Project Description

1.1. Instrument Location & Type

Instrument Location: Ron & Linda Yanke Family Research Park, Room 300, Boise State University
Instrument Code: MRI-31

The Office of Sponsored Programs, and the Office of Information Technology at Boise State University (BSU) have committed to house the requested instrument, a 32-node GPU/CPU cluster with a storage array and a 5×8 foot tiled display in a visualization theater setting. They will maintain power and cooling.

1.2. Research Activities

The proposed instrument integrates high performance computing (HPC), large-scale visualization and parallel file storage technologies in a single platform. The intended primary users are PI from five different departments—Mechanical & Biomedical Engineering, Biological Sciences, Geosciences, Computer Science, and Materials Science & Engineering. They and other major users will use the instrument in their externally funded projects. PIs' major research activities are summarized below with research briefs, followed by a table. The section closes with results from prior NSF MRI support.

CUDA Research Center at Boise State University

[redacted]

Boise State University has been recognized as a CUDA Research Center by NVIDIA Corporation since 2010 for embracing and adopting GPU computing across multiple research fields. The primary goal of the center is to develop and apply computational methods to applications in science and engineering where rapid and real-time computations can transform the current practice. The proposed tiled display GPU/CPU cluster will advance the GPU computing activities of five faculty members at the center.

CAREER: Multi-scale modeling of short-term forecasting and grid integration of wind energy over complex terrain

[redacted]

The proposed acquisition will help improve data analysis for multi-scale wind forecasting research over large geographic areas with complex terrain (see Fig. 1). There is a growing interest to increase the utilization of wind energy resources for electricity production, but the intermittency of the wind creates further problems in balancing the load and generation on the electricity grid. The research goal is to better understand turbulent flow characteristics in complex terrain with canyons under different atmospheric stability conditions. This fundamental understanding will then be used to create a *short-term wind forecasting engine on heterogeneous computing clusters, such as the one requested in the present MRI proposal*, to harness wind energy resources reliably.

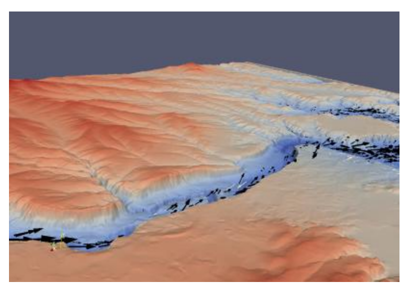


Figure 1: Parallel rendering of GIN3D simulation results of wind flow over complex terrain using Paraview.

PI [redacted] and his students develop a multi-scale wind forecasting approach that connects atmospheric processes at the meso-scale down to the micro scale where complex terrain features can be resolved. Specifically, the goal is to forecast wind power at the turbine level for the short-term (e.g., 0–6 hours). In the forecasting engine, a meso-scale atmospheric model (e.g., the Weather Research and Forecasting model) will be executed in parallel on central-processing units (CPU). A microscale terrain-resolving CFD model (see GIN3D description on the next page) will be executed on the GPUs of the same cluster concurrently with the mesoscale model. The meso-scale model will provide boundary and initial conditions to the micro-scale model. The micro-scale simulations will also be used to improve the surface layer parameterizations in the meso-scale model to establish a one-and-a-half-way coupling between the simulation models. Simulations will be validated against measurements that are continuously gathered from a complex terrain area, as shown in Fig. 1, instrumented with 14 weather stations by Idaho Power Corporation.

The proposed CPU/GPU cluster with a parallel file storage system will greatly accelerate the meso- and micro-scale computations to realize forecasting (i.e., faster than real-time predictions). The large eddy simulation (LES) technique with the dynamic procedure will be applied at the micro-scale. The complex terrain will be represented with the immersed boundary approach on a Cartesian mesh, which fits well to the execution model of CUDA on GPUs. LES of turbulent flows is computationally expensive. The turbulent channel flow simulation shown in Fig. 2 takes nearly 45 hours to complete on 8 Tesla M2070 GPUs [1]. The time-dependent nature of LES makes it an attractive modeling approach for estimating the variability in wind forecasting. However, simulations typically produce massive amounts of data that require parallel rendering and fast storage capabilities for interactive analysis of simulation data.

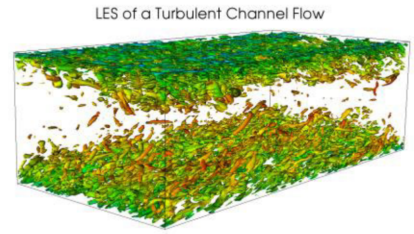


Figure 2: LES of turbulent channel flow using GIN3D

The multi-scale nature of this research calls for a multi-scale analysis on a large display wall as well. Fig. 1 shows only a small portion of the area simulated at the micro-scale. The PI expects to analyze a meso-scale weather simulation that covers a large geographical area alongside a micro-scale model simulation (GIN3D) that covers a much smaller area where terrain features are resolved. A large tiled display driven by a GPU cluster can support multiple instances of parallel rendering software (e.g., ParaView or VisIT) where researchers can study flow structure visualizations as they move from meso-scale to micro-scale.

There are several **broader impacts** for this research activity. Substantial technology gaps exist in short-term wind power forecasting and grid integration. Improving the accuracy of short-term forecasts is of importance to utility companies to balance load and generation on the grid while minimizing investments in the form of balancing reserves to smooth out the variability in wind power. The tiled display wall in a decision theater setting will greatly supplement PI's planned education and outreach activities and serve a much broader audience to create awareness of supercomputing and scientific visualization technologies. PI will use wind energy applications to motivate student interest in computational sciences. PI considers a tiled display as the most tangible aspect of a supercomputer. Therefore PI has been promoting a 4×4 tiled-display visualization cluster (built in-house with used and new parts, see Fig. 5 for an application in biological sciences) in his research laboratory for research, education and outreach. The cluster is also serving graduate and undergraduate students in PI's Parallel Scientific Computing class (Spring 2012). The tiled-display is also going to be used at the Discover Engineering Day at BSU on January 28th, 2012 and thereafter annually. PI and an NSF STEP Scholar undergraduate student Nick Cordell planned an activity entitled "Space Shuttle Atlantis – The Last of a Legacy," where participants will be presented high-resolution NASA imagery of the last shuttle mission while asked questions related to aerospace sciences. Plans for supercomputing booth are also underway for e-Girls, e-Camp, e-Day events at BSU.

GIN3D: GPU-accelerated Incompressible Navier-Stokes Solver

PI [redacted] has been leading the development of an incompressible flow computational fluid dynamics (CFD) solver for multi-GPU computing platforms [2-8]. GIN3D is the work horse in several ongoing and proposed projects. GIN3D is the first multi-GPU parallel incompressible flow solver, which has been acknowledged independently by other researchers [9] that demonstrated substantially faster CFD simulations on the Lincoln Tesla Cluster at the National Center for Supercomputing Applications (NCSA) and the Longhorn Visualization Cluster at the Texas Advanced Computing Center (TACC). GIN3D adopts explicit second-order accurate numerical methods in space and time and a parallel geometric multigrid solver [4]. Multi-GPU parallelism in GIN3D is achieved by interleaving MPI with CUDA and overlapping communication and data transfer with computations [7]. The largest simulation of a benchmark fluid dynamics problem with 17 billion mesh points has sustained 4.9 Teraflops using 256 GPUs on TACC Longhorn cluster [5].

GPU-Accelerated Atmospheric Transport and Dispersion Modeling

PI [redacted] adopts GPU computing in two projects to accelerate atmospheric transport and dispersion modeling. In the first project (NSF-DMS-1043107) [redacted] collaborates with Prof. [redacted] (Dept. of Mathematics, BSU) to locate the source of a chemical and biological (CB) agent dispersion event that is detected by a sensor network [10]. The proposed mathematical approach combines fast inverse methods with CFD-based forward simulations of CB agent dispersion on GPU clusters to reconstruct a dispersion event within a short turnaround time. Event reconstruction is critical to decision makers and emergency responders [11]. Once the dispersion event is backtracked in time, the dispersion can be projected forward using high-fidelity GPU-accelerated CFD models to predict the hazard-zone for emergency response and hazard mitigation. The project extends the methodologies in the χ^2 method [12] to CFD based plume dispersion models. CFD simulations are computationally more expensive than approximate plume models, but are expected to do a better job in predicting dispersion in urban environments. Therefore, [redacted] further develops the GIN3D CFD code to simulate turbulent dispersion of contaminants over complex geometry on GPU clusters.

In the second project, [redacted] collaborates with the NOAA Field Research Division in Idaho Falls to port NOAA Air Resources Laboratory's widely used HYSPLIT Lagrangian particle dispersion model to GPU computing platforms. The parallelization is done with CUDA-Fortran and the research team develops best practices to address issues that arise when porting legacy software to emerging architectures. A future project goal is to introduce multi-GPU parallelization in HYSPLIT.

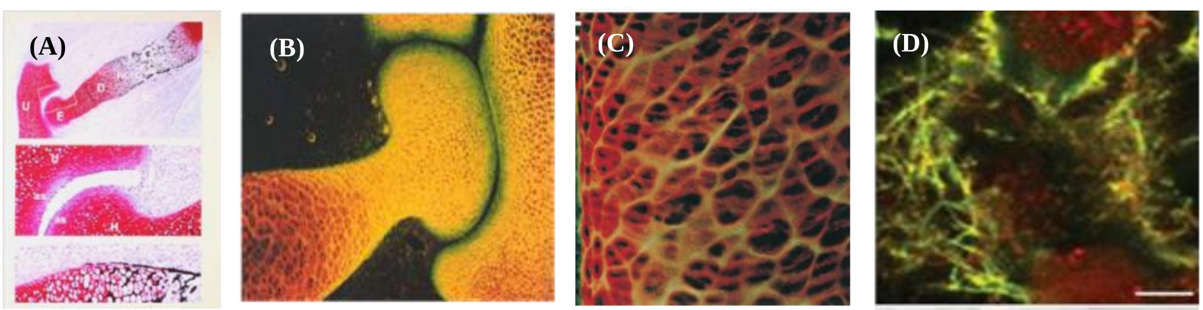


Figure 3: Analysis of developing vertebrate skeleton over multiple scales. (A). Saffranin O and von Kossa staining of e17d rat humerus indicates regions of cartilage (pink) and that undergoing conversion to bone (black). (B). Distinct differences in protein expression patterns are seen by immunofluorescence microscopy (green-permanent cartilage versus red-transitioning to bone). Yellow indicates regions of protein colocalization. (C) Zoomed-in view of epiphyseal region showing that the two proteins co-distribute (yellow). (D) Fibrils (green) detected around the cells (red nuclei) using laser scanning confocal microscopy. Scale bar = 5 µm.

Extracellular Matrix Molecules in the Transition from Cartilage to Bone

The proposed acquisition can support multi-scale biological analysis currently hindered by slow visualization and low resolution display and a setup that it not optimal for concurrent evaluation by multiple researchers. [redacted] is the principal investigator of multiple projects addressing the structure and function of the extracellular matrix (ECM). She has served as PI and Co-PI on four NSF-funded MRI grant proposals for instrumentation necessary to generate high resolution data files at multiple scales ranging from nanometer to millimeter in size. [redacted] is also the PI on an NIH project to investigate the mechanisms of skeletal development using a zebrafish model system and subproject PI on a second NIH project to investigate the role of ECM in cell signaling processes. Finally, [redacted] serves as PI on a project to investigate the role of ECM in the molecular mechanism of cellular mechanotransduction, funded by NASA.

Skeletons are variable in structure, function and evolutionary history. However, they share common features at the molecular level. Visualizing vertebrate skeletons in three dimensions aids both the understanding of physical appearance as well as the explanation for evolutionary molecular and cellular transition from one life-form to another. Although a fundamental idea, we do not yet understand why many invertebrates such as annelids and squids have evolved to take advantage of a cartilaginous rather than bony skeleton, and what the evolutionary and functional relationship is between cartilage and bone in vertebrate animal skeletons. To understand these fundamental questions, we perform macro- and microscopic level analysis. Fig. 3a–c, above, shows a developing long bone at increasing magnification. Early in development, the structure consists primarily of cartilage (Fig. 3a) [13]. Most will transition to bone, leaving only a thin layer of permanent cartilage at the joint surface. Expression patterns of proteins predict this differentiation before it happens, as shown by the thin green-staining region of future permanent cartilage and red staining region that will be first to transition to bone (Fig. 3b–c) [14]. Collagen fibril networks can be observed by laser scanning confocal microscopy, and at highest resolution (Fig. 3d) [15, 16]. We hypothesize that the fibrillar structure and surface features are essential for molecular function and ultimately determine the materials properties of the biomaterial (cartilage/bone) [17-21]. The surface features of individual collagen fibrils will be analyzed at the nanometer scale by TEM. [redacted] group's goal is to define the mechanistic details that differentiate between cartilage that remains as permanent cartilage, versus that which will be replaced by bone.

Fig. 4 shows X-ray microCT (Fig. 4a–b) and TEM (Fig. 4c) images during the transition from cartilage to bone and the earliest stages of mineralization in the ECM (Fig. 4c) [13, 22, 23]. Data on the trabecular features of the nascent bone are acquired by X-ray microCT and analyzed through high resolution

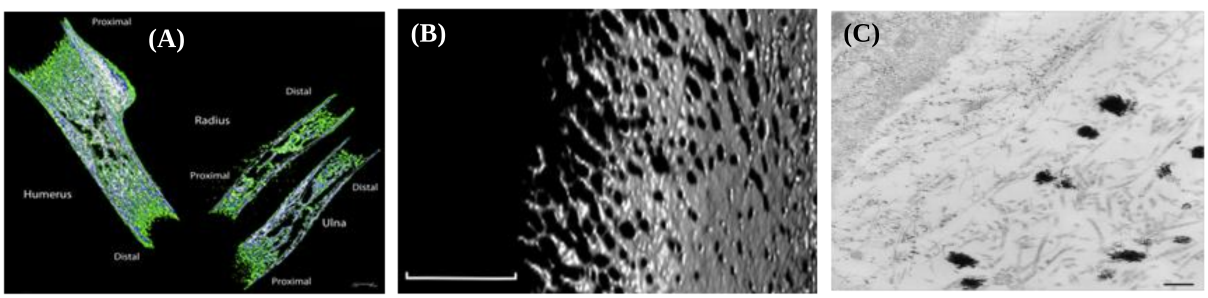


Figure 4: Mineralization of skeletal tissue using multiscale analysis. (A) X-ray microCT image of forelimb showing mineralized tissue. Bar = 160 micrometers. (B) Higher magnification of trabecular structure of newly formed mineralized tissue. Bar = 500 micrometers. (C) Mineralization foci shown by TEM. Nascent bone is represented by electron-dense (black) crystals of hydroxyapatite scattered within the large-diameter collagen fibrils of the perichondrium. A portion of a cell is visible in the upper left corner. Thin diameter fibrils of cartilage between the perichondrium and the cell are visible but not mineralizing. Note the sharp transition between the collagen fibril architectures of the perichondrium (thick) and the cartilage (thin) Bar = 200 nm.

microscale imaging, which is also used for 3D volume reconstruction. The instrumentation for skeletal tissue molecular structure analysis generates large, high resolution, multiscale data files (up to 64 MP each) that may span from nanometer to millimeter. Researchers perform current analysis on individual CPUs and a small, four CPU cluster. Image data rendering and volume reconstruction can require over 24 hours of processing time per image. Visualization display technology at [redacted] lab includes a 3-D mini-CAVE with conventional HD resolution, and workstations utilizing typical computer display technology. A visualization cluster is expected to accelerate this process substantially.

The collagen fibrillar structure and surface features shown in Fig. 5 represent a compilation of numerous studies [17, 19-23]. An overall view of the essential collagen fibril structure and glycosaminoglycans with which the collagens interact is shown. To better understand the spatial distribution and organization, a closer view within the context of the "big picture" is required. The biochemical and spatial parameters of surface features of individual collagen fibrils were viewed on the tiled display in [redacted] laboratory. The proposed visualization cluster with a 5×8 tiled display will support high resolution visualization and parallel data rendering required to better define mechanistic details that dictate transition from cartilage to bone. This research will benefit significantly from parallel rendering technology on the visualization cluster proposed here. The research proposed aligns with the NSF Developmental Systems Cluster of the Division of Integrative Organismal Systems. Additionally, investigation of cartilage and bone materials properties falls under the NSF Biomaterials Program within the Division of Materials Research. Results from the visualization cluster use will enable us to pursue future funding to address these NSF program missions.

Figure 5: Visualization of ECM molecular model showing collagen fibrillar network and ECM carbohydrates.

Mechanics of Magnetic Shape-Memory Alloys

The proposed acquisition will help facilitate materials science research at varying scales, and make better use of high resolution experimental data. [redacted] is the principal investigator for several projects on magnetic shape-memory alloys (MSMAs) including three collaborative, NSF-funded projects [redacted] which entail high-resolution in-situ deformation experiments providing a vast amount of high-resolution data as information is required on a large scale (e.g., the foam architecture, Fig. 6a) and on the microscopic scale (e.g., twin microstructure, Fig. 6b) requiring 20 to 100 MB resolution. [redacted] is also the PI on a project to investigate the inverse magnetoplastic effect of MSMAs, funded by Department of Energy's (DOE) Basic Energy Sciences program [redacted].

Magnetic shape-memory alloys (MSMAs) display giant magnetic-field-induced deformation, more than 50 times larger than the largest magnetostriction available in commercial Terfenol-D. These extraordinary properties originate from a strong coupling between magnetic and crystallographic "twin" domains. MSMAs deform by the (magnetic-field-driven or mechanically driven) motion of twin boundaries, which form a hierarchical pattern with characteristic lengths ranging from nanometer to millimeter. [redacted] leads several projects on MSMAs including two collaborative, NSF-funded projects that both entail high-resolution in-situ deformation experiments, and which will provide a vast amount of high-resolution data.

The first, highly successful project focuses on the magneto-mechanics of MSMA foam (together with Dr. Dunand, Northwestern University, Evanston, Illinois) [24-29]. The porosity enables the magnetoplastic effect in polycrystalline materials, while otherwise this effect is found only in single crystals. Polycrystalline MSMAs show no magnetoplastic effect because grain boundaries suppress twin boundary

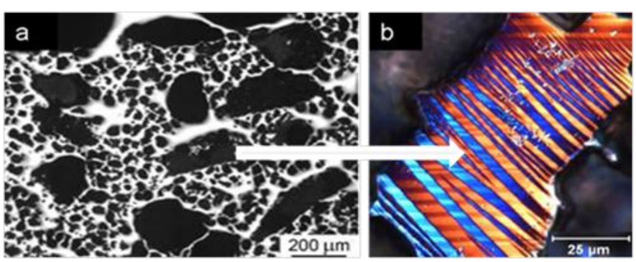


Figure 6: Ni-Mn-Ga foam with bimodal pore size distribution. (a) Optical micrograph of a polished cross section with two populations of pores (black);
(b) Zoomed-in Optical micrograph of strut with polarized light shows twins (orange and blue).

motion. Pores decouple grains such that small struts contain no grain boundaries (Fig. 6a). In these struts, twin boundaries span from pore to pore and are highly mobile (Fig. 6b).

Though large magnetic-field-induced strain was found for many foam samples, the amount of strain varies from sample to sample and depends on crystallographic texture and grain size. To gain a quantitative understanding of the relationship between grain size, texture, pore size, and pore size distribution on the one hand and magnetic-field-induced strain on the other hand, we will perform in-situ experiments where we will observe the deformation of struts and pores on the large scale (Fig. 6a) and the motion of twin boundaries on the small scale (Fig. 6b). Data evaluation will include quantifying pore deformation at the large scale to pinpoint active regions, where a visualization of the entire image on a large display at its native resolutions can help greatly. Simultaneously, we will zoom-in on those active regions to characterize the twin geometry and twin boundary motion. This process requires acquiring images such as those shown in Fig. 6a at a high resolution, permitting quantitative analysis of twin boundary motion on the small struts (white in Fig. 6a and colored in Fig. 6b). Twin boundary analysis calls for a resolution of about 0.1–1 megapixel, which translates to at least 100 megapixels for the image shown in Fig. 6a. Currently, [redacted] uses a 21 megapixel camera and anticipate acquiring a high-resolution high-speed camera to generate high-resolution videos to better visualize pore deformation and identify active regions concurrently. Therefore, a large display that can provide a resolution on the order of a 100 megapixel resolution will facilitate evaluation of a vast amount of data, and make better use of the high-resolution cameras used in the experiments.

The second project is a NSF-Materials World Network collaborative effort with the Ruhr University Bochum in Germany. The project goal is to gain a transformative understanding of the deformation mechanisms of materials with highly complex microstructures such as hierarchically twinned martensite. Self-accommodated martensite consists of a system of twinned martensite variants. Volterra disclinations are located where twin boundaries intersect (Figs. 7a-b, [30-35]). In-situ deformation experiments will be

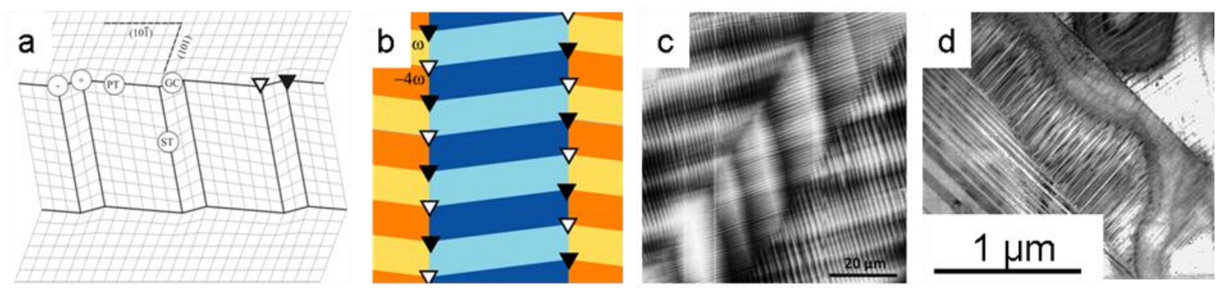


Figure 7: Hierarchical twin microstructures. (a) Schematic of the lattice distortions caused by intersecting twin boundaries. A disclination (indicated with a triangle) is located where three twin boundaries meet. (b) In hierarchical twin-microstructures, disclinations form walls. (c) Atomic-force microscopy image show three orders of hierarchical twins. (d) Transmission electron microscopy bright-field image showing two orders of hierarchical twins at the sub-micrometer length scale.

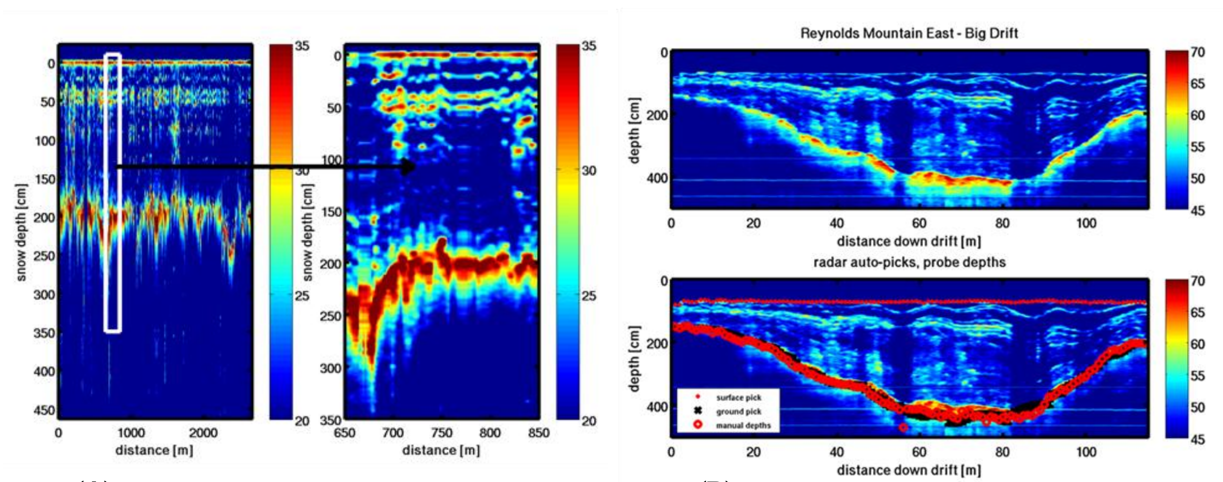
performed with transmission electron microscopy, atomic-force microscopy, and optical microscopy, spanning the length scales form atomistic to full sample size (Figs. 7c-d). The experimental study, which will be performed at Boise State University, will provide the distribution of elastic line defects, which then will be used as input data for the numerical study to be performed by colleagues in Germany. The hierarchical multi-scale nature of the microstructure requires the simultaneous observation of the rearrangement of twins at multiple length scales. This can only be achieved with high-resolution cameras and by displaying the full data set at once on a large display such as the one requested in this proposal.

Data evaluation will include quantifying martensite domain deformation at large scale to identify active regions. Simultaneously, we will zoom in on the active regions to characterize the twin geometry and twin boundary motion at length scales down to a few nanometers. The total dynamical range of twinning is 10^6 (from nanometer to millimeter) and cannot be covered with a single method. In-situ TEM will cover a range of 10^4 (from nanometer to 10 micrometer) which requires a 100 megapixel image size.

These projects can potentially have a widely felt impact at the university, within industry, and in our local economy. The proposed acquisition would be instrumental in data analysis and research, and in advancing MSMA technology towards marketability—a current effort of our Technology Transfer Office. Boise State University holds three MSMA patents, with three further patents pending. Boise State collaborates with a local spin-off company (Response Magnetics) which will likely provide technology jobs in Idaho.

Remote Sensing of Snow

[redacted] has a need to study high resolution data and visualize large distances when he estimates *snow water equivalent* (SWE), the amount of fresh water that a given area of snow contains. Accurate knowledge of SWE is essential for water resource management, hydro-power and flood forecasting. Over a billion people worldwide depend on snowmelt for water; and temperature and precipitation increases will significantly alter snow distribution, greatly complicating predictions about this already poorly understood but important water resource. [redacted] research has five major objectives, which focus on improving our ability to measure snow properties from space: 1) Test and improve retrieval algorithms and inversion models for snow with high-resolution data; 2) Quantify spatial variability of snow at a range of scales and explore the effect of variability on remote sensing for a range of footprint sizes; 3) Use data assimilation to improve snow property estimates between site visits and to use backscatter directly for predicting snow properties, and 4) Create a public awareness on the issue by



(A) **(B)**

Figure 8: (A) Example 2.5 km profile on the left, with an order of magnitude shorter distance (200m) extracted on the right from the white box in the left figure. Radar data must be viewed at this resolution to accurately pick layers, but seeing profiles at the km scale on a large resolution display help identify important layers to be picked. **(B)** Ground-based radar image of large snow drift. Upper image shows processed data, and lower image shows radar picks of the snow surface (red dots), radar picks of the ground surface (black X's), and 116 manual measurements of snow depth (red circles). Manual ground-truth measurements required 8 hours of manpower. Radar profile was performed in the field in 10 minutes, but required more than 5 hours of processing on an 8-core I7 desktop processor. Using a Tesla 1060 GPU board, the same image was processed in less than 15 minutes.

developing outreach program, in collaboration with the Discovery Science Center of Idaho, Bogus Basin Snow School and a strong education component through a long-term NASA Space Grant Undergraduate Research Program.

Although researchers can currently accurately estimate snow covered area (SCA) from space, they can only identify location, and not how much water the snow stores. Estimating SWE with remote sensing techniques remains problematic, as manual ground-truth measurements in typically highly variable snow conditions are time-consuming. Microwave remote sensing has great potential for giving scientists and practitioners ongoing SWE information at a global scale. Active radar sensors have the potential for high spatial resolution, and the technique has been chosen for the current European Space Agency CoreH20 mission concept. Results from the second NASA Cold Lands Processes Experiment (CLPX-II) campaigns in Colorado [36] and Alaska show demonstrate technique promise in a wide range of snow conditions.

[redacted] research focuses on active microwave radar measurements from ground-based, airborne, and spaceborne platforms to improve our ability to estimate SWE from space [37-39]. His research produces extremely large datasets that require substantial computational power to process and analyze. In particular, the bottleneck in the group's algorithms is the large Fast Fourier Transform (FFT) computations. [redacted] group currently uses 2 Tesla 1060 GPU cards in their work, which have resulted in a 50x speed up over a high-end desktop I7 processor. Every radar trace must have a 2^{14} point FFT applied, and these traces are all completely independent. Therefore, with 64 GPUs on the proposed cluster, it is expected that radar data will be processed an order of magnitude faster than one GPU, and several orders of magnitude faster than on a high end desktop machine. The proposed acquisition will also enable Marshall's group to explore inversion algorithms of high complexity, and to use radiative transfer modeling and unique datasets to study the effect of the variability of snow properties on microwave radar.

Aside from the FFT computations mentioned above, the slowest part of radar analysis is picking layers, which requires that users interact with visualized data. Radar analysis also requires user-driven quality control and interpretation, in which users must view every radar image, evaluate automated layer picking algorithms, and select control points. Fig. 8a shows a profile of several kilometers, with 200 meters extracted. Radar data must be viewed 200 meters at a time to accurately pick layers on a normal monitor. Fig. 8b shows an example of a 120 meter profile—[redacted] work involves radar profiles at scales of 10's to 100's of kilometers. High-resolution visualization on a large display wall is expected to enable several kilometers to be viewed at once, at the resolution necessary for picking layers accurately and enable Marshall's group to quickly identify layers of interest that are continuous over multiple kilometers.

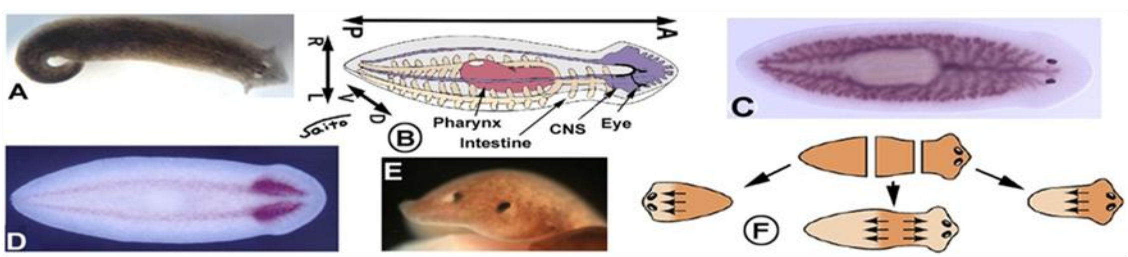


Figure 9: Planarian anatomy and regeneration

Biological Modeling and Sequence Analysis

[redacted] associate professor of computer science, has been helping biologists for some time to leverage high speed computing so they can improve hypothetical modeling and data analysis. The proposed acquisition will further enhance data analysis. [redacted] is collaborating with [redacted] from Boise State University and [redacted] from Tufts University to develop a computational model of planaria (flatworm) development and regeneration [redacted]). Planaria are well-known model organisms, each having eyes, a mouth, a central nervous system, a digestive system, and a tail (see Fig. 9). Most interestingly, it has a remarkable ability to recover from damage to its tissues, and is able to regenerate two complete organisms if split lengthwise or crosswise. This project aims to integrate experimental results stored in a database with a computational platform that will enable researchers to construct and test computational development and regeneration models. This project requires a computer cluster for model development using a genetic algorithm-based search process, and for model validation. The proposed instrument will also enable us to visualize at a high resolution and interact with (perturb) in real time with 3 dimensional models of developing virtual planaria.

[redacted] is also working with [redacted] from the Chemistry Department at Boise State University to study alpha-conotoxins (work funded in part by [redacted]), short peptides consisting of 10 to 30 amino acids that are found in the venom of marine cone snails, with the ultimate hope of developing a novel model of a membrane bound nicotinic acetylcholine receptor (nAchR) found in the human brain, and known to be important in a number of neurological diseases such as Alzheimer's. To this end, we have constructed computer homology models of the $\alpha_3\beta_2$ nAchR and validated our computational results using the α_3 and β_2 amino acid sequences from rat plasmids expressed in *Xenopus oocytes*. The template structure files for the homology models were the *Tm*-nAchR (accession number 2BG9) and the *Ac*-AchBP (accession number 2W8E) [40]. In order to facilitate high throughput virtual screening, we have developed computational tools that enable scientists to quickly set up and run computational molecular binding assays on a cluster of computers for high throughput virtual molecular screening [41]. Recently, work has been done to port the modeling algorithms that we plan to use to GPU-based architectures [42], and we anticipate extensive use of both the regular CPU cores and the dual Tesla 2075 GPUs for this project for both our computational needs as well as to further software development. This project will also take advantage of the proposed display wall, allowing scientists to compare results from different virtual screening runs, and visualize receptors and bound ligands at high resolution.

Research Activities for Major Instrument Users

Table 1 summarizes the current funded research for the PI, co-PIs and major instrument users. The proposed acquisition will support externally funded research that exceeds $13,200,000. Note that researchers would apply the total funding amount to projects with multiple investigators.

Results from Prior NSF MRI Support

NSF awards made since 2007, in which the PIs participated as PI or co-PI, are summarized below.

[redacted], 8/19/09, *MRI: Acquisition of an LC-MS for Multidisciplinary Research and Education,* [redacted]
MaXis time-of-flight mass spectrometer with Dionex UPLC and a Bruker Ion Trap MS were installed with funds from this grant. A Ph.D.-level facility director has been hired, and training courses for faculty and students have been offered. The facility has been used to support research programs for ten faculty members in Biological Sciences and Chemistry, and used to enhance teaching in CH432 biochemistry lab

[redacted], 1/15/2011-12/31/2015, *"CAREER: Multi-scale modeling of short-term forecasting and grid integration of wind energy over complex terrain,"* PI: [redacted] Two undergraduate students, one majoring in computer science, and one in mechanical engineering have been recruited. An undergraduate female computer science student worked on level-set methods for complex terrain for 6 months. A conference paper has been submitted to the 2012 ASME Fluids Engineering Conference related to this project [43]. A research poster has been presented at NASA Day at BSU, an event open to public.

[redacted], 10/01/2010-09/30/2012, "*Data-driven Stochastic Source Inversion Algorithms for Event Reconstruction of Biothreat Agent Dispersion,"* PI: [redacted], co-PI: [redacted]. A first generation mechanical engineering student with Hispanic heritage has been recruited as a graduate research assistant for this project. A mechanical engineering veteran student has been hired as an undergraduate student. The graduate student made a presentation and published a conference paper [1] which is currently under review for publication in a future special issue on GPU computing in Computing in Science and Engineering journal.

[redacted], 5/15/2008-4/30/2012, *"Collaborative Research: Enabling magnetoplasticity in polycrystalline Ni-Mn-Ga by reducing internal constraints through porosity,"* PI: [redacted]**.** This highly successful project (collaboration with [redacted], at Northwestern University) focuses on the magneto-mechanics of MSMA foam. The porosity enables the magnetoplastic effect in polycrystalline materials, while otherwise this effect is found only in single crystals. Results were published in high-impact journals including Nature Materials and Physical Review Letters [24-29, 44] and two further journal publications are in preparation. Furthermore, results were presented at numerous conferences, including two invited presentations [45, 46]. This project resulted in one patent [47].

Table 1: Funded research activities. The amount available to co-PIs may be less than indicated.

[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
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[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
				[redacted]

[redacted], 7/31/2013, *"NSF-Materials World Network: Deformation via the Transformation of Hierarchical Microstructures,"* PI[redacted] [redacted]). The project, in collaboration with the Ruhr University Bochum, is in its most productive phase. Mutual visits and visits with partner institutions have taken place. Results of the first year have lead to four manuscripts and two presentations, including one invited presentation [48].

[redacted], 9/15/2011-8/31/2014, "*Mechanics of Magnetic Shape-Memory Nanostructures*," PI: [redacted] (co-PI: [redacted]). This project is in its starting phase. Two undergraduate students have been recruited and a graduate student will be recruited with the next academic semester.

[redacted], $228,963, 9/2010-8/2013, *"Quantifying lateral flow of water in alpine snowpacks using high resolution geophysical techniques"*, PI: [redacted], Co-PI: [redacted]. The project currently supports a master's student. Geophysical instrumentation for measuring snow and soil water content has been deployed and is currently being used during our first winter/spring season. An undergraduate presented results at a May conference, as did a graduate student at the December 2011 American Geophysical Union conference. One publication is in review and another in preparation.

[redacted], *$300,000, 9/12/2011-9/12/2014, "Collaborative Research: CDI Type-1: A Computer Framework for Modeling Complex Pattern Formation,"* PI: [redacted] The project currently supports a master's student and undergraduate student. We have installed the modeling platform on a small 16 node Beowulf cluster and are working on genetic-based search algorithms, and have used them to produce flatworm models capable of simple head and tail regeneration when severed.

1.3. Description of Research Instrumentation and Need

The requested instrument will be a shared campus resource and expand current Boise State high performance computing initiatives managed by our Office of Information Technologies [49]. PIs propose to acquire the instrument specified below to integrate parallel computing, visualization, and storage needs of university and other local researchers in a single platform, and to promote it as a cyberinfrastructure resource to regional users using existing professional networks. Salient features of the instrument are discussed below. The quotations from Microway offer more details on the cluster and storage array.

32-Node CPU/GPU Linux Cluster

- *Node configuration:* Two AMD Opteron 6272 2.1 GHz 16-Core CPUs with 64 GB memory
- 20 NVIDIA Quadro 6000 graphics cards to populate 10 nodes (2 per node) to drive the tiled display. 44 NVIDIA Tesla M2075 cards to populate the remaining 22 nodes for GPU computing
- Infiniband QDR cluster interconnect and 1 Gigabit Ethernet
- Parallel LUSTRE storage array (5 nodes) with a usable storage of 64 TB high capacity storage for for large sequential I/O operations, and 3TB high-throughput storage to provide good throughput for small and random I/O operations. Maximum theoretical throughput is 4.7 GB/s

5×8 Tiled Display —40+5 24" professional HP LED backlit monitors (1920×1200) with a custom order aluminum frame for the tiled-display. Five additional monitors are requested as spare monitors because it is very common for monitors with specific bezel designs to go out of production. This particular monitor has a 178° off-angle viewing, which is critical for a large display. 25m long DVI cables and signal boosters are needed to drive the tiled display afar. Combined resolution of the tiled display is 92 MP.

Software Environment—The cluster will be managed with the Rocks Cluster Toolkit and Viz Roll. A suite of compilers (C/C++, Fortran, CUDA, OpenCL) and libraries (scaLAPACK, PETSc etc.) will be available on the Linux cluster based on user needs (e.g., OpenFOAM, WRF, Amber, Gromacs, etc.) The following middleware will be available for high-resolution visualization applications: *Chromium*, *CGLX*, *DMX*, *VisIT*, *Paraview*, *SAGE*, *Magic Carpet*.

Server Room—The cluster and storage array will be housed in a server room to meet power and cooling requirements indicated in vendor quotes. The floor plan for the envisioned visualization theater is included in the supplemental Facilities document. High-speed networking to connect the cluster to the Idaho Regional Optical Network (IRON) will be available at the building as part of the renovation plan.

The proposed instrument is designed based on hands-on experiences of PIs [redacted] and [redacted] on HPC systems and pioneering examples (e.g. NASA hyperwall-2, TACC Stallion and Optiportals) that are discussed in literature [50, 51]. [redacted] and his students built in-house a 4×4 tiled display 8-node GPU cluster at BSU using new and used parts. [redacted] has been operating the cluster since 2010. [redacted] and his graduate students have also built a 21 node Beowulf cluster for storing and performing statistical analysis of biological sequence data.

The total number of GPUs and CPUs and available memory per node addresses the needs of PIs and several major users. Performance results obtained by executing the GIN3D CFD code on the TACC Longhorn and NCSA Lincoln GPU clusters using as many as 256 GPUs [7, 5] guided some of our design choices related to the size of the cluster. PIs selected NVIDIA Quadro 6000 and Tesla M2075 cards to have uniform computing environment for scientific computing. The GPU architecture is identical in these cards and both cards provide 6 GB of global memory. Quadro 6000 cards provide dual DVI output and will be connected to the tiled display. PIs will review the hardware technologies at the time of ordering the instrument and use latest CPUs and GPUs within same price range. With 32 CPU cores per node, a total 64 GB memory per node provides 2 GB per core and enables shared memory applications to realize decent performance.

1.4. Impact on Research and Training Infrastructure

Intellectual Merit: Today's science and engineering research projects, whether computational or experimental, increasingly rely on availability of modern cyberinfrastructure for tasks such as parallel computing and rendering, data storage, and high-resolution imaging. As evidenced by the research activities listed in this proposal, the situation is no different at Boise State University.

The requested instrument will impact PIs' on-going research projects in several ways. PIs [redacted] and [redacted] generate high resolution images in their research that exceed current resolution of desktop monitors. Dr. [redacted] research has a transformative effect on various sensor and actuator technologies. [redacted] group produce and study novel magnetic shape-memory foams and alloys that exhibit strains and response times comparable to Terfenol D, the best commercial magnetostrictive material on market. [redacted] currently uses a camera of 21 MP and has plans to acquire a 100MP camera. [redacted] expects to use the proposed tiled display to better explore the micro structure of magnetic shape-memory alloys in high resolution

A visualization cluster with a large tiled display will significantly advance Dr. [redacted] fundamental research in understanding the evolution of invertebrates. Micro CT scanner in [redacted] laboratory can generate images up to 64 MP but there is no instrument available at BSU to visualize images at that native resolution. Fig. 5 shows [redacted] and her research staff member exploring a model of collagen fibril for the first time on the experimental tiled display in PI [redacted] research laboratory. [redacted] admitted that they avoid high-resolution images because they are too large for a desktop monitor, but she was convinced about the benefits of a high resolution display after discovering new details about their model as a result of using a tiled display.

The requested instrument will be a convincing demonstration of a wind forecasting engine for renewable energy industry. PI [redacted] research builds entirely on the availability of a CPU/GPU cluster to forecast winds at the meso- and micro-scale in a multi-scale coupled fashion. [redacted] will also use the instrument to rapidly compute chem-bio agent dispersion in complex environments. The instrument will also enable parallel rendering of simulation data that are expected from these projects. [redacted];s research will lead to a better understanding of atmospheric flows and contaminant dispersion over complex terrain, which is one of the least understood topics in atmospheric sciences.

The requested instrument will support Dr. [redacted] highly popular (a podcast of [redacted] was featured on Discovery Channel on Jan 23rd 2012) remote sensing of snow research aimed at improving our ability to measure snow depths. Marshall's research help determine the fresh water amount in a given area which is essential for water resource management, hydro-power and flood forecasting. This instrument with 64 GPUs and a large display wall will help eliminate major bottlenecks in [redacted] research. [redacted] expects to accelerate FFT calculations by several orders of magnitude faster than on a high end desktop machine. Equally important, a high-resolution large display wall will enable [redacted] to view several kilometers at once and at the resolution necessary for picking snow layers accurately and therefore enabling [redacted] group to quickly and precisely identify layers of interest that are continuous over multiple kilometers. [redacted] and his colleagues have traveled from Antarctica to Greenland to Alaska collecting huge amounts of data to be analyzed in their research.

The requested instrument will enhance PI [redacted] collaboration with biologists to develop a computational framework based on artificial intelligence on parallel computers to better understand what mechanisms living systems use to establish and maintain complex 3-dimensional shapes during embryonic development. The instrument will also help [redacted] research on developing computer models for data mining and storage to work with mountains of molecular and cell biological data.

The proposed instrument will be a tremendous asset for computing education and the planned Computational Science and Engineering (CSE) undergraduate minor degree at BSU. Students taking the 500/400 level *Parallel Scientific Computing* course, offered by PI [redacted] in the mechanical engineering department and the *CompSci430 Parallel Computing* course offered by the Computer Science department will be trained in the fundamentals of multi- and many-core computing and contribute towards a sophisticated workforce savvy of the-state-of-the-art cyberinfrastructure for computational science and engineering.

Broader Impacts: With two new Ph.D. programs in Biomolecular Sciences and in Materials Science & Engineering, Boise State understands the increasing cyberinfrastructure needs of researchers at different departments, therefore supports the acquisition of the requested instrument as a campus-wide resource, and commits a large space for the requested instrument in the highly visible Ron and Linda Yanke Family Research Park building that is open not only to university researchers but also to local technology companies and partners, with the goal of stimulating faculty-industry interactions. To this end, the acquisition of the proposed instrument will bring BSU closer to realizing NSF's Cyberinfrastructure Vision for 21st Century Discovery [52] and will help BSU recruit new faculty members with computational research into existing and new graduate programs.

Boise State University is emerging as a metropolitan research university of distinction and is both the largest and fastest-growing institution of higher education in the state of Idaho and an important regional economic engine. While the university continues to increase graduate and doctoral programs, it remains an undergraduate institution at its core, and maintains an 88 percent undergraduate student population. Many are non-traditional students. 81 percent are from Idaho, with a substantial number among the first in their families to attend college. As a result, exposure to cutting edge cyberinfrastructure and research can not only benefit researchers, but can also have profound effects on local and regional students who might otherwise never gain exposure.

The availability of a state-of-the-art HPC cluster will help BSU researchers to team up with other Idaho researchers. For example, the Center for Advanced Energy Studies (CAES) is a public/private partnership that includes the three Idaho public universities (Boise State University, Idaho State University and the University of Idaho), private industry, and the Idaho National Laboratory. CAES was established with the goal of improving collaborative and cross-disciplinary research and there is currently a strong effort to flourish modeling and simulation research throughout the state. PI [redacted] was the co-organizer of the *Second Annual CAES Workshop on Modeling, Simulation, and Visualization* that was held on September 08-09, 2011 in Boise. The workshop brought together researchers across Idaho. A panel was dedicated on expanding HPC capabilities across universities. To this end, the instrument will be available to CAES researchers and therefore it will serve as a cyberinfrastructure resource not only to researchers at Boise State but also at the State of Idaho.

PIs of this proposal are committed to using the instrument as part of their planned outreach activities. As part of his NSF CAREER grant, [redacted] is going to develop a supercomputing booth for ongoing K–12 outreach programs at Boise State University (e.g. e-Girls, e-Camp, e-Day). The first of these activities has already been prepared for the Discover Engineering Day event (January 28th, 2012) and will be presented by a freshmen NSF STEP Scholar student. These events are centered on the small tiled-display platform in PI [redacted] laboratory. A much larger display will greatly enhance these outreach activities. Since 2007, [redacted] and graduate students in his research group have reached out to several elementary and high schools in Boise to educate students on materials science, nanotechnology and materials characterization. The proposed high resolution display will be excellent platform to fascinate students on material characterization. [redacted] expects to leverage the proposed GPU cluster and the large tiled display in his outreach activities to initiate a long-term NASA Space Grant Undergraduate Research Program and develop a strong education and public outreach program, in collaboration with the Discovery Science Center of Idaho and Bogus Basin Snow School. [redacted] laboratory works with high school students from Medical Arts Charter High School in Meridian, Idaho. MMACHS has a student body of ~ 66% female, allowing us to address the under-representation in the STEM disciplines. The second program that [redacted] is involved through the University of Idaho is the Summer Research Scholars, a two-week program at Boise State providing an intensive research experience to students who have never done research before. Participants in this program are from 2-4 year colleges that do not offer graduate programs. Partnership with these programs will provide an opportunity for students to use the large tiled display wall to visualize their data.

Participation of Underrepresented Groups and Women: Southwestern Idaho has a sizable Hispanic population. Latinos/as comprise the largest ethnic minority in Idaho with nearly 10.7% of the state population, according to 2009 US Census Bureau data. The Boise region is home to an underrepresented population significantly higher than the state average (e.g., 28 % in Caldwell and 18% in Nampa). BSU has well-defined programs to attract and support women and students from underrepresented groups. A $782,272 grant from NSF (DUE-0856815) provides engineering scholarships for 30 undergraduate students a year in engineering and computer science to help advance the College of Engineering’s goal to attract and retain talented women and men from diverse backgrounds. BSU’s Women’s Center focuses on access and equal opportunity in educational and research programs, as well as in their personal development [53]. The Ronald E. McNair Post Baccalaureate Program at BSU is designed to identify and cultivate young scholars from underrepresented groups who demonstrate strong academic potential and promise for doctoral success [54].

PI and co-PIs for this proposal have a history of involving underrepresented students in their research projects at the graduate and undergraduate levels. [redacted] has recruited a first generation graduate student with Hispanic heritage, and an undergraduate veteran student to conduct research on his NSF funded projects and also supervised several undergraduate students and high school summer interns on computational science projects. 50% of the graduate (2 out of 4) and undergraduate (3 out of 6) students in [redacted] research group are female students. [redacted] has advised female undergraduate students on two separate CREW (Collaborative Research Experience for Women) grant funded projects. [redacted] is mentor to Dr. Liliana Mellor, a Hispanic woman and life science researcher, who is focused on space-related biomedical/biotechnical research through the NSBRI Postdoctoral Fellowship Program. [redacted] has a major outreach program with Bogus Basin Snow School, which provides warm clothing, transportation, and snow science instruction in a winter environment to at-risk and underrepresented K-12 students.

1.5. Management Plan

Office of Information Technologies (OIT) at BSU has started offering HPC services to campus researchers. The R1 cluster, a 12-node cluster with 5 nodes dedicated to GPU computing was brought on line in July 2011. An HPC system administrator position, with experience in networking, parallel file systems, remote systems administrations, and clustering software, has been created permanently, and a wiki page [49] has been developed to provide documentation and updates on HPC systems. Researchers have access to web based weekly training sessions and real time support are through the “BigBlueButton”. The proposed instrument will become a part of HPC resources at BSU and will directly

Table 2: Project tasks and timeline.

	Project Tasks	Year 1				Year 2			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1	Purchasing & space renovations	x	x						
2	Tiled-display & Linux cluster hardware integration			x					
3	Software installation & user accounts. Cluster is ready				x				
4	User accounts & support, research software installations					x	x	x	x

benefit from these existing services. As mentioned in *Section 1.3*, PI [redacted] and co-PI [redacted] have hands-on experience building tiled display GPU clusters and Beowulf clusters for storage, respectively.

PI [redacted] will lead instrument acquisition in collaboration with co-PIs. [redacted] and the system administrator [redacted], who is the senior personnel in this project, will manage instrument technical aspects, instrument acquisition. [redacted] has 10 years HPC system administration experience. Co-PI [redacted] is a recipient of a previous NSF MRI grant and the Director of the Boise State Center for Materials Characterization. His experience with instrument acquisition and user facilities will be leveraged towards efficient acquisition and implementation. Co-PIs [redacted] and [redacted] will be responsible for informing the major users at the College of Arts and Sciences. PIs and the OIT system administrator will form a *steering committee* to set policies on usage, priorities and oversee compliance with project goals and data management plan. Steering committee will meet quarterly to review the status of the instrument.

The assembly and integration of the tiled-display platform with the CPU/GPU cluster will be performed by the system administrator in collaboration with the vendors and in consultation with [redacted] and [redacted] according to the schedule shown in Table 2. Operations and maintenance will be performed by the same system administrator at OIT. 0.5 FTE support for the system administrator is requested in the first year and 0.25 FTE is requested in the second year. Rocks and Viz Roll will be the cluster management tool. Instrument time will be allocated using the Sun Grid Engine Scheduler (SGE). A priority parallel-queue based on a user-group consisting of the five PIs of the grant will insure priority job run time. BSU researchers and students in scientific computing classes will have free access to the instrument. Steering committee will review and add new users to the priority or subordinate queues to ensure maximum usage of the instrument. All users will be asked to submit a research activity summary every six months, describing instrument use in their research. 5% down time is expected for yearly maintenance. Steering committee will review and allow external organizations to make use of the instrument with the goal of providing a cyberinfrastructure resource to the region.

The instrument will be located in Room 300 of the Ron & Yanke Research Park Building at Boise State University. The instrument is expected to draw 36 kW of peak power, which has been discussed with facility engineers and estimates for renovations to the space, power and cooling have been obtained and the administration at BSU is fully committed to house the instrument as a visualization theater setting. The floor plan is available in the supplemental Facilities document.

***Plans for Continuous Operation and Maintenance*:** Boise State University is committed to the continuous operation and maintenance of the instrument beyond the project timeline. This commitment is granted by the Vice President for Research and Associate Vice President of Information Technology (see the commitment letter in the supplemental documents). OIT at BSU has already created HPC services and a permanent system administrator position in charge of the effort. Therefore OIT is committed to maintain and service the instrument to researchers during its useful lifetime (estimated as a minimum 5 years). The existing HPC wiki page [49] will be expanded to feature the proposed instrument with detailed documentation and instructions.

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