Acquisition of Infrastructure for Research in Grid Computing and Multiscale Systems Computation

1. Research Activities

This proposal requests a 374-processor campus-area grid testbed to represent the core of the Rensselaer Grid. The resulting set of distributed heterogeneous computing clusters interconnected via a hierarchic network infrastructure will provide a research testbed consistent with technologies to be available in the future national cyberinfrastructure [8]. This testbed will support research on the development of grid middleware and multiscale computation technologies, and the computational needs of seven large-scale scientific and engineering research projects. By the concurrent consideration of the middleware advances needed to support scientific and engineering applications and the use of these technologies to provide grid computing for scientific and engineering applications using multiscale simulations, the Rensselaer Grid will:

- Support the advancement of technologies central to meeting the massive computational needs of critical application simulations using grid computing.
- Support the advancement of generalized multiscale computational methods that can be effectively used by others in many applications run over the national grids.
- Provide the simulation tools and computational power needed to advance several on-going research application areas.

The research projects already planning to use the requested grid testbed involve 38 faculty from 11 academic departments in the Schools of Science and Engineering. The funding for these research projects, which comes for ARO, DARPA, DOE, NIH, NSF, ONR, New York State, two National Labs and four companies, is approximately eight million dollars per year.

This proposal has received extensive support both in terms of the required cost-sharing from Rensselaer’s Vice President for Research and networking and technical support from the Chief Information Officer and his staff. This level of campus support and integration underscores how critical this grid testbed infrastructure will be to RPI’s current and future computing research programs. Rensselaer has already developed a number of independent parallel computing clusters that are providing support to research groups. The overall campus strategy is to provide the network infrastructure to link these systems into the Rensselaer Grid and to the outside grid computing capabilities via Internet II (e.g., NSF, DOE and ETF systems). The Rensselaer Grid will interconnect the three clusters requested in this proposal, a fourth planned large cluster to supported by a recently awarded grant for Quantitative and Computational Bioscience and ten smaller existing campus clusters.

Current grid middleware infrastructures, e.g., the Globus toolkit, enable the utilization of distributed, heterogeneous, and high-performance computing resources as a virtual meta-computer. While substantial progress has been made, a number of key grid computing middleware technologies need to be developed, tested and integrated into test applications to provide needed for applications operate across the grid. The information technology component of the research to be supported by the Rensselaer Grid is focused on several grid computing middleware technologies associated with distributed programming technologies, grid network simulation and security, control of data flow, dynamic load balancing and real-time applications and devices.

Multiscale systems computation is a core Rensselaer research activity that represents an enabling technology for the application of predictive simulations in the advancement of applications in biotechnology, nanotechnology and homeland security. By taking a systems-level approach to multiscale computation, Rensselaer is developing generalized modeling methods and computational algorithms that can support the linkage of fundamental science discovery to engineering processes for the virtual design of optimized material and biological systems. In addition, this research can provide the types of model reductions needed to support real-time processes for ever more complex applications such as surgical training based on realistic models of biological material deformations. The Rensselaer Grid will not only allow us to develop and validate the multiscale computation methods, but will also support the effective advancement of applications.
that require multiscale simulations.

The core of the envisioned Rensselaer Grid consists of three clusters to be housed in distant physical locations. The architecture of each cluster will be selected to optimize the needs of the primary local research community within the constraints of being able to be connected together and providing a sufficient level of computational support to meet the needs of the largest applications that will run on the grid. The goal of this approach is to provide two levels of near optimality; (i) structuring clusters to optimize local computing usage, and (ii) providing an integrated grid system that can be applied to large simulations that require resources greater than provided by a local parallel cluster. At both levels, we will leverage commodity computing and network equipment that we would expect to find at other educational and industrial research centers. Unlike the “performance at any cost” focus of a supercomputer center, we wish to examine how our multiscale parallel applications will perform in a “common case” grid computing environment. Integrated solution approaches to performance bottlenecks will be devised by both application and grid middleware researchers. By “common case”, our grid testbed architecture will use dual processor systems as the base compute node and a combination of 10 and 1 gigabit Ethernet as the physical network interface between hosts, both locally and between cluster sites.

One cluster will be managed by the Computer Science Department to support ongoing research on the development of grid computing middleware, and highly data intensive and real-time applications. The second cluster will be managed by the Scientific Computation Research Center (SCOREC) to support the development and application of adaptive multiscale simulations. The third cluster will be managed by the campus computing organization (DotCIO) to provide parallel computing capabilities to address Rensselaer’s research computing needs. The distributed nature of the Rensselaer Grid will provide an effective environment to investigate the middleware technologies needed by the diverse set of applications to be supported.

The descriptions of grid computing and multiscale computation research projects discussed in the remainder of this section include an indication of the faculty involved with abbreviated departmental designations which are defined as follows:

- BIOENG - Biomedical Engineering
- CBE - Chemical and Biological Engineering
- CEE - Civil and Environmental Engineering
- MANE - Mechanical, Aerospace and Nuclear Engng.
- DSES - Decision Sciences and Engineering
- BIO - Biology
- CS - Computer Science
- MATH - Mathematics
- MSE - Materials Science and Engng.
- PHY - Physics

The number of researchers, sponsors and collaborators for each project are also indicated.

### 1.1 Grid Computing Technologies Research

The Rensselaer Grid will implement Basic Grid Services and Core Grid Services using the NSF Middleware Initiative's software that includes the Globus Toolkit [42,43,50]. Using this common base will enable the integration of the Grid into larger grids. While the current grid services development represents an excellent starting point, there remain a number of important challenges largely unaddressed by the grid computing community. These include:

- Programming models that simplify application development by providing high-level abstractions and algorithms so programmers do not have to explicitly deal with distribution issues such as data placement and replication, load balancing, quality of service and fault-tolerance.
- Middleware infrastructures that support the aforementioned programming abstractions, profile the network, and adapt programs to dynamic grids to meet applications needs that range from real-time requirements, to massive levels of computation.

We are investigating advanced programming models and a new generation of grid computing middleware [2] to improve the programmability and flexibility of next-generation grid applications without sacrificing performance, standardization efforts, and global resource utilization.

Current research is addressing the programmability and scalability of scientific applications when moving from traditional tightly-coupled homogeneous clusters using MPI to the loosely-
coupled distributed and heterogeneous clusters connected by grids [32]. Satisfying quality-of-service requirements (e.g., real-time constraints) on grid computing environments is a challenging research goal considering current network infrastructure. In addition, most existing middleware infrastructures inherit the lack of support for real-time and QoS in most widely available operating systems. The Rensselaer Grid will concurrently support both production and experimental middleware prototypes to develop and evaluate distributed programming technology and algorithms while satisfying the computational needs of scientific applications.

We plan to work actively with the grid community so that our middleware research prototypes use and influence standards such as the Open Grid Services Architecture (OGSA) [106], and so that the software prototypes becomes an integral part of future releases of the NSF Middleware Initiative and other important open-source efforts.

1.1.1 Distributed Programming Technologies
To effectively address non-functional concerns of applications running on a grid, such as data distribution, process scheduling, fault tolerance, load balancing, security, and quality of service (including timing constraints), it is critical to provide high-level programming to developers. These programming languages must support the abstractions need to enable middleware layers to dynamically choose resource management strategies that optimize both applications throughput and resource utilization on highly dynamic, unreliable computer networks.

Rensselaer is actively researching programming models, languages, and tools for grid computing. Projects include; (1) SALSA, a programming language that provides abstractions to facilitate the development of dynamically reconfigurable distributed systems [107], (2) OverView, an Eclipse plug-in that supplies run-time visualization of Java-based dynamically reconfigurable distributed systems [54], (3) Transactors, a programming model designed to maintain a consistent distributed state over unreliable networks [34], (4) IO, a smart middleware layer that dynamically profiles the conditions of a large-scale network and decides key distributed execution issues to balance load and improve overall system throughput [26,97], (5) GSC, a grid scientific computing project that uses SALSA to tackle problems with huge distributed data sets such as Principal Component Analysis (PCA), and (6) Generic Code-Carrying Proofs (GCCP), a concept-based approach to enforcing security policies on mobile code.

The SALSA programming language has been used for over two years to introduce both undergraduate and graduate students to concurrent and distributed programming, as well as a research platform for projects such as generic distributed algorithms, distributed garbage collection, decentralized naming services, dynamic load balancing, and grid scientific computing. Open source code is available at http://www.cs.rpi.edu/wwc/salsa/.

Faculty: Varela, CS; Musser, CS; Symanski, CS; Luk, CS Researchers: 8 graduate students
Sponsors: IBM Eclipse, IBM SUR, NSF NGS, RPI Seed Funding, DARPA, ONR MURI.
Collaborators: UIUC, IBM Research, and Williams College.

1.1.2 Grid Network Simulation and Security
A major barrier to fast data access on a Grid is the high latency of communication in wide area networks. To address this difficulty, we are investigating automated techniques for scalable replica distribution and consistency algorithms that require the least possible synchronization and communication between the nodes that hold copies of the replicated objects. The replica management services being developed offer transparent data replication based on a runtime system that evaluates the access cost and performance gains of replication before moving or copying any data. Our replication cost model is formulated as an optimization problem that minimizes the total sum of data access and replica maintenance costs on a given node. This runtime system will form the basis of Proactive Replica Management Services (PRMS), and will be integrated with the Globus Toolkit [42,43,50].

The simulation framework GridNet [65,66] is built on top of the network simulator ns [77] that models the network elements: nodes, links, and packets. GridNet introduces application-level services implemented on top of the existing ns protocols and extends ns object semantics. The
results of simulations show that dynamic replication improves (by 60% on average) the overall data transfer and response times within the Data Grid.

Sharing memory, bandwidth and CPU transparently and dynamically requires a security architecture integrated with open software tools to build grid systems. Security must be provided over multiple administrative domains each with its own access and protection rules. Currently, grid system security is based on PKI and Transport layer security protocols (TLS) [50]. The PKI system with X.509 certificates [81] has management overhead for maintenance of digital certificates and has potentially scalability problem. Furthermore in heterogeneous environments where wireless and wired networks interfaced, the capabilities to support PKI and TLS in an end-to-end fashion may not be possible. We are developing a 2-tier approach to provide for security in grid computing. In this scheme each grid node is considered as a Certificate Authority (CA) and a web of trust is established among the grid-nodes. Confidentiality and authenticity between a pair of grid-nodes are ensured by encapsulating a special header similar to IPSEC tunneling [53] which is secured by asymmetric cryptographic techniques. Within a grid-node, security is ensured using a distributed version of Kerberos system [59].

Faculty: Szymanski, CS; Yener, CS
Researchers: 3 graduate students
Sponsors: IBM Almaden Research Laboratory.
Collaborators: ISI USC, IBM Almaden Research Laboratory.

1.1.3 Data Flow, Extraction and Control

The importance of understanding and making effective use of large-scale data is essential in science, engineering, and business [118]. Key research questions are how to extract information from complex data sets, how to mine the structure of the data, and how to provide guarantees on the quality of the answers. There are critical issues related to the management and retrieval of massive datasets (e.g., data access and integration in dynamic and distributed environments). Data Science is the integration of the following activities: i) data capture, ii) data generation and synthesis, iii) data analysis and evaluation, iv) data storage, indexing and retrieval, v) data exchange and sharing, vi) data visualization, vii) data quality and consistency control.

Data mining over large data sets can take a prohibitive amount of time due to the computational complexity of the algorithms. The SPIDER (Scalable, Parallel and Interactive Data mining and Exploration at Rensselaer) data mining project is developing scalable algorithms that can efficiently handle terabytes of data, and that can scale to thousands of attributes and billions of transactions [80,117]. We are developing an extensible high-performance data mining (HPDM) system built over our Data Mining Template Library. The goal is to develop a systematic solution to a whole class of data mining tasks in massive, diverse, and complex datasets, rather than to focus on a specific problem. We are developing a prototype large-scale HPDM toolkit, which is: i) extensible and modular for ease of use and customization to needs of analysts, and ii) scalable and high-performance for rapid response on massive datasets. The Extensible HPDM system will be able to seamlessly access file systems, databases, or data archives.

The Rensselaer Grid will provide an ideal environment to develop and test large-scale high-performance data mining system on terabytes of data, as well as conducting research on integration of I/O, file systems and databases. The platform will provide ideal opportunities to develop truly scalable and online data mining methods, and allow us study the different components of the mining tasks from a large-scale perspective in terms of persistent (external-memory) data structures and algorithms, to external data layout issues and efficient I/O [116,74]. The insight and experience gained in designing and implementing a general purpose high-performance data mining library, will tremendously aid research in developing more generic data mining and analysis tools that are scalable to the terabyte (or in the future petabyte) range.

Faculty: Zaki, CS; Goldberg, CS; Magdon-Ismail, CS; Adali, CS; Drineas, CS; Bennett, MATH
Researchers: 1 postdoc, 6 graduate students, 2 undergraduate
Sponsors: NSF Career, NSF, NSF ITR, DOE Career, NIH
1.1.4 Dynamic Load Balancing

The adaptive selection and control of models, methods and discretizations is central to the effective and reliable solution of multiscale problems. Large scale parallel adaptive computations over non-dedicated grid clusters is complicated by the regular changes in both the distribution of computational load and the availability of distributed computational resources. Critical bottlenecks will form and parallel speed-up will be lost without dynamic control of the distribution of computations and data over constantly monitored grid processors. Therefore, grid-based dynamic load balancing is central to the success of adaptive multiscale computation.

Rensselaer researchers have been leaders in the development of parallel adaptive continuum methods employing dynamic load balancing. This includes structures to house a distributed mesh [10,101], and a distributed octree [40,41]. These structures have been combined with dynamic load balancing to support parallel adaptive analysis [40,41,85] and parallel mesh generation [23,24,25] and are currently being extended to support parallel adaptive multiscale simulations.

Our current research is focused on dealing with heterogeneity resulting from different hardware capabilities and non-dedicated usage of the machines executing the computation [33]. The added complexity and constraints introduced into load balancing optimization mandates techniques to dynamically measure machine capabilities and utilization. The Dynamic Resource Utilization Model (DRUM) is being constructed building on grid technologies such as MPICH-G2 [58] and Globus to (i) automatically determine and encapsulate the details of the execution environment, (ii) provide facilities for dynamic and minimally-intrusive monitoring the environment and (iii) provide a tree structure for the execution of hierarchical partitioning [101,102].

SCOREC faculty are members of the Terascale Tools and Techniques Center (TSTT) [103] supported through the DOE SciDAC program. TSTT is developing interoperable mesh and discretization technologies to be made available in open source form. As part of this effort the Algorithm Oriented Mesh Data structure [83] and its parallel version [84] have been made available on the web (http://www.scorec.rpi.edu/AOMD/). Dynamic load balancing is supported by the Zoltan dynamic load balancing library [27,28] from Sandia National Laboratories.

Faculty: Flaherty, CS; Jansen, MANE; Shephard, MANE; Symanski, CS; Varela, CS

Researchers: 1 postdoc, 5 graduate students, 1 undergraduate

Sponsors: DOE SCIDAC program, ARO, Sandia Nat. Labs., Simmetrix Inc.

Collaborators: Sandia National Laboratories and Williams College.

1.1.5 Support of Real Time Applications and Devices

The fundamental property necessary for any real-time system is execution time predictability. Most existing grid middleware infrastructures (e.g., Globus[42]) inherit the lack of support for predictable, real-time execution in most widely available operating systems. While dedicated networks of mostly homogeneous computers running real-time operating systems can provide a good starting point for supporting hard-real-time applications, we will initially target only applications which have soft-real-time constraints on controlled (dedicated) grid environments, such as (a subset of) the Rensselaer Grid.

A haptic device, which provides force feedback to the user while s/he controls a real or virtual remote device (e.g., a robot working in a garden or a virtual surgical tool) requires hard-real-time support (a new signal every millisecond) when controlled in the most straight forward way. However, with good dead reckoning the device can operate in a user-friendly manner with control signal updates every 10-100 msec. This real-time constraint can be satisfied by reserving dedicated grid computing resources ahead of time. An alternative is to profile the use and availability of grid resources to make accurate forecasts of end-to-end performance. The former strategy requires real-time support from the hardware and operating systems, while the latter strategy can be modeled with existing middleware, such as the Network Weather Service [111]. An alternative strategy that will also be explored on the Grid is to build device controllers that are synchronized by events rather than by time [31]. For example, the surgical tool driven by the haptic device will stop moving downward when the force sensor value exceeds a given thresh-
old. All three strategies can be applied to a wide variety of real-time applications. The proposed Rensselaer Grid will afford us the opportunity to leverage current research on robotics and haptic devices for virtual surgical planning and assembly planning. Integrating this into the Grid will facilitate its transformation from a purely computational grid into a next-generation cyberinfrastructure such as those envisioned by the National Science Foundation.

**Faculty:** Carothers, CS; Stewart, CS; Trinkle, CS; Varela, CS  
**Researchers:** 2 graduate students, 2 undergraduates  
**Sponsors:** RPI Seed Funding.

### 1.2 Multiscale Systems Computation Applications

Fundamental advances in physical and biological sciences have made it possible to understand spatial and temporal phenomena on the atomic, molecular, microscopic, and macroscopic scales. The ability to translate these advances into new products and industries requires a transformation in the methodologies of modeling, simulation, and design. Interactions at all scales affect the ultimate behavior of the complete system, practitioners must model and design across this range of scales (Figure 1 shows three such applications considered below). While many physical and biological principles are specific to their domains, the challenge of representation across scales, automatic synthesis of reliable simulations, optimization of design decisions, propagation of uncertainty across scales, and validation of multiscale methods are core issues that map across applications, and can best be addressed by a systems approach to design across scales that we refer to as multiscale systems design.

A major component of reaching the goal of multiscale systems design is providing the computational environments and tools needed to support the development and application of this new approach to engineering. In our interactions with industry, we have found that many groups within corporations are developing cost effective parallel computer clusters and other distributed processing capabilities. However, these corporations have clearly indicated they do not want to invest in extremely large centralized parallel computing systems. Thus, the only effective means for them to meet the computational requirements of multiscale systems design is through the application of grid computing technologies in which the distributed computing capabilities of the corporation are put to effective use around the clock. The ability to enable the needed levels of grid computing requires the grid enabling technologies discussed in Section 1.1 to be developed and used in the development of grid enabled applications. This section describes a set of applications currently under development at Rensselaer that will be grid enabled.

#### 1.2.1 Interoperable Adaptive Multiscale Computation Tools

To be effective, multiscale techniques must locally apply the largest scale models that can provide the requested level of accuracy and link information between interacting scales. Since there are few situations where *a priori* specification of the appropriate scales throughout the space/time domain is possible, adaptive techniques based on *a-posteriori* measurements are being developed. Adaptive methods complicate parallel processing for these massive calculations due to the changing computational loads. The adaptive multiscale simulation procedures being developed at Rensselaer address automatic construction of interacting models, effective parallel computation, fast algorithms, extendable multiscale simulation software, and the interoperability

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**Figure 1. Example multiscale applications.**
with different meshing and discretization technologies. At the fine scales, fully discrete models are used. To support adaptive discrete methods and irregular placement hierarchic trees [89] are under investigation. At larger scales discretized continuum models are employed. To support these discretizations SCOREC has developed automatic adaptive meshing techniques [23,24,29,44,63,70,71,85,86,90,91]. Continuum scales linking [12,109] is available and discrete-to-continuum methods are under development [13,18]. The efficient solution of the systems associated with a multiscale simulation requires use of methods with optimal computational growth rates. New explicit time marching methods are under development that effectively remove high frequency components from the solutions [3,30,35]. A key to the definition of optimal multilevel methods is to separate frequency ranges and operators to communicate between levels. Such procedures have been developed and demonstrated for continuum-continuum multiscale simulations [36]. Efforts to extend them to include linkage with discrete simulations are under consideration [13,18].

To facilitate the development of new adaptive multiscale analyses an object-oriented framework based on careful decomposition of the geometry, physics, mathematical model, discretization and numerical methods has been developed [11]. Discretization techniques implemented to date including mixed finite elements, stabilized finite elements [64], partition of unity methods [63,72], discontinuous Galerkin methods [85]. Atomic level simulation based on discrete model representations have also been integrated into the system [13,18].

Faculty: Anderson, MANE; De, MANE; Fish, CEE; Flaherty, CS; Jansen, MANE; Kumar, CBE; Picu, MANE; Shephard, MANE

Researchers: 4 postdoc, 8 graduate students, 3 undergraduates


Collaborators: Argonne, Sandia, Los Alamos and Lawrence Livermore National Labs, Stanford

1.2.2 Multiscale Methods for Biomolecular Structure, Function and Assembly

The goal is to quantitatively model aspects of biomolecular structure and interactions critical to function. Quantitative modeling of biological systems involves a spectrum of lengthscales from atomic to microscopic, and timescales from picoseconds to minutes and hour, thus presenting challenges and opportunities for development of multi-scale methods. Our research explorations have taken three directions: (i) Understanding of Self-assembly: Biological self-assembly is driven by water-mediated interactions (e.g., hydrophobic interactions). We are quantifying and developing molecular level models of the role of water structure in mediating interactions of biosystems constituents (e.g., references [82,46,14,49,47,48,57,52]). A coarse-grained approach based on this knowledge will significantly speed-up biomolecular simulations. (ii) Quantum/Classical Scale-linking: We are developing approaches to combine quantum mechanical and classical (molecular dynamics) modeling to understand autocatalytic splicing reaction in a class of proteins called inteins. In combination with molecular biology experimentation, these calculations will lead to faster cleaving inteins that will be employed in affinity based one-step bioseparation process [114,112,113]. In addition, the hybrid QM/MD method is being applied to modeling enzymatic reaction of serine protease Subtilisin Carlsberg in organic media, which will be helpful in the development of functional biomaterials. (iii) Modeling of enzymes in non-biological contexts: We are performing large-scale molecular dynamics simulations of enzymes in a variety of non-biological contexts (e.g., organic media, solid salt matrices) to understand the key determinants of the nanoenvironment of the enzyme that are critical for maintenance of its function. This effort is aimed ultimately at the development of functional biomaterials [115].

The modeling approaches described above are computationally intensive and require input from researchers that may be distributed geographically. We have already adopted and implemented algorithms (such as replica exchange algorithm) that use several tens of computer processors to perform MD simulations of biological systems. A combination of molecular dynamics and Monte-Carlo analysis allows biosystems to overcome large barriers leading to excellent confor-
mational sampling. The replica exchange (or parallel tempering) currently takes advantage of a single Linux cluster environment. However, the number of processors present on a single cluster currently limits the application of this algorithm. We plan to employ the grid technologies discussed above to help effectively execute our calculations over the Rensselaer Grid gird that will include the clusters requested here in combination with our existing five distributed clusters that have a total of over 200 processors (the bio- and nano-technology clusters).

**Faculty:** Belfort, CBE; Bystroff, BIO; Dordick, CBE; Garde, CBE; Kumar, CBE; Nayak, PHY

**Researchers:** 4 postdoc, 6 graduate students, 2 undergraduates

**Sponsors:** NSF Nanotechnology Center, NSF NIRT, NSF CAREER, NSF ITR, NIH

**Collaborators:** NYS Wadsworth Labs., NIH NIDDK, Los Alamos Nat. Lab.

### 1.2.3 Soft Tissue Simulation and Virtual Surgery

The principal goal is to develop computer-based training tools for minimally invasive surgical procedures involving real-time force-feedback and visualization in which the trainee will see, touch, and manipulate 3D tissues and organs programmed into the system. A major complexity is the real time computation of the soft tissue deformations and reaction forces. An update rate of 1kHz is typically required for the haptic interface to deliver a stable smooth sense of touch [88].

A unified technique of rendering volumetric objects using points and solving the partial differential equations governing the interactions between surgical tools and soft tissues [9,19,20,21,22,60,61,62] is under development. In vivo determination of soft tissue mechanistic properties poses a formidable challenge and a mathematical and computational method is being developed which uses an ultrasound imaging system and interior displacement data [56,75,79,87,98] for a single low frequency pulse as it travels through the imaging domain.

Using recently developed hybrid and multiresolution algorithms [61,62] it is possible to simulate a few thousand particles in real time (with force extrapolation) on single processor machines. However, for realistic calculations of complex organs obtained from the Visible Human Project [1], a global discretization on the order of a million particles with no extrapolation is needed. Parallel versions of the numerical procedures will be constructed to determine how fast the required level of calculations can be executed. For soft tissue property estimation, a three-dimensional inverse problem must be solved involving a large amount of data (the ultrasound imaging system provides 6,000 frames/second) and unknowns. For the imaging technology to be competitive, the problem must be solved in real time.

The discretization of the organ models by computational particles is achieved using an octree-based technique [72]. Complex organ models will require parallel adaptive computations building on the tools discussed in Section 1.1.4.

**Faculty:** De, MANE; Maniatty, MANE; McLaughlin, MATH; Jeff Trinkle, CS; Xu, MANE

**Researchers:** 2 postdoc, 9 graduate students, 3 undergraduates

**Sponsors:** NSF FRG, NSF DMS, NIH, Electric Power Research Institute, NIH NLM

**Collaborators:** MIT, Harvard, Albany Medical College, ESPCI

### 1.2.4 Simulation-Based Medical Planning for Cardiovascular Disease

The current paradigm for interventional and surgery planning for the treatment of congenital and acquired cardiovascular disease relies exclusively on diagnostic imaging data to define the present state of the patient, empirical data to evaluate the efficacy of prior treatments for similar patients, and the judgment of the surgeon to decide on a preferred treatment. The individual variability and inherent complexity of human biological systems is such that diagnostic imaging and empirical data alone are insufficient to predict the outcome of a given treatment for an individual patient. We are developing a new paradigm [100,99] of predictive medicine in which the physician utilizes computational tools to construct and evaluate a combined anatomic/physiologic model to predict differential changes in blood flow for alternative treatment plans for an individual patient. The predictive medicine paradigm can be realized in Simulation-Based Medical Planning Problem Solving Environments. These environments will provide an integrated set
of image segmentation, geometric solid modeling, automatic finite element mesh generation [90], computational multiscale mechanics [55,110] and scientific visualization tools accessible through an intuitive human-computer interface.

Grid computing is necessary for this project to have an impact on surgical planning. It is doubtful that every hospital that carries out vascular surgery will have the computational resources for virtual surgical planning in the near future. The grid presents a pooled resource that could be made available to hospitals to enable the necessary detailed computations. Furthermore, we are proposing comparing several virtual surgical plans. Each of these distinct plans could be carried out virtually on non-overlapping resources of the grid, further accelerating the surgical planning. The computational needs at various stages are intense and varied making grid computing a natural choice. The most intense stage (the flow solution) has already been proven to scale well on parallel computers. Maintaining this capacity while integrating error estimation and more automated adaptivity (while staying faithful to extremely complex geometric models) is a challenge.

Faculty: Jansen, MANE; Shephard, MANE; Spilker BIOENG
Researchers: 2 postdoc, 4 graduate students, 2 undergraduates
Sponsors: NSF ITR, NSF CAREER Collaborators: Stanford, University of Texas

1.2.5 Multifunction Polymeric Nanocomposites

Nanofilled polymers result in materials with unique combinations of tunable properties not achievable with traditional composites including the opportunity to create transparent coatings that are scratch resistant, anti-static, UV filtering, antifouling, etc. [69]. Such properties would be useful for contact lenses, windshields and finishes [6,7,15,108], in optical data storage [69], etc. The ultimate goal is to determine optimal material composition, processing conditions, and process control strategy to achieve a prescribed functionality without entering the laboratory.

To achieve this, computationally intensive multiscale modeling is necessary. The high surface area ratio of nanofillers and large size of polymeric molecules means the entire volume is influenced by interface properties. Atomic scale and coarse grained discrete simulations are needed to model the interaction of the polymer-chains and the nano-particles. These models will provide the molecular scale structure, and the dynamic and transport properties. This requires modeling the polymer entanglement [94]. At the material (micron) scale, filler dispersion and distribution influence the macroscopic behavior. Process modeling of the melt at this scale is needed to understand the effect of particle size and shape on the rheology of the melt and to model the clustering behavior of the nano-particles. Macroscale continuum models driven by finer scale information and interaction needed to predict overall performance must be developed. Adaptive model error control will be necessary to guide the multi-scale analysis is required. Homogenization [37,38] and stochastic methods [45] will be used in addressing these issues.

Several of the individual component simulations indicated above can only be addressed effectively with parallel implementations. The ability to combine these simulation technologies to support adaptive modeling processes dramatically increases the total level of computation needed and requires the effective control of heterogeneous parallel computing components, which when run over a set of grid clusters, need to take advantage of the heterogeneous nature of the grid to place the right classes of calculation on the right systems (e.g., Monte Carlo based molecular simulations on processors with slow interprocessor communications while adaptive mesh-based finite elements on a parallel cluster with fast interprocessor communications.)

Faculty: Fish, CEE; Jansen, MANE; Keblinski, MSE; Kumar, CBE; Maniatty, MANE; Millard, ECSE; Nayak, PHY; Ozisik, MSE; Picu, MANE; Shephard, MANE; Wen, ECSE
Researchers: 2 postdoc, 8 graduate students, 3 undergraduates
Sponsors: NSF Group Grant, P&G, ONR, NY State
Collaborators: Howard University, Princeton University

1.2.6 Planning Dynamic Contact Tasks with Application to Disaster Recovery

We are actively engaged in research on mathematical and computational methods for multibody
contact problems (e.g., [92,95,104,105]), with particular interest in both automatic and human-aided planning. An example contact problem of great interest is the rescue of survivors trapped in a rubble pile resulting from a building collapse. The objective is to determine which chunks of rubble can be removed to create a stable survivor extraction corridor while maintaining the stability of life-sustaining cavities. Planning uses a mathematical model of the pile for motion prediction combined with search algorithms in a high-dimensional state space. This approach requires the solution of contact problems that are mathematically nonsmooth (due to stick-slip behavior and complex deformation mechanics) and therefore difficult to solve. However, given information about structural elements of the pile and approximate geometric and physical, one can formulate a dynamic model as a complementarity problem [17], suitable for stability analysis and the prediction of pile motion if it destabilizes [4,5,78,93,96]). Material removal and survivor extraction plans can then be determined using model-based computation of the reachable pile states using LaValle's RRT (Rapidly-exploring Random Trees) method [67,68].

To obtain plans under time constraints, models and search strategies of varying resolution are employed for analysis and planning. For purely automatic planning, when the pile is large, hundreds of thousands of simulation steps will have to be taken to construct a sufficient number of RRTs such that a robust extraction plan can be found, and each step can require up to several hours on a modern CPU. Fortunately, each RRT and each arc within each RRT can be computed independently. For user-aided planning, a first-responder with good intuition could significantly speed the process by testing hypotheses on a virtual pile. A haptic device can be used to "grab" and remove virtual pieces of rubble much as a crane would in a real situation. The challenge with a haptic device in the loop is that they typically require a controller set-point update every millisecond (although this can be extended to 10-100 ms with good dead-reckoning). Haptic interaction is possible today only for overly simplified rubble piles with ten to fifteen chunks. Virtual interaction with large rubble piles could be feasible on a grid after the exploitation certain structural properties of the complementarity problem.

Increasing the number of compute nodes at RPI will allow us to automatically plan extraction plans for more complex piles, but the exponential complexity of the search problem will be a limiting factor. On the other hand, increasing the number of nodes and connecting them with the multi-gigabit network links as requested in this proposal will allow us to explore fundamental questions that will arise in many real-time grid applications, while extending the size of the survivor extraction problem we can solve by supporting haptic interaction with a virtual pile.

**Faculty:** Anderson, MANE; De, MANE; Pang, MATH; Trinkle, CS

**Researchers:** 6 graduate students  
**Sponsors:** NSF Math., RPI faculty start-up  
**Collaborators:** Univ. Pennsylvania, Univ. Iowa, Univ. Maryland (Baltimore County)

### 1.2.7 Evolution of Social Groups in Communication Networks

The objective of this research is to provide new scientific methodologies for the analysis of social groups. A comprehensive set of models, encompassed by a unified framework, is being developed to study the evolution of social groups. This framework provides tools that could be used for the identification, detection, and explanation of behaviors of social groups over time. Important applications of our models are to the identification of (abberant) groups that camouflage their functioning in a large communication network such as the Internet, and to the prediction of how the communication needs of a society will evolve with time so as to more effectively allocate communication infrastructure. In our approach, societal evolution is governed by a set of parameters that are to be learned, or reverse engineered from the observed evolution [51,73]. The knowledge of these parameters is the basis for the analysis of the evolution of social groups including prediction of future behavior [16].

Reversed engineering requires optimizing a function that computes the probability of observing a given societies evolution, which takes time that is a quadratic function depending on the number of nodes (actors) and the number of active groups. Currently, we can simulate societies with up to 10,000 actors in a matter of hours. The reverse engineering portion of this simulation takes several days even for societies with several hundred actors. Our algorithms are highly paralleliz-
able, since the probability can be broken into a sum of independent terms that could be computed on different machines. The access to clusters of computers will allow us to analyze realistic-sized societies, with millions of actors and thousands of groups. The Rensselaer Grid will make it practical to apply the analytical tool-box to predict the behavior of evolving groups and to discover new communities in large societies.

**Faculty:** Goldberg, CS; Krishnamoorthy, CS; Magdon-Ismail, CS; Wallace, DSES; Yener, CS

**Researchers:** 6 graduate students  
**Sponsors:** NSF ITR, NSF Math

2. Description of the Rensselaer Grid

This proposal requests three grid clusters with a total of 374 processors. The clusters are the Information Technology Cluster, the Multiscale Computation Cluster and the Multi-purpose Applications Cluster. The equipment requested for each cluster includes a set of gigabit interconnected dual processing nodes, and a gigabit ethernet switch. Multi-terabyte storage systems are requested for two of clusters (the third will use existing storage systems). The three clusters will be connected via dedicated 10Gbit links. Table 1 gives more information on the clusters including summary prices. (Detailed cost information and quotes are included in the supplementary documents). The cost of the requested equipment is $998,278. The current cluster configuration presented should be considered only representative systems based on current quotes. If this proposal is funded we will rebid each cluster accounting for two important factors. The first is that there are likely to be improvements in the price/performance ratio by the time of the award. The second is based on past experience which indicates that once an award is given the ability to negotiate with vendors for greater discounts is substantially increased.

**Table 1. Proposed Rensselaer Grid Components.**

<table>
<thead>
<tr>
<th>Cluster</th>
<th>Item</th>
<th>Description</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Information Technology</td>
<td>Cluster Nodes</td>
<td>One Apple Xserver G5 head node with dual PowerPC G5 2GHz processors, 8GB memory, 80GB disk and dual Gigabit ethernet. 41 Apple Xserve G5 nodes, each dual PowerPC G5 2GHz processors, 8GB memory, 60GB disk storage and dual Gigabit ethernet.</td>
<td>$256,334</td>
</tr>
<tr>
<td></td>
<td>Network Switch</td>
<td>Cisco Catalyst 6506 with Supervisor 720, four 10Gigabit ethernet ports, 96 10/100/1000 ethernet ports, redundant power supplies.</td>
<td>$61,737</td>
</tr>
<tr>
<td></td>
<td>Disk Storage</td>
<td>Two Apple Xserve RAID, each with 2.75TB of disk storage, 1GB of battery-backed cache and dual 2Gbps fibre channel connections.</td>
<td>$17,698</td>
</tr>
<tr>
<td>Multiscale Computation</td>
<td>Cluster Nodes</td>
<td>One Microway Navion-N head node, with dual Opteron 2GHz, 4GB memory, 152GB disk storage, dual Gigabit ethernet. 64 Microway Navion-A nodes, each with dual Opteron 2GHz, 3GB memory, 80GB disk storage, dual Gigabit ethernet.</td>
<td>$241,892</td>
</tr>
<tr>
<td></td>
<td>Network Switch</td>
<td>Cisco Catalyst 6506 with Supervisor 720, four 10Gigabit ethernet ports, 96 10/100/1000 ethernet ports, redundant power supplies.</td>
<td>$61,737</td>
</tr>
<tr>
<td></td>
<td>Disk Storage</td>
<td>One Nexsan ATABeast RAID array with 7TB of storage, 512 MB of battery-backed cache and 2Gbps fibre channel host connection.</td>
<td>$27,500</td>
</tr>
<tr>
<td>Multi-Purpose</td>
<td>Cluster Nodes</td>
<td>One Microway Navion-N head node, with dual Opteron 2GHz, 4GB memory, 152GB disk storage, dual Gigabit ethernet. 80+ Microway Navion-A nodes, each with dual Opteron 2GHz, 2GB memory, 80GB disk storage, dual Gigabit ethernet.</td>
<td>$267,123</td>
</tr>
<tr>
<td></td>
<td>Network Switch</td>
<td>Cisco Catalyst 6506 with Supervisor 720, four 10Gigabit ethernet ports, 96 10/100/1000 ethernet ports, redundant power supplies.</td>
<td>$64,257</td>
</tr>
</tbody>
</table>

The requested clusters will be integrated with existing and planned clusters through the campus network to form the Rensselaer Grid for research computing. Table 2 summarizes the existing campus clusters that are focused on research in information technology, multiscale computations, biotechnology and nanotechnology. In addition, Rensselaer has recently been awarded a
grant for Quantitative and Computational Bioscience that includes the purchase of the projected cluster summarized in Table 3.

Table 2. Existing Clusters

<table>
<thead>
<tr>
<th>Num. Processors</th>
<th>Num. Nodes</th>
<th>Node Type</th>
<th>Node Memory</th>
<th>Node Interconnect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Information Technology</td>
<td>128</td>
<td>Dual 2.4 GHz Xeon</td>
<td>1.5GB</td>
<td>100 Mbit</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>800 MHz xSeries</td>
<td>2.0GB</td>
<td>Myrnet 2000</td>
</tr>
<tr>
<td>Multiscale Computation</td>
<td>66</td>
<td>Dual2.0 GHz Xeon</td>
<td>2.0GB</td>
<td>Myrnet 2000</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>400 MHz Nextra-XI</td>
<td>640MB</td>
<td>100 Mbit</td>
</tr>
<tr>
<td>Biotechnology</td>
<td>48</td>
<td>Dual 1.2 GHz Pentium 3</td>
<td>1GB</td>
<td>10/100 Mbit</td>
</tr>
<tr>
<td></td>
<td>72</td>
<td>Dual 1.0 GHz Pentium 3</td>
<td>1GB</td>
<td>100 Mbit</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>550 to 750 MHz Pentium 3</td>
<td>256 MB</td>
<td>10/100 Mbit</td>
</tr>
<tr>
<td>Nanotechnology</td>
<td>64</td>
<td>Dual 2.2 GHz AMD Athlon</td>
<td>512 MB</td>
<td>1 Gbit</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>Dual 2.26 GHz Pentium 4</td>
<td>1 GB</td>
<td>100 Mbit</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>800 MHz to 1 GHz Pentium 3</td>
<td>512 MB</td>
<td>10/100 Mbit</td>
</tr>
</tbody>
</table>

Table 3. Planned Quantitative and Computational Bioscience Cluster

<table>
<thead>
<tr>
<th>Item</th>
<th>Description</th>
</tr>
</thead>
</table>
| Cluster Nodes      | Microway Navion-T dual Opteron 2GHz, 4GB memory, 2x146GB disk storage, dual gigabit ethernet, QLogic fibre channel 2Gbps host bus adapter.  
|                    | 80 Microway Navion-A dual Opteron 2GHz, 4GB memory, 80GB disk, dual gigabit ethernet.                                                                 |
| Network Switch     | Cisco Catalyst 6506 with supervisor 720, four 10Gig ethernet ports, one 10Gig ethernet optical module, long reach, 144 copper gigabit ethernet ports, one free slot for expandability. |
| Disk Storage       | Two Nexsan ATABeast RAID arrays, each with 7TB storage, 512 MB of battery-backed cache and 2Gbps fibre channel host connection                   |

Figure 2 shows the Rensselaer Grid and indicates how it will be linked through the campus network. The requested Rensselaer Grid clusters and the planned Quantitative and Computational Bioscience Cluster will be connected over dedicated 10 Gigabit Links. The existing Information Technology and Multiscale Computation clusters will be linked by a dedicated Gbit connections. The existing biotechnology and nanotechnologies clusters will be connected over the campus backbone that consists of a set of shared Gbit lines. The campus backbone also provides a 155Mbit link to Internet II.

![Proposed Equipment](image_url)

Figure 2. The Rensselaer Grid.
The heterogeneous nature of the Rensselaer Grid is critical to Rensselaer’s research on grid computing middleware. Although small test facilities can provide important information to guide initial efforts, it is only through operation on full scale systems running real applications that the type of information needed to properly guide such research can be collected. In the majority of situations, it is only this type of experimentation that will lead to the development of the best concepts and resulting technologies.

The importance of the computational power of the Rensselaer Grid to the multiscale system applications can be demonstrated considering any of the application areas. We give two brief examples here. Simulating the hydrodynamics of the collapse and rebound of a single 10 micron bubble in water required a mesh with over 3M elements and 6000 time steps. This simulation took 48 hours on 32 2GHz P4 processors. Since this finite element code used has excellent scalability, this same simulation could be run in approximately seven hours on the largest of the three requested clusters (accounting for a 1.5 speed increase and the increased number of processors). Since this simulation resolved only a single bubble and multiple bubble sonoluminescence is of great interest, the desired next set of simulations will start with at least one order of magnitude larger system. These simulations would then be back up to 3 days on the largest cluster.

Distributing these calculations (which do require substantial, but carefully optimized, interprocessor communication) over the clusters connected by the dedicated 10 Gbit should decrease the required times with essentially no loss in parallel efficiency. Employing additional clusters with dedicated Gbit connections should show small degradation, while the effectiveness of distributing to those over the shared campus Gbit backbone will be measured and optimized.

The second example involves multiscale quantum/molecular mechanics simulation of the interactions of biological molecules with carbon nanotubes. In these simulations 50 to 150 atoms are modeled at the quantum level and 1000 to 8000 at the molecular level. The current code being used has acceptable scaling to 32 processors. A single run, which requires 30 to 60 optimization steps, takes two hours on 32 processors. However, a proper study for a single biological molecule will require 600 such runs or 12.5 days. Using the capabilities of the Rensselaer Grid this time can be effectively reduced by distributing these simulation over the clusters taking-up available computing cycles. Such capabilities will allow the effective consideration of more biological molecules.

3. Impact of the Rensselaer Grid

Rensselaer is following a comprehensive strategic plan that has identified focal areas for investment and growth within Information Technology, Biotechnology, Nanotechnology and Homeland Security. Rensselaer’s plan has a specific focus on interdisciplinary research programs within those areas. Information Technology research is focused on technologies needed for the cyberinfrastructure with grid computing middleware as a central component. The development of multiscale systems technologies to provide the modeling and simulation technologies needed in biotechnology, nanotechnology and homeland security is a campus core research area. Rensselaer’s ability to advance cyberinfrastructure research and multiscale systems simulations applied to critical applications is supported by institutional commitments to focused faculty hiring, program development, and the creation of new resources and infrastructure. The Rensselaer Grid represents a unique opportunity to bring together science and engineering applications research with computer science in a synergistic research environment.

Rensselaer’s information technology research is focused in the Department of Computer Science, the Department of Electrical and Computer Engineering and in the Center for Pervasive Computing and Networking. The impact of the Rensselaer Grid on these programs is to enable the evaluation of new middleware infrastructures for grid computing and to study the feasibility of supporting multiscale scientific applications over distributed heterogeneous and dynamic environments. The Grid will enable evaluation of heterogeneous computer architectures, with different processor power, memory and interconnect capacities, and linked though both dedicated and shared network infrastructures. Separate administrative domains will also help us model realistic security and shared resource policies in larger grids. New middleware and algo-
gorithms to deal with heterogeneity, distribution, security, multiple scales, and resource administration issues will facilitate application migration into larger national and international grids of the cyberinfrastructure, ultimately enabling scientific discoveries not possible otherwise. The Scientific Computation Research Center provides expertise in multiscale theory, modeling and computation. The Nanotechnology Center and National Science Foundation Center for Directed Assembly of Nanostructures supports major nanotechnology research programs with an emphasis on bio-systems. The Center for Integrated Electronics at RPI has a well-established clean room facility for micro and nanoelectronics, and the New York State Center for Advanced Technology and the Center for Polymer Synthesis provide supporting capabilities in polymer and nanocomposite synthesis and micromanipulation and micromanufacturing. Rensselaer is constructing a new building and forming the Biotechnology and Interdisciplinary Studies Research Center that will include facilities dedicated to biotechnology and nanotechnology, and related biochip and nanoelectronics research. In addition, Rensselaer has announced the search and recruitment of six sets of one senior and two junior chaired faculty to head new research programs in information technology and biotechnology. The Rensselaer Grid will provide a critical core resource to enhance Rensselaer research in support of our strategic research thrusts. It is well recognized that computation has joined the classic pillars of observation, experimentation and theory to form the four pillars of modern scientific investigation. The importance of the computation pillar is clear for many critical applications where the multiple scales of behavior of importance do not allow the direct application of observation and experimentation to define and validate all the needed theoretical models. This is why one of Rensselaer’s information technology research constellations is focused on the development of the effective multiscale computation methods that promise to provide the technologies and tools required to link information between scales as needed to increase understanding of many critical areas of scientific investigation. There are 38 Rensselaer faculty (8 of them current NSF CAREER award recipients) from 11 academic departments in Science and Engineering involved with the projects already planning to use the Rensselaer Grid. There are 16 post doctoral associates, 71 graduate students and 18 undergraduate students working on those projects. These research projects are supported by scores of grants from 7 federal agencies, NY state, and 6 companies/foundations. These projects include collaborations with 13 universities, 6 national laboratories, and a state agency. Rensselaer has a strong pro-active program for the recruitment and retention of women, members of underrepresented minority groups, and individuals with disabilities at both the faculty and student level. As part of its strategic plan 50% of all new faculty hires will be from underrepresented groups. The Rensselaer Office of Minority Affairs, established in 1979, has taken a leadership role in recruitment and provision of support for academic, social, and cultural needs of minority groups. With 10 active programs, Rensselaer’s cultural diversity has improved over the last decade as shown by increased representation of African Americans, Latin Americans, Asian Americans and native Americans by 7% to 12%. Gender diversity also improved by 40%. Retention rates for minorities have improved dramatically over the last decade to now nearly equaling the 91% of male students (retention rates for females are higher at about 95%). Graduate programs addressing the needs of minority students include the Collegiate Science and Technology program (C-STEP), Patricia Roberts Harris Fellowship Program, National Consortium for Graduate Degrees for Minorities in Engineering (GEM Fellowship Program), GE Summer Bridge Program for Minority Graduates, and the OMSA Graduate School Seminars on Graduate Opportunities. Success at improving graduate student diversity through these programs is shown by 30% to 100% increases in representation by category over the past decade. These programs will continue to be refined and expanded under the direction of Rensselaer’s recently hired Vice-Provost for Diversity. The 71 graduate and 18 undergraduate students working on the projects already planned for the Rensselaer Grid will develop and/or apply software on the requested grid clusters thus making the Grid an integral part of their education. The grid will also have a substantial influence on the education of a wide number of students through its impact on graduate and upper level under-
graduate courses. Several of the growing course offerings on cyberinfrastructure will take advantage of the Rensselaer Grid. In many cases, the methods developed through this research and data obtained from studies performed will be used. In specific courses relating to grid computing, parallel processing and networking students will be involved with course projects that use the Grid and tie directly to the research projects. The first course on multiscale systems computation is being given this semester, the second is planned for the fall and more are under development. These courses will take advantage of the Grid to support course projects. Courses focused on the applications areas will employ results obtained from simulations performed on the Grid. An increasing number of undergraduate research projects will be linked to the research programs using the Rensselaer Grid. Results produced on the Grid will also contribute to outreach programs for students at all levels. For example, some faculty involved with applications projects are already partnering with the Junior Museum in Troy, NY to develop modules that are part of the Molecularium visual education demonstrations. In addition to teaching children about the wonders on the molecular world, we can include information showing how the molecular world links to their world and to let them know that massive simulations run on grids of parallel computers are needed to analyze these interactions.

4. Project and Management Plans
The project principal investigators will be responsible for the construction and operation of the Rensselaer Grid. Trinkle (Chairman of Computer Science) and Shephard (Director of SCOREC) will be responsible for the administration of the project. Carothers and Varela will coordinate the grid computing technologies research, and Shephard and Garde will coordinate multiscale systems computation applications. All the principal investigators will be involved with interactions between the grid computing technologies and applications research activities to ensure the greatest possible synergy.

The principal investigators will coordinate with the Rensselaer Research Computing Committee (RRCC) that will be charged with defining overall directions, operational structures, and long-term planning for Rensselaer’s research computing capabilities. The RRCC will be headed by the Vice President for Research (Arthur Sanderson) and the Chief Information Officer (John Kolb). It will include faculty members (including at least two of the PI’s from this project) and key computing professionals from the Division of the Chief Information Officer (DotCIO) and computing intensive departments and research groups.

The RRCC will be responsible for defining the campus level mechanisms for structuring cluster interactions and for allocating and monitoring the usage of the Rensselaer Grid. The structures defined to control the interactions of the clusters will be designed to protect the stability and usefulness of the entire cluster while supporting the needs of the research programs responsible for that cluster. Access to the machines will be based on a two level process. The top level is defined at the level of individual grid clusters where allocation processes will be developed depending on the needs of the sponsors supporting the research performed on those clusters. These policies will be reviewed by the RRCC and depending on sources of funding for the cluster and its continued support, some percentage of that cluster will be made available to the campus community using dynamic allocation methods. A simple proposal process open to the campus community will be used to allocate the resources to the general campus level clusters.

The Rensselaer Grid will be installed, operated and maintained by technical support staff from DotCIO, Computer Science and SCOREC. Technical, systems level software and specific research software libraries will also be supported.

The computing hardware purchased will be put under maintenance for from two to three years at the time of purchase. All core equipment, which includes servers, primary disk systems, network controllers and front nodes will be kept under continuous hardware maintenance. Decisions on the continued hardware maintenance of cluster processors and secondary disk storage will be based on a risk analysis comparing vendor maintenance to self-maintenance.
5. References


[77] ns network simulator; http://www-mash.cs.berkeley.edu/ns


