborative research. There is an important piece of cost sharing: The Center for Relativity commits one postdoc (letter attached) supported by State of Texas funds as a match to the funded postdoc position requested here. This amounts to a *real* costsharing (salary, fringes, and overhead) of $354,775 over the five-year proposed duration of this grant.