CYBERINFRASTRUCTURE FOR TRANSFORMATIONAL SCIENTIFIC DISCOVERY IN ARKANSAS AND WEST VIRGINIA (CI-TRAIN)

1.0 Introduction

Imagine – a funded project with scientific impact so deep and broad that it could help design communities, change the way that new materials are invented, transform surgical procedures, and even refine the analysis of ancient artifacts. Research institutions across Arkansas and West Virginia, shown in Table 1, are partnering to transform the practice of information technology services, enabling breakthroughs in scientific discovery, advancing the frontiers of knowledge and improving the economic competitiveness of both states. Through advanced cyberinfrastructure training we position ourselves to be competitive and stand ready to apply for anticipated new levels of federal funding for science and technology [a1].

The Arkansas and West Virginia CI-TRAIN project is a strong partnership that builds on common research in geosciences, virtual environments, nanosciences, and computational sciences, and leverages complementary expertise in two states. West Virginia leverages expertise in the deployment and operation of shared high performance computing resources in Arkansas, and Arkansas leverages expertise in West Virginia related to visualization and modeling. The perspective of similarly-sized institutions and states brings common experience and vision of the value of an advanced cyberinfrastructure that is shared across multiple smaller institutions, including two HBCUs. The full set of resources requested in this proposal will create a nationally competitive computation and visualization environment in Arkansas and West Virginia that will enable a broad range of scientific research and educational activities across several computational science and engineering domains. The project will also dramatically grow the cyber-workforce in both states with initiatives at the high school, college undergraduate, and graduate levels, with professional information technology staff, and research faculty.

Table 1: Participating Research Institutions in Arkansas and West Virginia

UAF	University of Arkansas, Fayetteville; Campus Leads: Amy Apon, Fred Limp
UALR	University of Arkansas at Little Rock; Campus Lead: Srini Ramaswamy
UAMS	University of Arkansas for Medical Sciences; Campus Lead: Gal Shafirstein
UAPB	University of Arkansas at Pine Bluff (an HBCU); Campus Lead: Mansour Mortazavi
ASU	Arkansas State University; Campus Lead: Hai Jiang
MU	Marshall University; Campus Lead: Anthony Szwilski
WVU	West Virginia University; Campus Lead: Don McLaughlin
WVSU	West Virginia State University (an HBCU); Campus Lead: Robert Huston

2.0 The Current Status of the Cyberinfrastructure Landscape

EPSCoR RII Track-2 requires, as a foundational first step, an understanding and description of the partnership's cyberinfrastructure landscape. Cyberinfrastructure consists of computing systems, data storage systems, data repositories, advanced instruments, visualization environments, and people, all linked together by software and advanced networks to improve scholarly productivity and enable breakthroughs not otherwise possible [a2]. The cyberinfrastructure status at research institutions in Arkansas and West Virginia as expected at the time the grant is awarded is summarized in Table 2.

The states' institutions have significant cyberinfrastructure capability in the area of computational resources and Internet access. However, we recognize cyberinfrastructure needs in several areas that cannot be met by EPSCoR Track-2 funding alone. Arkansas and West Virginia have formulated strategic plans for cyberinfrastructure, and science and technology [a3, a4]. Cyberinfrastructure needs will be met through several sources including this project, access to national resources, targeted federal proposals, state funding, and commitment to cyberinfrastructure by the institutions.

In addition to the capabilities at the individual institutions, the Arkansas Research and Education Optical Network [a5] is being deployed to connect twelve institutions of higher education in Arkansas with a minimum bandwidth of 10Gbps. (More details are in the Facilities section.) In West Virginia, a new state network was funded in FY06 that uses improved switching for point to point traffic. The network will reach higher education institutions in West Virginia with data rates of 1Gbps. A grant from the Federal

Table 2: Cyberinfrastructure Status by Institution						
	Data Center Capacity	Computers	Networks Bbone;Links;I2	Storage; Archives	Infrastructure Software	Personnel for CI; Policy; Support
UAF	2000SF avail. 220KVA UPS avail., 120 tons AC@ 80%, no chilled water	1256-core 10.75Tflops shared cluster; shared clusters since 2005	10Gbps redundant; 1Gbps to most desktop; 10Gbps I2, NLR	20GB per user backed up; 17TB scratch	Campus LDAP SSO, Moab site license, no campus CA, GSI, or Shibboleth	3.5 FTE; $1.15M Active CI grants; $100K/year sustained; CI reports to VPR, MOU with IT
UALR	Campus 440SF avail., 80KW 60%; ETAS 312SF,5T AC, 13KW @100%	512-core shared cluster being installed; smaller workgroup clusters	10Gbps redundant; 10/100/1000 to desktop; 10Gbps to I2 and NLR.	4.5TB scratch	Campus LDAP, Moab site license, SSO in progress, no campus CA, GSI, or Shib	.25 FTE for CI; $400K active CI grants; CI reports to CS Dept, to Dean of EIT
UAMS	2240SF, 415KVA UPS, 84T AC, at capacity	8 node Mac cluster	10Gbps; 1Gbps to buildings, 10/100/1G links	30GB/user backed up; 2TB image app, 4GB to off-site SAN	Campus LDAP SSO, campus CA, WebSSO and Shib in process	.25 FTE for IT and HIPAA and security policies
UAPB	UPS and AC at capacity	No clusters	10Gbps backbone; 1Gbps to all servers;	No research storage	Active Directory for faculty; AD for students F09	CI awareness through CS Department; 0 FTE for CI
ASU	1376SF (300SF avail),100KV A UPS at 45%,20T AC w/ backup	8-core 12Gflops experimental cluster	10Gbps backbone; 1Gbps links; 155Mbps I2, tol be 1Gbps	850GB scratch on prototype cluster	Campus LDAP SSO, no campus CA, GSI or Shibboleth	.5 FTE for CI; CI through CIO, reports to VC for F&A
MU	1800SF, 1000SFavail 150KVA UPS@80%, 60T AC @21%	2 16-processor workgroup clusters; WV Global Grid Exchange	10Gbps backbone, 10Gbps to labs; 1Gbps other;1Gbps I2	75TB SAN storage	Active Director, I2 eduPerson schema, campus CA, Kerberos	0 dedicated FTE for CI; no current CI grants; CTO reports to CIO, CIO reports to President
WVU	2800SF, 1000SF avail, UPS 30KVA@80 %, 32T AC@25%	224 processors in workgroup clusters; a few shared clusters, TeraGrid use	1Gbps campus backbone; 100Mbps links; 1Gbps to I2	Multi TB on per cluster/ project basis	Campus Active Directory, beginning Shibboleth, InCommon	0.4 FTE CI, CI reports to VPR
WVSU	2400SF; EdPAC HVAC units, 30KVA UPS	14 processor cluster in Math & CS; WV Global Grid Exchange	1Gbps Bbone; 100Mbps links; 14Mbps to Internet	No archival services	Campus LDAP SSO, no CA, GSI, or Shibboleth	0 dedicated FTE for CI; Comp. Services reports to VP for Admin

Communications Commission will provide Internet2 access to MU in 2009. WVU has a 1Gbps connection to the Pittsburgh Supercomputing Center and is a member of the Three Rivers Optical Exchange [a6].

3.0 Results from Relevant Prior Support

Several significant funded projects have demonstrated the ability of the UAF team to lead a collaborative cyberinfrastructure project of the scale and complexity proposed here. In 2004, Educause funded $75,000 to the UAF (PI Apon) with partners in the Great Plains Network (GPN) consortium to create a working regional test bed implementation of Shibboleth among several participating institutions of higher education [a7]. A follow-on project created GPNGrid, a virtual organization within Open Science Grid. Many publications resulted [a8-a22] and UAF has participated as a contributing member to Open Science Grid and to the Southeastern Universities Research Association Grid (SURAGrid).

Prior to 2004, scientific computation at UAF was primarily conducted in individual research labs. NSF grants [MRI #0421099, $213,334, 2004-2008][MRI#072265, $803,306, 2007-2010] (PI Apon, UAF) deployed the two most powerful supercomputers in Arkansas. The systems have been highly utilized and UAF cyberinfrastructure has been significantly enhanced. More than five dozen research articles have been published that utilized these resources, including journal and high-quality conference publications, Ph.D. dissertations, and master's theses. More than $12M has been granted to new projects that are supported, at least in part, by the resources purchased with these grants. A concurrent grant at UALR [NSF MRI #0619069] (PI Ramaswamy, UALR) has been used to purchase a cluster using the same vendor and specifications as at UAF. Ten research publications have resulted from the award to date.

Supplemental funding in 2007 of $20,000 to MRI #0421099 supported the Arkansas Cyberinfrastructure External Advisory Committee. As a result, $250,000 from Governor Mike Beebe has been provided in support of cyberinfrastructure. The Arkansas Cyberinfrastructure Advisory Committee, with participants from public, industrial, and research institution partners in the state, delivered the strategic plan for cyberinfrastructure in Fall, 2008 [a3]. A funding request will be presented by Accelerate Arkansas [a23] to the 2009 state legislature. These grants and activities have enabled the formation of a community for computation, including the establishment of the Arkansas High Performance Computing Center under PI Apon, and have changed the way that UAF views computational research. The CI-TRAIN effort will bring even more visibility to cyberinfrastructure and expand the computational research community in both states.

[MRI BCS #0321286, $349,452, 2004-2007] (PI Limp, UAF) The High Accuracy, Resolution Landscape and Structure system supported the acquisition of a number of instruments including long and short range terrestrial laser scanners, multi-spectral scanners, and surveying instruments for the capture of geophysical and structural data at multiple levels of resolution. These instruments have dramatically expanded the research at UAF, and they have been central in the award of six grants totaling more than $1.8M. These include a high performance computing award (NSF IIS #0431070, $1,068K) (co-PI Limp) that funded development of methods to fuse multi-modalities of data and to extract relevant architectural details [b1-b8]. The experience gained in the use of these instruments will play a key role in this project.

[NSF EPS#9871990] established the SEPSCoR network in 1998. With Department of Energy funding in 2003 WVU joined with Pittsburgh Supercomputing Center (PSC) and others in the SuperComputing Sciences Consortium. This effort provided computational resources at PSC, a modest shared cluster at WVU and the network infrastructure to connect WVU research programs to PSC. This became the foundation for the WVU connection to the Three Rivers Optical Exchange and Internet-2.

[NSF EPS #0082984] (PI Harris, WVU) and a multi-year West Virginia Research Challenge Grant funded the acquisition of the MechDyne four wall immersive visualization system, a stereo-enabled GeoWall system, and custom software solutions for geovisualization. These and other sources of support have permitted completion of a newly renovated $32 million building for the Department of Geology and Geography at WVU that now provides four teaching labs containing 100 laboratory computer stations and a 17 seat high-end visualization lab. The infrastructure built through these initial NSF grants has been used to secure additional federal, state, and private funding of several million dollars. The infrastructure supports undergraduate and graduate education in STEM tools and technologies, extensive research grant acquisitions, and has generated five patent awards.

Funding [$4M, 2007-2010] from the Economical Development Administration (EDA) and industry is being utilized to build a new visualization laboratory at MU that includes an immersive visualization system (MechDyne) and motion capture technology as part of a new engineering laboratory building. A principal objective of the EDA grant is to advance innovation and develop the next-generation of training technologies by investing in core capabilities of the institution, such as visualization and the application of collaborative, interactive, web-based virtual environments. The initial applications are in mine safety and rescue training and simulations. The new capability is establishing collaboration opportunities across the MU campus and generating significant interest from industry, companies and institutions in the region.

[NSF EPS #0554328, $8,999,903, 2006-2009] to West Virginia resulted in radical cultural changes at the state and university level. These changes improved scientific output, broadened participation in STEM, transformed state and institutional policies and expectations, and provided considerable new state funding to build the academic research base and recruit eminent scholars, which, in turn, is changing WV's economic base. These changes encourage continued growth in nanoscale science and engineering and provide future opportunities for West Virginia to maximize NSF and state investments.

4.0 Proposed New Cyberinfrastructure

The proposed new cyberinfrastructure will create or deploy:

1. A multi-faceted self-renewing workforce empowered to apply, sustain, and create cyber-based systems, tools, and services over the long-term. Education and training of cyberinfrastructure human resources is a long-term permanent investment to the institutions – *cyber-enabling the workforce*,
2. A nationally competitive computational and visualization environment shared across the partnership, comprised of approximately 900 new computing cores to be located at UAF, new medium-sized clusters for computation, visualization, and training at MU and WVU, a Graphics Processing Unit (GPU) cluster at ASU, and the EnVision system for remote visualization of scientific data,
3. Visualization display resources to be located at eight institutions in both states, including medium-scale stereo display devices not currently available, and enhanced immersive visualization capabilities at two locations, MU and WVU,
4. Software and high-end data capture devices in support of the creation of new digital content, and
5. Networking upgrades at WVSU that will allow full access to remote cyberinfrastructure resources.

4.1 Cyber-enabling the workforce

A careful look at cyberinfrastructure enablement at institutions in Arkansas and West Virginia reveals that one of the greatest needs is an educated and trained workforce that will supply the operational support and training for cyberinfrastructure resources. Thus, development and execution of a strategy for cyberinfrastructure education and training that is self-sustaining over the long term at the participating institutions is a central objective of this EPSCoR Track-2 proposal. Not only will it yield improved opportunities for competitive research funding, it will improve the economic well-being of the residents. The proposal defines a strategy for education and training on multiple levels: 1) faculty researchers and educators and their students, 2) Information Technology (IT) professionals, 3) undergraduate and graduate pedagogy, and 4) high school students.

4.1.1 CI Campus Champions: Pairing Researchers and Educators with CI Resources

The NSF is making enormous investments in Track 2 and Track 1 supercomputers that can operate up to tens of petaflops, and all integrated into the TeraGrid [a24]. However, there is a significant and growing "cyberinfrastructure gap" in the level of access to TeraGrid between EPSCoR and non-EPSCoR jurisdictions [a25]. In 2007, 89% of TeraGrid allocations of time went to non-EPSCoR states. CI Campus Champions address this challenge directly.

The strategy behind CI Campus Champions is simple – pair researchers and educators with local and national cyberinfrastructure resources. The CI Campus Champions concept is an extension of the TeraGrid Campus Champion program, which has very strong community support, including a formal Memorandum of Understanding with TeraGrid [a26]. UAF has been participating in the TeraGrid Champions program since August, 2008. Getting a new allocation and a new research application running on TeraGrid is a labor intensive process that may take several weeks or more. At UAF four new researchers have obtained TeraGrid allocations in the past few months, in part through the UAF TeraGrid Champion program. Two large applications are targeted for the January, 2009, application deadline.

Larger institutions in the CI-TRAIN partnership are in the process of joining the TeraGrid Champions program formally. Smaller institutions with fewer researchers may leverage the activities of the larger campuses, or may join the TeraGrid Champions program.

A strong letter of support from Scott Lathrop, Director of TeraGrid Education, Outreach, and Training, is included in the supplemental documents. It is through his office that the TeraGrid Champions program was launched. We look forward to working closely with the TeraGrid and supercomputing (SC) education communities in the CI-TRAIN project, including sending CI Campus Champions and other faculty to summer and November SC Education workshops, submitting our developed training materials to the Computational Science Education Reference Desk repository, and active participation in the newly launched HPC University virtual community. TeraGrid has committed to providing at least one workshop each year at one of the CI-TRAIN partner sites – a very strong commitment.

Complementary to NSF TeraGrid funding is a view of campus-level “Track 3” resources, including clusters in the 1000-core range, visualization, data storage and collections, and instruments for data collection. Campus resources cannot and should not attempt to compete with TeraGrid at scale. Rather, campus resources can enable nationally competitive research by providing local systems for development and “small” runs, advanced user support for both local and campus resources, and mechanisms that leverage both campus and national resources, effectively a ladder with multiple rungs and a support system that facilitates the transition from one level to the other. The CI Campus Champions strategy is to assist researchers on “small” problems and activities on local resources, and to leverage economy of scale on large or remote resources where appropriate.

CI Campus Champions will become a part of the institution’s permanent investment in cyberinfrastructure. The CI Campus Champions will form a support community, leveraging each others' skills and knowledge. CI Campus Champions will become broadly familiar with the range of local and national computational, visualization, and scientific resources that are available. Each CI Campus Champion will become an expert in the use of at least one local and at least one national computation, visualization, or scientific resource. Examples include: the use of various computational and visualization resources; TeraGrid Science Gateways; Open Science Grid; SURAGrid; Condor; and others. In this project there are two types of CI Campus Champions, both of which have a passion to engage colleagues:

- Faculty Campus Champions typically hold positions as tenured or tenure track faculty.
- IT Campus Champions typically hold IT staff positions, such as system administrators.

The two roles address different aspects of cyberinfrastructure adoption. The Faculty Champion position serves as a vehicle to connect to faculty researchers, motivating them to expand the use of high-performance computing and advanced visualization in their research. A Faculty Campus Champion will first enable his or her own research through the use of advanced cyberinfrastructure, and then be a source of information through at least one training session and for a couple of hours each week for others to use advanced cyberinfrastructure resources. Faculty Campus Champions will become familiar with NSF infrastructure, instrumentation, and research grants in their area of expertise, and will lead in proposals utilizing cyberinfrastructure during the project period.

The IT champion will provide campus expertise on the operational and technical aspects of using HPC resources. The IT Campus Champions will commit to attending monthly CI Training Days events, and will coordinate, advertise, and recruit additional participants from his or her campus to the event as appropriate. IT Campus Champions assist users to quickly get start-up allocations of computing time on TeraGrid systems, to login and use the systems, to port codes to the systems, and to move data. They will also work closely with the partnership’s visualization staff to train local faculty and students on the use of the CI-TRAIN visualization tool kit. They will also serve as a campus point of contact for the scheduling and management of the shared partnership resources.

Each CI Campus Champion will prepare or adapt, in collaboration with project partners, module materials that can be delivered in seminar and/or course form to staff, faculty, and/or students on their own campus, as a part of a formal course, at regional events, and/or at one of the monthly CI Training Days sessions. Each CI Campus Champion will deliver at least two training sessions or course modules during the year. Module materials will be made available on the project web site and may be contributed to community collections.

Each funded Campus Champion will commit to attending two project meetings during the year, including a fall meeting and a Project Review meeting in the late spring or summer. The Project Director will serve as "Champion of Champions" to coordinate activities for champions across the campuses. With the assistance of the partnership, a CI Campus Champion can shepherd one or more CI Days events on his or her campus during the project period.

4.1.2 CI Training Days: CI Technology and User Support Training for IT Professionals

CI Training Days will bring together IT professionals for the purpose of training and perfecting leadership skills that will lead to a sustainable cyberinfrastructure. Participation in CI Training Days is a mechanism to engage the Campus Champions and also the broader community, including IT professionals and faculty that can utilize CI resources.

Each participating institution will select at least one IT Campus Champion committed to participation for at least one year. Participants will attend at least 50 hours of common meetings during the year, which may be in the form of multi-hour electronic seminars or multi-day in-person training. Training may be vendor supplied (such as from Redhat), and additional funding will be sought for these opportunities as needed. Training may also be supplied using the massive amount of web resources available on these topics. Project experts (e.g., Apon, Cothren, Harris, Limp, Pummill, and Szwilski), as well as new CI Campus Champions, are prepared to deliver training. The curriculum for the first year will be determined during the Project Kick Off Meeting at the start of the project, as described in the Assessment section. Topics for CI Training Days may include, and are not limited to:

- Basic Linux use and administration; Basic Linux cluster architecture and administration; Rocks
- Cluster monitoring, alerting, and testing using open source tools
- Visualization architectures and workflows; using EnVision tools for remote visualization
- 3D laser scanning principles and equipment and software operation
- InfiniBand and other high performance and low-latency networks
- Parallel and network file systems; Storage architectures and management
- Overview of scientific computing codes and programming languages
- Application profiling, optimization, and scalability
- Strategies for integrating multiple data streams into visualization
- Condor deployment, including recruiting appropriate applications and users for Condor
- Authentication and authorization architectures, including Globus, Shibboleth, and GridShib; Staying apprised of national trends, TeraGrid best practice, and NSF recommendations for deployment

4.1.3 Complementary Efforts in Undergraduate and Graduate Pedagogy

The CI-TRAIN project will have a dramatic impact on undergraduate pedagogy in many disciplines. CI Faculty Campus Champions, trained in the use of advanced cyberinfrastructure, will be empowered to take their skills back to the classroom. Furthermore, complementary expertise among participants will allow us to leverage curricula and course materials across all participating institutions. Faculty will drive the use of immersive and synthetic environments for the visualization of scientific, engineering, medical, forensic, and mathematical data and models. There are applications of virtual environments in non-technology areas such as the use of virtual classrooms for teacher training and the reconstruction of historical and archeological sites to study past cultures. Efforts to tie computing education to meaningful applications in many disciplines will help to attract today's students to pursue studies in high technology fields, which is important generally and particularly critical to energize interest in traditionally underserved communities. For example at UAF, educators will utilize new visualization resources in the delivery of undergraduate courses such as “Visualizing the Roman City.” This course allows students in a wide range of disciplines to interrogate and grow their understanding of the architecture and life of Romans in the imperial harbor city of Ostia. Students study Roman life and architecture and create visualizations that reflect their understanding of the past [b13-b14]. A second class, “Digital Pompeii,” utilizes complex visualization to create a web-accessible interactive Pompeii (via the Unity game engine [b15]) with the extensive recovered artworks in their original locations. This database will further the investigation of essential research questions about Pompeii: what did the Romans paint on their walls, and why? Does it change according to wealth and social class? The UAF Department of Classics is developing a Heritage Visualization degree that will utilize visualization.

At MU, The Edwards Comprehensive Cancer Center will use the visualization resources in the clinical education of medical and other health profession students. They host a weekly tumor board conference wherein particularly challenging current cases are reviewed. This tumor board meeting is multimedia intensive and requires simultaneous display of digital radiographs, laboratory reports, and microscopy images of tissue biopsies. The multi-screen, media-rich capabilities of the visualization node, along with Access Grid to share with remote sites, will add significant value to the learning experience.

The WVU Department of Geology and Geography offers many courses in Geographic Information Science (GIS) that directly utilize geovisualization concepts, the Cave Automatic Virtual Environment (CAVE), and the GeoWall in their classes. For example, the course “Geovisualization and the CAVE” exposes students to software and hardware technologies used in visualizing spatial information on a range of devices from the desktop and handheld devices to full immersive environments. Students learn to identify and utilize current visualization and geovisualization techniques, to utilize spatial data visualization in scientific inquiry, and to share that information with specialist and general audiences.

To date, humanities scholars have made only tentative forays into the use of GIS and related technologies. At WVU, “GIS and the Humanities” courses will include humanities students and concepts, such as those required in building GIS and related databases that may be utilized to support humanistic studies, and assesses the manner in which current research in GIS for history and archaeology (as exemplified above in the ‘Visualizing the Roman City’ and ‘Digital Pompeii’ courses) can be more broadly used in the humanities. Two other courses, “3D GIS” and “Digital Cities” are under consideration at WVU to provide students with important GIS and geovisualization concepts and methods related to the development of 3D models and spatial analysis within a variety of disciplinary domain areas. The CI-TRAIN project will enable UAF and WVU to build on one another’s progress in GIS and the humanities and extend these resources to other institutions.

Apon and Limp have been very successful in using Access Grid to offer multi-campus/institution formal university classes. For example, “Introduction to High Performance Computing” has been delivered to UAF and UALR from LSU via Access Grid, and will be delivered for the third time in spring, 2009 [a27]. This highly collaborative course has been supported by NSF [OCI #0634064] (PI Sterling) and is available to participating institutions. One of the outcomes of the project Kick Off Meeting will be identify opportunities to leverage partnership instructional capacities to add new Access Grid based courses. Through these virtual offerings we anticipate reaching necessary class sizes across the partnership where an individual campus might not, and to leverage expertise across the partnership for advanced courses.

At UAPB, the Faculty Campus Champion (Walker, Chair of the Computer Science Department) will work with other science departments to create a new computational course with the broadest reach possible.

The UAF CSCE department is addressing declining enrollments and promoting student diversity in several ways that complement the CI-TRAIN project objectives. First, in the redesigned Bachelor of Arts degree students take three courses in a different discipline (e.g., business, geosciences, etc.) that allow the incorporation of an application area into their studies. Second, a new introductory course, "Explorations in Computing", encourages non-majors to investigate computing in a visually-oriented course. Third, a restructured minor allows more students in the other STEM degrees to add appropriate and relevant courses to their degrees so that they have a stronger computational education. For CSCE majors at both the undergraduate and graduate levels, there are efforts to create more courses in high-performance computing which have, at their heart, some of the most important scientific problems (e.g., genetics, pharmacology, economic forecasting). New hiring is targeted towards this area.

4.1.4 Outreach and Education to High School Teachers and Students

As studies from sources such as the National Research Council demonstrate, to create a cyber-workforce it is essential to “prepare the educational ground” at even the middle school level and definitely at the high school level [b9-b11]. It is much too late to begin an educational focus only at the university level.

Because of the structure of accountability in place in most school systems, creating materials for public education students requires close coordination with state education administrators and integration with the current curricular requirements. This project addresses these challenges by drawing upon the extensive relationship that the UAF group has had since 1997 with the EAST Initiative. The EAST

Initiative is “a performance-based learning environment utilizing community service, project-based, service learning, integrated with advanced technological applications in an interdisciplinary environment where the intellectual and problem-solving growth of students is the focus.” [b12] It is a recognized element of existing curriculum in seven states. Robust research has shown that the following can occur with this model:

- Technology is used to promote collaboration, higher order thinking, and problem solving
- Professional development is an important component of the education technology program
- Technology is effectively integrated into the curriculum
- Students are allowed to select appropriate technology tools to obtain, analyze, synthesize and assimilate information
- Effective use of technology allows the creation of new learning environments
- Teachers encourage students to utilize technology to find and make sense of information

A multiple year research effort funded by the US Department of Education found:

> *Among the 16 student outcomes that were studied, analyses indicated that participation in EAST appears to have a* ***positive, statistically reliable impact in five domains****. These included three problem solving domains (defining the characteristics of a problem, assessing the outcomes of a solution, and revising strategies in response to the assessment of outcomes), one motivation domain (motivation for school derived from accomplishment), and self-directed learning style. The preponderance of evidence for program effects in the area of problem solving skills seems consistent with one of the most central goals of EAST, and may point to a particular strength of the program. ..* ***[T]he domains on which EAST has been shown to have an impact are widely recognized as being important for both academic and career success*** [b12].

EAST is in nearly 200 schools in Arkansas, and eight other states with more than 17,000 students participating. The Center for Advanced Spatial Technologies (CAST), with Director Limp at UAF, has worked closely with the EAST Initiative since its founding and supports programs in areas such as GPS, geospatial applications, visualization, and animation, through on-site school visits, web-based resources, [b24] and an extensive suite of short courses [b25].

In West Virginia outreach efforts will focus on expanding the Governor’s School for Mathematics and Science (GSMS) to include concepts from the EAST program as well as offering to secondary school teachers and students workshop experiences that present high-performance computing and visualization concepts. Through a cooperative relationship between WV EPSCoR, WVU, the NSF National Radio Astronomy Observatory, and the National Youth Science Foundation, the GSMS annually offers 120 students across the state the opportunity to participate in hands-on, investigative, small group experiences conducted by teams of teachers and university faculty in student group sessions during one- or two-week summer residential programs. The GSMS program at WVU annually serves sixty rising 8th and 9th grade students who work in research groups at WVU to learn math and physics.

We will build on these foundations in Arkansas and West Virginia. As part of this project, a half-time position in the EAST Initiative will be supported who will work with the GSMS cooperative and the CI-TRAIN and EAST projects. The Outreach individual, who has had extensive experience in K-12 education and the EAST model, will develop specific educational content focused on EAST and the GSMS cooperative that uses the CI-TRAIN project’s research. These will include web materials to be placed on the EAST resources web site and live demos via web delivery of visualization products. In particular the visualization activities that are part of CI-TRAIN will serve as powerful attractors for students. In the past these types of efforts have been used to first attract and then motivate students to attend computer science training at the university level and to pursue employment in the field later. Students attending EAST sponsored short courses at the UAF’s EAST Training center or GSMS sponsored workshops and courses at WVU or MU will have a tour and experience the visualization capabilities.

The project will fund two annual summer programs for 10-12 EAST/GSMS students who will participate in a service-learning community oriented project hosted on both the WVU and UAF campus. Through this project they will learn computational science and visualization skills and also serve as ambassadors to the larger community after the project.

The EAST Initiative has an animation and visualization component, including training in Soft Image XSI (offered by UAF-CAST staff). As a result all 17,000 students have been at least exposed to high-end animation content creation and some 1,200 students are actively involved. The animation "track" of this proposal is a valuable conduit from the high schools to higher education.

4.2 Support for high performance computing and rendering

We propose to address computation needs in multiple ways. The CI Campus Champions developed by the CI-TRAIN partnership will provide a "ladder of access" that will introduce and then grow use of HPC by a wider range of researchers. Several types of local computational resources will be acquired and made accessible to all partners. Furthermore, the CI Campus Champions will enable researchers to access large scale resources on the TeraGrid. Several investigators, described in Section 5, are keenly positioned now to utilize large-scale computational resources on TeraGrid, including support for the integration of computation and remote visualization.

A portion of the funds will purchase three types of resources for computation and rendering in Year 1. A shared capability cluster will be located at UAF. The cluster architecture will be an integrated system, a type currently found at only a few institutions nationally, and will allow processes running across the cluster to compute scientific data, render directly from the same file system, and then view the data from the same file system via Internet access. Lustre/DDN storage systems are proposed for fast file throughput and higher capacity. At least eight nodes, configured with graphics cards and external network connections, will support the EnVision software package from TACC for remote data visualization. Professional services from TACC will assist us in building this hardware and software architecture. This comprehensive platform will be a nationally competitive resource that can be shared among investigators in the project and will be a substantial resource for outreach to smaller institutions and projects. The bandwidth required for remote access for visualization is less than 100Mbps.

Secondly, at ASU a small GPU cluster will be purchased that will be network accessible to the CI-TRAIN community. The ASU Faculty Campus Champion has agreed to deliver Access Grid lectures and create other materials for the partnership on GPU programming. Finally, medium-sized shared clusters at MU and WVU will provide cluster training and support for computation. Although MU and WVU have had a number of clusters owned by individual investigators, they do not currently have a capability cluster that is shared among investigators. The new cluster will provide training on cluster tools, scheduling software, and sharing policies, and prepare West Virginia for a competitive MRI or other proposal for a larger capability resource during the project timeframe. Funds are requested in Years 2 or 3 of this proposal for data centers upgrades at MU and WVU in anticipation of these acquisitions. Representative quotes for the clusters are included in the supplemental documents and described in the Budget Justification.

A fair-share scheduling system, proposed to be Moab or Maui, will be used to manage access to the shared clusters among a number of investigators across multiple institutions and two states. An objective and simple starting point for allocations is to prorate the number of shares on the system to the PI proportional to the dollar value of all funds in force as PI. The PI can distribute the shares equally or not equally among his or her user group as desired. Every PI, whether externally funded or not, will start with a minimum "base" funding. Startup packages will be used to attract new faculty into the partnership. Allocations or usage on TeraGrid will be included as external funding (for example, counting as a grant valued at $0.20/cpu hour). The incentive will be to utilize national resources, since the more investigators use national resources, the higher their priority will be on local resources. Every user will have some level of access. Initial allocations procedures will be developed in consultation with the TACC staff and the project's External Review Team (Ahalt, Boisseau and Roskies – see Sec 8.0 Evaluation Plan) and regularly reviewed and approved by the CI-TRAIN Board of Advisers (see Sec. 10.0 Management Plan).

Initially, users will authenticate to shared clusters via campus mechanisms (e.g., LDAP or Active Directory) and each campus will maintain individual user accounts. We are familiar with grid and community solutions such as Globus and Shibboleth. We will stay apprised of national trends and TeraGrid practice regarding these technologies and will incorporate them as they benefit the project.

4.3 Visualization and display resources

Visualization centers have become an essential capability for research universities. Visualization is rapidly moving beyond its initial scientific applications and becoming a critical research tool across and between disciplines as varied as business, the creative arts, and the humanities, as well as expanding its central role in science and engineering. We propose to create strong scientific visualization capabilities across the entire partnership community to include the conventional interactive 2D/3D display of scientific, engineering, medical, forensic, and mathematical data while also providing immersive virtual environments for better viewing and interaction with 3D modeling and simulation applications, such as geospatial, urban infrastructure, computational fluid dynamics, and molecular modeling.

In this project the visualization components will involve (a) placing base visualization nodes at all the partner institutions, (b) creating staffing capabilities to support and expand usage of the capabilities at all the partners, and (c) building on the existing Mechdyne immersive facilities at MU and WVU. While all partners will have substantial facilities as a result of this and earlier support, various locations will take the lead in selected areas to reduce duplication and increase the overall partnership capabilities. MU, WVU, and UALR will have key roles in immersive and experiential display research while UAF will focus on data ingest, process modeling, and linking network accessible visualization with supercomputing resources.

Every participating institution will have a base visualization node, consisting of a networked facility with a stereo-projection system (DepthQ) and supporting hardware and software and two high-end (e.g. quad-core, 16GB memory) stereo-display enabled workstations, digitizer, and visualization/3D development software. Each node will have 3D content creation software that includes solutions such as Blender and ArcGIS. Each partner will also have access to the EnVision software that utilizes the cluster at UAF and will allow partners to visualize scientific data and analyses running on the EnVision server. Each of these location's nodes will be co-located with Access Grid, and instruction and support will be provided to all CI Campus Champions.

A visualization staff person will be funded at each of UAF, MU, and WVU to assist CI Campus Champions at each of the institutions and other faculty and students at the partners in the use of the visualization hardware and software and to prepare instructional materials. The project also will support animation and visualization content creation. Each partner will have appropriate animation content software (e.g., Soft Image, Vue 6 and others). Partners will then be able to use either workstations or one of the clusters to perform final renderings of complex animation products using open source/freeware rendering applications (e.g. Pixie, POV or others) that can be spread over the multiple cores.

Currently MU and WVU have MechDyne immersive Virtual Reality capabilities. Staff at MU and WVU will provide support for these systems. UALR has a Virtual Reality system that is used in research activities.

4.4 Software and high-end data capture devices for creation of new digital content

In addition to rendering, process modeling, and visualization, data ingest and processing is a central element in the proposed effort. In the past one of the primary limitations to many visualization efforts was the difficulty in the acquisition of accurate "real world" 3D details on buildings, infrastructure, objects, etc [b18-21]. The last decade, however, has seen development of a number of new technologies to both rapidly and accurately measure 3D objects at a range of scales – from the city (100 km^2) to human and object (<0.5 m^2) scales. 3D point-cloud data acquisition (or scanning) is a key technology in the CI-TRAIN project as it is the vehicle through which many aspects of the external world are captured and introduced into visualizations and made available for modeling. The scanning portion of the project at UAF is led by Jackson Cothren who has a PhD in photogrammetry and more than a decade of experience in scanning and scanning applications. Equipment to be acquired at UAF and shared with all project partners includes three types of scanning systems: 1) a 3D motion-compensated long-range (e.g., an Optech ILRIS), 2) a high-speed mid-range (e.g., Leica HDS6000), and 3) a short-range (e.g., Konica-Minolta Rapid7). Several data capture components, also to be shared, will be acquired at MU, including a mobile (mountable) PanoScan Mark III panoramic camera, a mobile (mountable) Velodyne HDL-64E scanner for high-speed mid-range mid-precision scanning of large interiors and outdoor scenes, a hand-held small-object ZScanner 800, and a mobile all-terrain ActivRobots Pioneer 3AT robot with SLAM and autonomous navigation software to facilitate data capture in confined, remote or hazardous areas. MechDyne Conduit Modules linking existing software from ESRI, Autodesk and others to the multi-plane immersive displays that are already in place at WVU will be acquired at MU.

These different systems are necessary as they vary in capabilities, especially range and precision. For example the Optech has a range of 10-1,000 m while the K-M operates in the 0.5-0.8m ranges. The Optech, Leica, and KM are fixed, high precision (6mm and better) units while the Velodyne scanner is designed for very large area, mobile acquisition but at much lower precision (e.g. 2 cm). The suite is needed to acquire the range of data needed by the partnership. Technical specifications and vendor quotes for each are provided in the supplemental materials. These scanning systems together will acquire detailed three-dimensional point cloud data over large outdoor areas or communities, buildings, interior rooms, and items. These 3D data, in combination with electro-optical data from traditional multi-spectral sensors and photographic cameras, can be fused into highly detailed characterizations. The acquisition of these instruments is transitioned over the three years of the project. In the first years existing UAF instruments will be used, including an older Optech, and Konica-Minolta Vivid 9i short range systems. As these current devices are now reaching their effective life-spans the timing for their replacement is ideal.

In addition to these instruments the partnership will also acquire data ingest processing software (e.g. RapidForm, PolyWorks, RockWorks). The instruments and software will be shared among the partners. UAF CAST has had a sharable research instrument pool in place for more than four years, based on NSF MRI BCS #0321286, and they have developed effective strategies to enable wide sharing of equipment by multiple faculty in many locations. A half-time staff person funded by the project will maintain and manage the equipment distribution and sharing, train new users, and increase capability across the community.

4.5 Networking upgrades at WVSU

The project will enhance local network capacity in order to expand to researchers on the WVSU campus use of the proposed Internet2 connection and the interstate and intrastate network connections between the participating institutions. WVSU is the smallest land grant institution in the country, and although it has a robust agricultural and environmental research component, it has struggled to keep pace with networking technology upgrades. The main campus is composed of 26 buildings, eight of which primarily house research facilities and/or research faculty. The primary equipment upgrades requested for WVSU in this proposal are focused on upgrading the campus research network backbone from 1Gbps Ethernet to 10Gbps Ethernet. This backbone upgrade will permit a new level of national research network access and interactivity on the campus by providing the foundational framework for campus Internet2 connectivity. A new network switch that supports quality-of-service and IPv6, with a minimum of six 10Gbps Ethernet trunks, will be purchased. These trunks will reach all research facilities on the campus. In addition, existing Fast Ethernet switches at each research facility will be replaced with 1Gbps Ethernet switches that also support quality-of-service and IPv6.

5.0 Cyberinfrastructure-enabled Science and Engineering Projects

The full set of requested resources, including CI Campus Champions that can assist in the access to an almost unlimited set of national computational resources, along with the computation and visualization resources that will be shared across the partnership, has the potential to enable the broadest possible range of scientific discoveries. Writing this proposal has uncovered a large number of scientists who could benefit from access to advanced computational resources in their research, but who are typically not aware of these resources or how to access them, and who can be positively impacted through the CI-TRAIN project. A sample of the most compelling of these is described in this section.

5.1 Geovisualization, GIS, and infrastructure and community modeling

Investigators: Limp (UAF Lead), Szwilski (MU Lead), Harris (WVU Lead) Apon, Cothren, Dixon, J. Gauch, S. Gauch, Hagstrom, Fredrick, Huneycutt, Johnson, Johnston, Rardin, Smith-Blair, Hapgood, C. Thompson, Tullis (UAF); Srini, Yoshigoe, Ye (UALR); Fuller, Gudivada, Smith (MU);

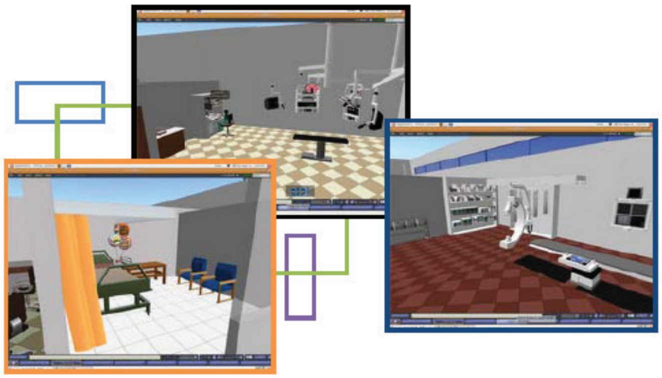
The advanced visualization resources in this project, which include high-end data capture equipment along with enhanced computational resources and display capabilities, will significantly expand a number of on-going research efforts at UAF, WVU, MU and UALR.

Digital communities. One growing area of interest in visualization is the concept of 'digital cities'. WVU has been focusing on the development of digital city models for smaller communities utilizing 3D modeling of structures and landscape, infrastructure and demographic data. The WVU team will partner in this effort with the UAF CAST and UAF CSCE programs. The UAF team efforts have increasingly focused on individual buildings, infrastructure (e.g. utilities) and using the ANSI infrastructure specification SDSFIE [b26] and Open Geospatial Consortium's (OGC) CityGML semantic format [b21] as well as the integration of both of these with Building Information Management systems [b27]. One of the UAF project Co-PI's (Limp) was a founder (1994) of OGC, and this group has continued to develop interoperable specifications for a range of data, many of which have resulted in ISO standards (c.f. ISO 19115). The multiscalar CityGML specification addresses many issues in the acquisition, storage, and representation of spatial data from the region to single structure [b21-b23]. The WVU group will use small communities as a test bed, and the UAF team will work with the UAF campus as its test bed. The focus by WVU on small communities will have the added benefit of contributing to public cyberinfrastructure development and encourage technology integration and employment opportunities in West Virginia.

Data ingest from the real world. Another key goal of the proposed effort is to develop tools and strategies to link intensive and extensive mensuration of the "real world" to computationally-based visualization and analysis. To date the source of much urban and infrastructure visualization has been Computer Aided Design (CAD) files or traditional mapping (GIS). This will be extended though the integration of a wider range of high resolution mensuration processes. An initial goal is to expand ongoing work to create tools and workflows that will merge traditional data sets such as CAD or GIS files with laser scans, motion-capture, high resolution photogrammetry, and other sources to create and populate highly detailed virtual buildings or communities. Prior work at the UAF from a 2004-2007 NSF-IIS sponsored project developed strategies to integrate data from such disparate sources as CAD/GIS (point, line and area features), aerial photography (raster Cartesian data), terrestrial laser scanning (both long-range and close range – 3D point clouds), magnetometry and resistivity (arrays of values), and ground penetrating radar (cross sectional high density returns) [b1-b8]. Key additional data to be used in the research will be (a) airborne and mobile terrestrial LiDAR (especially the Optech and Leica instruments), (b) semantically structured building and other urban data (using CityGML), and (c) real-time data feeds from RFID and other sensors. Work by Cothren [b4] has developed methods to ingest and manage very large aircraft LiDAR data sets in an Object Relational Database Management System and this has been coupled with tools that allow integration of these data with terrestrial photography for automatic feature extraction [b16]. The capabilities in this proposal will allow us to dramatically expand this research.

A related research program, currently funded by NASA, at UALR is developing algorithms for understanding photo-realistic 3D models as input to distributed unmanned ground vehicle (UGV) navigation within structures. The problem of 3D modeling includes data registration, texture mapping, and data reduction, and the problem of 3D scene understanding includes scene segmentation, multi-resolution data analysis, data enhancement, and object modeling. 3D scene understanding is essential for creating symbolic representation of the environment as input to UGV navigation. The UALR team has been developing an approach [q1-q6] that utilizes both texture and 3D point cloud data. The HPC and data capture capabilities that would be made available from this proposal will allow development of new algorithms and their application to a distributed UGV system. The computer cluster will support high fidelity hardware-in-the-loop simulation of the distributed UGV system. The visualization resources will be used to display the scene model and the results of data analysis. The combination of high performance computing and visualization infrastructure will enable new research discoveries in large-scale 3D scene modeling and conceptual understanding which would not otherwise be possible.

The above efforts also link closely with ongoing work by Szwilski's group at MU [s1], sponsored by the Economic Development Administration and WV mining interests, where an immersive virtual environment is being developed for mine safety and rescue training. This virtual environment, currently built in Second Life, is based on an actual mine safety training facility at the Mine Safety and Health Administration Academy. The reconstruction to date has been done manually, including the recreation of numerous pieces of mining and personal protection equipment. Some of the larger pieces of equipment (like vehicles) were converted from CAD files, but still had to be painstakingly textured and then scripted to be made operational. This work will benefit from the CI-TRAIN 3D content capture technologies (especially the Velodyne, SLAM and PanoScan instruments), sensor-linkages, and semantic models that incorporate dynamics. Virtual worlds and immersive environments have become especially useful for training and experiential learning in many types of situations that are difficult, hazardous, or even impossible to construct in the real world.



Smart Worlds. In separate, but closely related, recent work Thompson (UAF) and associates have investigated a family of technologies relevant to pervasive computing and the merging of these into virtual world representations. General methodologies have been developed for pervasive computing [c1-c9], RFID middleware has been created that provides real world identity tagging technologies [c10-c17], practical natural language interfaces have been implemented for human/machine communication [c18-c23], representations to automate workflow have been designed [c24-c28], a grid indexing technology for querying distributed datasets has been proposed [c29-c34], and a synthetic data generator for creating large (i.e., terabyte scale) realistic datasets has been written [c35-c39]. To investigate integration of real-world data sensor feeds in a virtual world, in fall, 2007, Thompson and associates acquired a Second Life (SL) island and a pilot project to model virtual RFID focusing on *Healthcare Logistics in a Virtual World* was launched. This domain was selected because hospitals contain sophisticated equipment and a complex supply chain [c8, c40]. The results are encouraging. However, the geography, building plans, and equipment available in SL are synthetic and restrictive. The team is expanding their work to utilize OpenSim rather than SL and building translation capabilities between sources such as CityGML and OpenSim. Efforts that focus on moving from high resolution scanning of objects (Konica-Minolta instrument and software) to rooms (Leica instrument) and then exterior structures (Velodyne and Optech instruments and photogrammetric cameras) into CityGML and then to OpenSim are a course of action for moving extensive real-world content into OpenSim, SL, and many other virtual worlds such as the Unity and Havoc game engines.

One shortcoming of most of these virtual environments is their inability to realistically model air and water (or other fluids) – neither their flow dynamics nor compositional makeup. A critical element of mine rescue (and other hazardous environment training) is the ability to monitor and control the flow and composition of gases (such as nitrogen, oxygen, methane, carbon monoxide, and carbon dioxide) throughout the mine. This requires a realistic real-time simulation of air flow, the mixing of components from multiple sources and their dispersion over time and space, and the ability to determine its breathability and/or its combustibility. This has led to an effort at MU by Smith to incorporate a new level and type of physics into the virtual environment. The proposed physics is based on smoothed particle hydrodynamics [s2], a fast particle-based (mesh-free) dynamics method, and will be incorporated into OpenSim and/or the underlying Havoc or Unity physics engine. All these efforts will accelerate the development of content needed by the growing web accessible virtual communities. The results of this work will have substantial impact since populating these virtual communities with "real world" content is now seen as a major constraint to their continued growth. The structure of CI-TRAIN will allow these groups to share data ingest capabilities and leverage each other's efforts.

Enhancing humanities research through geovisualization. The recent dramatic developments in GIS have had significant impact on engineering, the physical and biological sciences and the social sciences, but GIS has made only limited inroads into the humanities. Part of the reason for this lies in the epistemology of GIS and the issues that arise in merging scientific methods with humanities approaches [d1-d5]. The proposed project continues an ongoing focus at WVU on exposing researchers and students from humanities disciplines to the capabilities of visualization for exploring art, history, and the social sciences. Data visualization is especially powerful when representing spatial relationships that are difficult, if not impossible, to explore in tabular, textual, or map forms. The visual processing of spatio-temporal data in particular is challenging. Geovisualization is beginning to be used as an important tool for understanding the conjunction of time and space that can be informative to both humanities scholars and, arguably even more so, to the general public [d6]. Dynamic visualization transforms the static tabular record in digital textual databases to visual representations that illustrate historical processes.

This project will continue work in the spatial humanities using geovisualization, and immersion tools to provide data analytical approaches that are sensitized to the traditions of humanities disciplines and yet can utilize the rich resources that the humanities provide. Spatial story telling through geovisual immersion is one such avenue of enquiry [d7]. Thus humanities scholars and students will be exposed to spatial concepts, geospatial technologies, geovisualization and immersion in research and educational training contexts, and they will develop spatial analytic skills that will help them apply these STEM technologies to gain new insights within their own domain areas [d8, d9]. The WVU efforts are paralleled by UAF activities such as the “Visualizing the Roman City” and “Digital Pompeii” initiatives [b13-b15].

Enhancing local and virtual geocollaboration. Virtual collaboration is an important theme of this project and ties together the implementation of the visualization infrastructure. At WVU specific attention will be paid to virtual geo-collaboration: the real-time sharing of geovisualizations in multiple locations to support research and decision making. Currently this is possible through a loose coupling of technologies such as sharing KML files between institutions and viewing them in Google Earth and communicating via peer to peer communication services such as Google Talk [d6]. This approach, however, does not allow for real-time updates, or editing information or shared navigation. A step toward a tightly coupled geocollaboration system has been developed at WVU based on ESRI's ArcScene and enterprise geodatabase technologies that allows for participant-driven navigation and near real-time interaction with data. (The local system syncs the current state of the database at chosen time increments, generally set from 45 to 60 seconds.) With the development of the new XNA Game Studio based Spatial Experience Engine at WVU [d6], geocollaboration is being constructed on networked video game technologies that allow for real-time interaction, 3D immersive environments, and real-time communication. In addition to being available in the MechDyne FLEX systems in West Virginia and on the visualization platforms acquired as part of this proposal, each of these technologies is available for use on desktop computers, increasing access, though decreasing the level of experience and local collaboration. These efforts parallel the work being done at UAF using the Unity game engine and MU with the Havoc system, and all three groups will be able to use the CI-TRAIN setting to leverage their prior work.

A smart world is the desired outcome. Visualization and virtual worlds are approaches for getting there. Early intellectual challenges will involve understanding these virtual world architectures, and how to scale them dramatically. Disciplinary boundaries can be breached and innovative investigation accomplished through the co-location and visualization of previously separate data sets. Processes that are frequently the domain of particular disciplinary silos are brought together because they occur at the same geographic location. The potential opportunities and benefits to be gained from the integration of geospatial sciences with immersion and geo-visualization are demonstrable and substantial [d2-d4].

The work proposed will be a significant step toward the realization of Wade Roush’s “Second Earth” [s3], a visually immersive environment rich with real-world content and real-time responses to real-world events, bringing a better sense of presence to mirror world applications and a better sense of place and time to virtual world applications.

The work proposed by MU will have a dramatic and direct impact on the applicability of virtual worlds to all types of training, experiential learning, and ad hoc discovery by bringing more realism to the virtual environment. The most immediate impact will be on training exercises that benefit from better dynamic modeling of air and water, such as first responder training for chemical leaks, biological attacks, flooding, and others. The multi-scale aspects of this work will have a significant impact on “hands-on” learning and discovery.

The broader impacts of this research are significant. Important public participation efforts centered on spatial information continue to be streamlined as new methods for utilizing contemporary web mapping applications and virtual globes gain greater acceptance. Combining geospatial data, 3D modeling, visualization, and spatial analysis technologies, digital cities can provide a powerful collaborative environment for managers, planners, utility units, emergency response personnel, and others to quickly and intuitively manage the city landscape. These visualizations can be used in day-to-day city management, infrastructure monitoring and maintenance, assessing proposed developments and analyzing their impacts, emergency response planning, and, importantly, public participation. The issue with collecting public perspective data is that it often remains separate from the data used to create models and make decisions.

Assessment, monitoring and modeling of transportation infrastructure (*Investigator:* Szwilski) is a significant research area of the Marshall University Rahall Transportation Institute. A U.S. Federal Railway Administration grant ($5.4M, 1999-2009, Szwilski Co-PI) [s4-s10] has developed multi-sensor technologies mounted on a mobile platform that assess and evaluate rail track superstructure and substructure. Integration of large-scale computation, visualization, and storage resources is a requirement of achieving the principle objective of the research – to fuse data from the multi-sensors in real-time to develop a valuable rail track inspection tool. In addition, Lidar scanning, HADGPS and geophysical sensor technologies are being applied to the mapping and monitoring of highway infrastructure. 3D modeling of bridges and mapping of geohazards (slope stability, subsidence) are a part of this effort [s11]. The Appalachian Consortium for Geohazards in Transportation, comprised of the the state DOT's, Geological Surveys, USGS, FHWA, US Corps of Engineers, CSX and Norfolk southern railroad companies, was established in 1999 to share information, best practices and technology (Szwilski, Chairman) [s12].

5.2 First Principles Investigation of Low-Dimensional Multiferroics

Investigators: Bellaiche, Salamo (UAF)

The objectives of this aspect of the proposal are to gain a deep understanding of multiferroic nanostructures, in general, and to reveal original, exciting phenomena in low-dimensional multiferroics, in particular. To achieve these objectives, *the entire* unknown or poorly understood issues mentioned above, as well as other related problems, will be investigated by developing and/or using state-of-the-art techniques from first principles.

Multiferroics are materials that can simultaneously possess ferroelectricity (that is, a spontaneous electrical polarization that can be switched by applying an electric field) and magnetic ordering [e1]. Such a class of compounds exhibits a magnetoelectric (ME) coupling that is of high technological relevance, since it implies that electrical properties are affected by a magnetic field or, conversely, that magnetic properties can be varied by an electric field. Therefore, they are key materials for actuators, sensors, and energy conversion and storage. They are specifically relevant to energy efficiency, and transportation, conversion, and storage technology.

Multiferroics, in their bulk and (thick) film forms, have been intensively studied in the last century, from the sixties to the eighties (see, e.g., refs. [e2-e6] and references therein), then "fell in disgrace" among the scientific community (mostly due to weak ME coefficients) until recently, experiencing a huge rebound in interest (see, e.g., Refs. [e7-e15] and references therein). Consequently, an extensive understanding of multiferroic bulks and films has been gained and numerous breakthroughs have occurred. For instance, one better understands why so few materials simultaneously exhibit ferroelectricity and magnetism [e7] and how their magnetic ordering can be efficiently controlled by the application of electric fields along specific directions [e11, e15]. Similarly, it is now clear that some multiferroics can possess a rather large electrical polarization [e8,e12].

On the other hand, little is currently known and/or deeply understood about multiferroic nanostructures -- e.g., ultrathin films, wires, nanotubes, and three-dimensionally confined multiferroic nanodots, despite their technological promise in tuning towards a desired behavior that is not always achievable in a bulk-like material and despite their fundamental promise in yielding novel, exciting effects. Note that such promises mainly stem from the fact that such nanosystems should be exquisitely sensitive to their morphology because: (1) the interactions that give rise to a spontaneous polarization and/or magnetism are drastically modified in the presence of surfaces and interfaces; (2) there is a strong coupling of ferroelectricity and magnetism to the mechanical boundary conditions; (3) the electromagnetic fields arising either from depolarization or demagnetization also interact strongly and directly with the ferroelectric or magnetic order parameter, respectively; (4) ferroelectric and magnetic order parameters are inherently coupled in a multiferroic, implying that the direct modification of one of such order parameters automatically affects the other order parameter. As a matter of fact, the precise effects of the substrate, growth orientation, surface termination, thickness, and electrical boundary conditions and dimensionality on the properties of multiferroic nanostructures are basically unknown.

For instance, one may wonder if the ME coefficients can be greatly optimized when going from bulk to nanostructures, and, if so, what are the microscopic origins of such desired optimization. Similarly, why the ferroelectric domains found in some multiferroics thin films [e14] are so different in morphology and size from those found in ferroelectric thin films [e16,e17] remains an unanswered question. It is also of large interest to determine if unusual phenomena found in ferroelectric or ferromagnetic nanostructures (e.g., the so-called bubbles, single and double vortices, and onion states [e18-e26]) still persist in low-dimensional multiferroics, or rather if their unique coupling between electric and magnetic dipoles yields original patterns that await to be discovered. Furthermore, determining the dynamics of ferroelectric and magnetic domains in a multiferroic nanostructure is an important issue that remains to be addressed. Are the motions of these domains governed by new laws because of the ME coefficients? Another research area, among many others, that needs to be pursued in multiferroic nanostructures explores the possibility of creating a material with a negative index of refraction (see Refs. [e27,e28] and references therein). As a matter of fact, it can be considered that some specific conditions associated with low-dimensionality (e.g., a particular thickness and well-given mechanical boundary conditions) can yield a nanoscale multiferroic system for which both the real part of the complex dielectric susceptibility and the real part of the complex magnetic susceptibility are negative within a frequency window. If this is the case, the quest for extraordinary devices, such as superlenses [e29] and “invisibility cloaks” [e30] will be fulfilled.

Collaborations with the Salamo group (UAF), which has an ongoing experimental program in multiferroics will be further strengthened. This will allow the grounding of simulations and to fully, deeply understand the complex materials under investigation. It is strongly expected that the results will significantly enhance the current understanding of multiferroics and nanostructures, by revealing their (anomalous) properties, identifying the microscopic features responsible for such properties, and by discovering new phenomena. These insights, as well as the direct use of the so-called inverse method, will have great impacts on the design of new and improved devices, for example, actuators, sensors, and data storage. Moreover, the publications in high-quality refereed journals, strongly expected (because of the huge, current interest in the proposed topic) if this proposal is granted, will certainly help the future career of the involved students. The resources proposed here will leverage currently funded grants from NSF and ONR totaling more than $9M.

These objectives will be achieved by further generalizing and/or using three complementary numerical techniques: direct first-principles techniques, first-principles-derived effective Hamiltonian approaches, and inverse methods. Computation time of 70 million hours (if performed on the UAF supercomputer) each year is estimated to accomplish the envisioned transformational research. Since the proposed shared computational cluster will only be one step toward meeting these goals, providing about 7.9 million hours each year, the CI Campus Champion is an essential component that will provide local skills sets for accessing local resources and also facilitate access to the unprecedented computing resources available on TeraGrid. CI Campus Champions will complement the research and significantly reduce the startup time for current and future students and postdoctoral associates to do research.

5.3 Atomistic Simulation and Advanced Computational Visualization of Defects in Nanocrystalline Materials

Investigator: Spearot (UAF)

This research, supported in part by NSF Grant #0800718 ($259,269, with PI Huang), focuses on the behavior of interfaces on the nanoscale and the development of multiscale structure-property relationships which are motivated by atomistic simulations [f1-f3]. The primary thrust of this work is to use molecular dynamics (MD) to identify the mechanisms associated with dislocation nucleation in nanocrystalline (NC) metallic materials. Of particular interest is the role of impurities or dopants on grain boundary behavior, an important aspect of material behavior, which is currently unresolved. For example, recent work by Spearot et al. [f4, f5] aims to use atomistic simulations to study the influence of dopant atom concentration and distribution on the mechanical properties of NC materials. Preliminary results are shown in Figure 3 for a Cu-Sb alloy with 12 nm average grain size and two different Sb concentrations [f5]. Figure 3(a) shows a section-cut of the initial grain structure of the sample. Figure 3(c) shows a snapshot of dislocation activity during tensile deformation. MD simulations indicate that Shockley partial dislocations are nucleated from the grain boundaries and propagate across the grain interiors (leaving a trailing stacking fault in their wake), in agreement with previous MD simulations in the literature. Interestingly, grain boundary sources for dislocation nucleation appear to correlate visually with the presence of Sb dopants at the grain boundaries [f5].

The proposed CI-TRAIN parallel visualization capabilities with appropriate storage facilities for visualization purposes enables atomistic simulation to study mechanisms associated with failure of nanocrystalline materials with larger grain sizes (closer to typical experimental samples) and more realistic grain size and disorientation distributions. Ultimately, the aim is to provide an understanding of the inverse Hall-Petch response in nanocrystalline materials with dopants or impurities distributed along the grain boundaries.

It is clear from the Figure 3 that advanced visualization is a key component in this field of research. Atoms in Figures 3(a) and 3(c) are colored by the centrosymmetry parameter [f6], which is commonly used to identify regions of local lattice distortion, such as around grain boundaries and stacking faults, in cubic materials. Molecular dynamics is capable of computing atomic stresses and energies; however, a molecular level picture of deformation is critical to correlate such quantities to the physical mechanisms that lead to mechanical failure. Current computational facilities are capable of performing simulations on

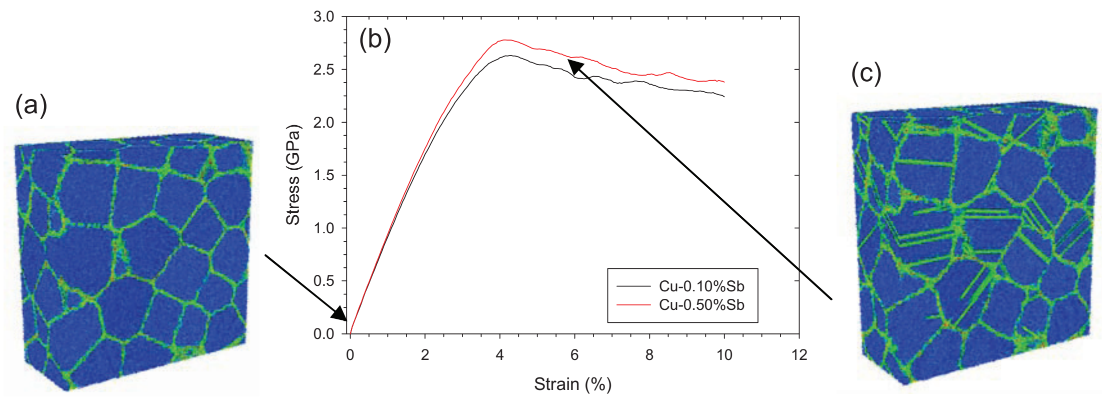


Figure 3: (a) Initial microstructure of a NC sample with 0.5 at% Sb at grain boundaries; (b) stress-strain response during uniaxial deformation; (c) dislocations nucleated from the grain boundaries in nanocrystalline Cu with 0.5 at % Sb.

tens of millions of atoms within the MD framework; however, future advancement of this research is limited by (1) the ability to store data required for resolving images of the atomistic output and (2) the ability to render three-dimensional models of the atomistic output in a parallel visualization environment. Accordingly, atomistic visualization is restricted only to smaller models (such as in the 3 million atom model shown). Data sets generated for larger atoms are in the range of 1TB in size, demanding the need for an integrated computation and visualization system. The estimated computing requirements in 1Q09 are 300,000 hours for just one of the 3 to 4 Ph.D. students working in this problem area.

5.4 Discovering new physics and phenomena in nanostructured materials
Investigator: Huaxiang Fu (UAF)

This research is focused on discovering and understanding new physics in novel types of nanomaterials. Access to high-performance computing facilities is required for understanding the following novel nanostructure materials that possess unusual properties of technological importance: (1) nanostructures of ferroelectric (FE) and piezoelectric oxides (which exhibit many electrical, mechanical, and structural properties that are not shared by other materials, see below); (2) semiconductor nanomaterials (which are currently one of the major pursuits in nano-technology [g1]). The state-of-art first-principles density-functional theory (DFT) [g2] will be the main computational tool. This theory is known to be very accurate. However, applications of this theory to nanomaterials are exceptionally difficult since meaningful modeling of nano-sized materials requires the consideration of several hundred (or even thousands) of atoms, which far exceeds the size range (~100 atoms) that normal DFT can handle. For this reason, many existing theoretical studies of nano-dots rely on semi-empirical or model approaches. By comparison, the first-principles approach has much greater prediction power and is able to handle a realistic atomic-scale environment. While the direct DFT study of nanomaterials no doubt poses a great challenge, overcoming it, on the other hand, implies a new area of unknown science to be explored and discovered.

Ferroelectric and piezoelectric perovskite oxides distinguish themselves from other classes of materials by being able to efficiently convert electricity into mechanical energy or vice versa. Consequently, they have been widely utilized in energy-conversion devices such as transducers and actuators, robotics, and micro-electric mechanical systems [g3]. These materials have also been ubiquitously used in ultrasonic imaging for human health, arrays for telecommunications, and military sensors for national security [g4], as well as in nonvolatile random accessed memories [g5]. Fundamentally, the spectacular modern theory of polarization using geometric phase [g6, h7] as well as the significance of polarization in density functional theory [g8, g9] are examples indicating the importance of the field.

Compared to bulk ferroelectrics, FE nanostructures (e.g., thin films, wires, nanotubes, dots) are poorly understood [g10-g12] (in fact, most of their properties remain entirely unknown). Recently, the Fu and Bellaiche group predicted that a novel vortex phase may exist in FE particles [g13], using first-principles derived effective Hamiltonian methods [g14, g15]. The properties in FE nanostructures were found to be very different from those of the bulk, indicating new physics and knowledge in nano-FE. The goal here is to be able to model the FE nanostructures using the direct DFT theory, since the direct approach is reliable and accurate down to very small size (e.g., a few atoms) and can also potentially take into account the realistic surface and boundary conditions. It is well known that the relevant energy scale of ferroelectric instability is only a few milli-eV, a property that requires very accurate modeling. Surface conditions are expected to be increasingly important when the size become smaller, in which the direct approach thus becomes necessary. Though an accurate and efficient mix-basis DFT code has been developed [g16] (which has been successfully applied to study electrical, dielectric, electromechanical, optical and elastic properties [g16-g22]), its applications to FE nanostructures have not been attempted because of the lack of sufficient computing power. This challenging problem in materials science can be tackled with access to high performance computing clusters.

5.5 Interactive visual exploration environment for real-time image guided surgery

Investigators: Shafirstein,Topaloglu (UAMS)

Recent advancements in computing power have made it possible to simulate minimally invasive and thermally based surgical procedures for the treatment of solid tumors, prior to surgery. However, to assist the surgeons during therapy, large parallel computing resources are required to perform real-time image guided surgery [h1-h4]. To that end, a 3D image of the target tumor, and adjacent anatomical tissue, must be processed and imported into the software simulation packages, computed, and sent back to the surgical suite within 1-3 seconds. As the surgery progresses this process must be repeated many times with feedback response time of 1-3 seconds. While some surgeries take hours to complete, a huge amount of data (terabytes) could be accumulated in a single surgery. The goal is to develop real-time multimodality image guided surgery that includes thermal ablation and endoscopic and robotic surgery for the treatment of cancer tumors [h5-h9]. Development and evaluation of advanced computer programs for an interactive visualization environment of multimodality image guided surgery is the objective of this study. The integrated computation and visualization environment will ultimately lead to: 1) safe development and testing of novel surgical techniques; 2) teaching and practice of multimodality surgical procedures, in real time and 3) real-time telemedicine for image guided surgery and treatment planning.

5.6 Near Field Scanning Optical (Fluorescence) Microscopy (NSOM)

Investigator: Norton (MU)

Near Field Scanning Optical (Fluorescence) Microscopy (NSOM) has the potential to provide multimode information (topography, mechanical properties, optical properties) simultaneously in near real time (noise limited). With sufficient signal, low density particle centers should be locatable with at least 1 nm resolution, using deconvolution methods similar to those of FIONA [j1]. However, the current reality, as can be seen by the lack of dominance of this superior technique for non-destructive analysis of nanometer objects, is that NSOM systems provide relatively poor AFM images and lower than anticipated optical resolution. Supercomputing could impact the ability to image with the current Nanonics NSOM system primarily in four ways. First, the fiber optic tip represents a massive, complex structured surface used for imaging. Because the target objects in Figure 4 are ca 7 nm in height (DNA objects = 2 nm, nanoparticles ca 5 nm), only asperities in the last ca 2 nm of the fiber tip "image" the objects. However there may be several such asperities in such a tip. Access to supercomputing resources gives the ability to obtain rapid "deblurring" of the images to make them interpretable.

The second mechanism through which supercomputer assisted visualization can impact NSOM is through real time determination of the center of the fluorescence signal. The asperities in the tip will negligibly convolute the optical field, therefore a Gaussian fit to the intensity distribution would yield a noise limited localization of the emitting object. Nanometer scale positional accuracy in the determination of the location of isolated particles should be possible. Real time knowledge of these positions is not currently possible because such determinations are made in post processing. Only a limited number of target samples can be characterized and real time triage of samples would advance the field.

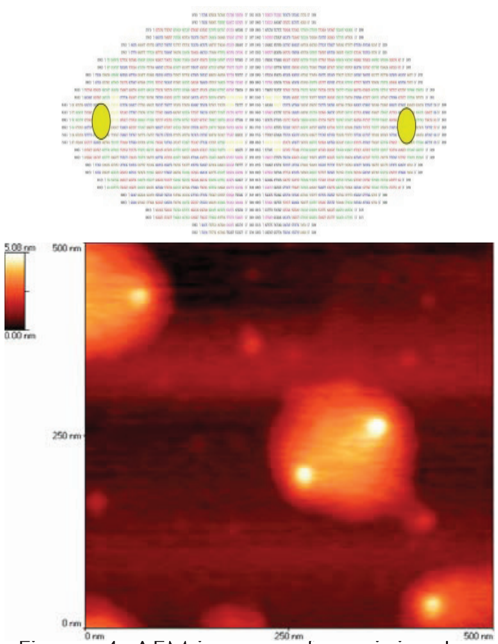


Figure 4: AFM image of semicircular "Origami" construct (diam. ca 100 nm) w 2 nanoparticles directed to the surface

A third contribution of real time computation would be registration of the optical and multitip (mechanical force) images. The determination of the offset of the optical center with respect to the imaging asperities on the tip would enable high resolution registration of these images, which is a requirement for progress in the field of nanoscopic multimode imaging. Such improved imaging has relevance not only to nanoelectronics, but also to molecular biology.

The fourth contribution through the combination of multimode scanning probe microscopy with supercomputer capability is real time 3D visualization as a human interface for this form of imaging. In addition to artifact and noise elimination (through averaging), which is almost unheard of in this field, the ability to encode 3D information in stereoptic, rather than color coding (the normal method of topographic representation in the scanning probe field), frees color to represent intensity and spectroscopic (wavelength) information in a manner more native to the viewer/scientist. This 3DI viewing at multiple scales in multi-mode is fully compatible with the objectives of the thrust in developing real world physics model in virtual representations of real systems. This web based approach provides a natural mechanism for distribution of image data, including the NSOM data discussed above, to a very broad audience.

5.7 Adaptive Simulation of Relativistic Particle Transport Systems

Investigator: Jiang (ASU)

Relativistic particle transport systems describe a large number of particles by phase space distributions, which are snapshots of where particles are and how they move at a particular time. When the system is in equilibrium and is able to maintain equilibrium, the Boltzmann equation can lead to macroscopic hydrodynamic equations, and can be used for the study of equilibration from non-equilibrium initial conditions and for the study of systems far from equilibrium [k1].

The focus will be on a system of massless ultrarelativistic partons which move at the speed of light. Different from classical billiard balls [k3, k4], space and time are related relativistically. Under semiclassical approximation and the Abelian dominance approximation [k2], the equations of motion become a set of equations that resemble classical transport equations. The Boltzmann equation will be solved by the test particle method. The phase-space will be sampled by point particles.

Realistic simulation is memory-consuming and computationally intensive [k5] and adaptive simulation schemes will be used. The proposed research intends to develop application-level resource management and scheduling mechanisms to take advantage of aggregate heterogeneous systems where each connected computer contains multiple GPUs to explore both task and data parallelism. Computing resources can be arranged automatically and dynamically so that the simulation will be conducted speculatively and aggressively to utilize any idle/unused computing units locally and remotely [k6,k7]. This application-level scheduler works with existing middleware to utilize computing power within computers and clusters.

In this research: 1) GPU clusters are utilized to hierarchically parallelize speculative simulation; 2) Multi-layer checkpoint/restart schemes will be applied for fault resilience, load balancing and platform reconfiguration; 3) Dynamic data/workload migration and adjustment will be supported. This research will demonstrate how full-fledged flexibility can be integrated into scientific applications.

The results include: 1) demonstrating how to hierarchically parallelize real applications using GPU clusters; 2) applying similar strategy in molecular dynamics [k8, j9, k10, k11] and other fields [k12, k13, k14] and deriving a generic approach for all scientific applications; 3) providing sufficient materials and environments to open a new course "Scientific Computing Programming" for non-Computer-Science researchers and students.

5.8 High Performance Cyberinfrastructure Driven Research in Software Visualization
Investigator: Gudivada (MU)

This research addresses the need for customizable and configurable tools to support the entire application lifecycle management -- requirements management, software design and architecture, software configuration management, build configuration management, release management, support for testing and bug tracking, and improving software quality through software metrics and measurements.

Software visualization naturally plays an important role in software engineering. Requirements can be visualized to assess their dependency and perform impact analysis. Software design can be traced back to requirements using visualization [m8]. Visualization can also be used for localization of code for bug fixing [m4, m7, m6, m11, m15, m16, m17], software design [m1, m5, m10, m12], software reliability [m18], project management [m9], testing and debugging [m2, m14], and to facilitate code and application comprehension [m3, m13]. Code version history, differences between releases, static properties of code, code profiling and execution hot spots, and dynamic program slices can also be visualized [m11]. A hierarchy-based visualization approach can be used for understanding software metrics. The ACM Symposium on Software Visualization (started in 2003, held in alternate years), attests to the importance of visualization in software engineering. However, most of the existing software visualization techniques have originated within the context of small software systems.

SourceForge.net is the world's largest open source software development web site, and has the largest repository of open source code and applications. It hosts more than 180,000 projects and has more than 1.9 million registered developers. The source code of several applications from SourceForge.net is used in MU software engineering courses: JUnit, Hibernate, Eclipse, Subversion, ImageJ, Derby, and Lucene.

This project utilizes computational and visualization resources and open source software to investigate innovative approaches to software visualization to support the gamut of application lifecycle management activities. The project uses a modest number of cores (e.g., 16) over time, will run well on the proposed new cluster at MU, and will provide a range of education experiences for software engineering students.

5.9 3-D Reconstruction of the Plant Secondary Cell Wall
Investigator: Hood (ASU)

The objective of this research is to reconstruct a 3D image of the secondary cell wall of leaf epidermal cells through microscopic and spectroscopic imaging. The enzyme work and mapping experiments are funded by the Department of Energy with cost share from the Walmart Foundation and the Walton Family Foundation. Techniques are being developed to observe the relationships of cell wall polymers within individual cell layers that have relatively uniform wall structure, such as epidermal cell layers [n1]. Antibodies to the major polymers of the wall—structural proteins, hemicelluloses, lignin, and cellulose, the latter using labeled cellulose-binding-domains—will be conjugated to different compositions of nanotubes in order to map the location of the unique molecules through localization of specifically associated metals [n2]. Mapping experiments will be conducted after treatment for various times with cell wall degrading enzymes to understand the interaction of the layers of polymers.

The second experimental system involves Raman spectroscopy. Different types of bonds within biological materials, for example, C-H and phenolic rings, can be detected via their Raman vibration signaling. Samples will be mounted in a “wet” cell that has microfluidic introduction capabilities. A “bond map” will be constructed of the original sample without treatment. High resolution images of the samples can be viewed and captured while samples are on the Raman stage. The same sample will be subjected to enzyme treatment, and a new bond map of the surface constructed at 15 minutes and 2 hours after enzyme treatment. These maps will indicate the changes in bond topography upon enzyme treatment. The goal is to coordinate results from the three instruments to partially reconstruct the process of enzyme deconstruction of secondary cell walls. Image reconstructions of the bond maps and the topography of the macromolecules mapped using the specific antibodies can be overlayed. Visualization of these complex overlays will begin to elucidate some of the more complex interactions in the secondary wall that are currently understood only through biochemical means, and will assist in the understanding of how to cost effectively recover the components of the wall for use in bio-based product development.

5.10 Nano science application to improve the performance of concrete

Investigator: Selvam (UAF)

Every year billions of dollars worth of concrete is utilized in the U.S. and around the world. At this time the durability of concrete is limited because the tensile strength of concrete is 1/10th of compressive strength. Because of this, property concrete fails due to corrosion, shrinkage etc. One of the key challenges to improving the tensile property knowing the atomic structure of cement or calcium silicate hydrate (CSH). For materials like copper and iron the atomic structure can be determined experimentally. However, CSH atomic structure cannot be determined experimentally because it has an amorphous atomic structure. Once the atomic structure is known, one can manipulate the atomic structure and improve the tensile strength. The Arkansas State Highway and Transportation Department is supporting a project to determine the atomic structure of CSH using computer modeling. In this project the atomic structure is determined by calculating the bulk material properties of the few proposed atomic structures of CSH. Access to large-scale computational resources will be required to accomplish these research goals.

5.11 Computational analytics, informatics, visualization and virtual reality

Investigator: Tudoreanu (UALR)

Protein folding. Protein rendering is extremely processor intensive due to the large molecular size of most proteins, and current techniques often do not render details but only the backbone. To analyze second- and third-degree folding types visually, a user needs all those details. Rendering can be performed concurrently on multiple processors, and what-if scenarios displayed to the viewer. Given the complexity of the geometry of protein surfaces, the best approach to understand them requires user immersion taking advantage of the innate abilities of the human visual system.

Visualization of processes. The design, implementation, and debugging of parallel processes, such as the ones developed to be run on a supercomputer, is not a trivial endeavor. Students and users of the supercomputer can benefit from animations of how these processes execute rather than from pieces of static code and mental projection of the system’s state. To create these highly interactive animations that put the users “inside” the running supercomputer, data from select running programs need to be collected, processed, and transformed into graphics. Additionally, large displays capable of handling large images provides a significant advantage.

5.12 Monte Carlo Modeling of Protein Structures and Polymeric Materials

Investigators: Tang, Darsey (UALR)

The goal of this project is to predict protein 3D tertiary structure. In a first step, a study of 27,000 proteins in the Protein Databank [y1] has generated a large number of secondary structures for a new protein using Monte-Carlo simulation. A novel clustering algorithm is used to find the most probable secondary structure. Each new protein requires up to one million simulations, each with very large memory and cpu requirements. A clustering algorithm of this magnitude cannot run on single computer and requires parallel processing. In a second step, the 3D structure that requires the minimum energy of formation is selected from among a large number of simulations using ab initio quantum mechanics between the atoms forming the protein.

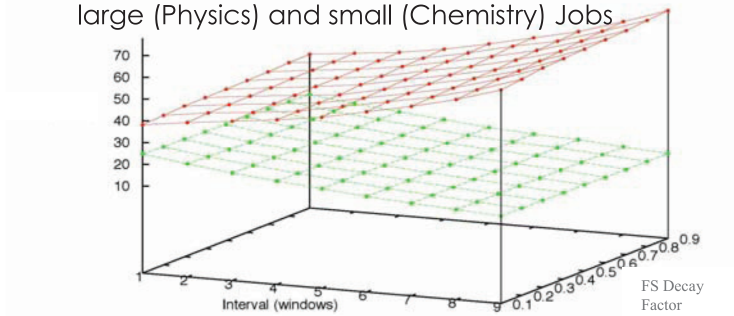
Finally, Monte-Carlo simulation is used to calculate the statistical properties of a large number of known polymers to form a polymer property database reflecting the co-existence of statistical and physical properties of the real known polymers. Data mining is used to find the association and link between statistical properties and physical properties of polymers from this database. The structures of the new polymers with the desired physical properties are found by calculating their statistical properties first and then predicting their physical properties using the results of data mining to match the desired physical properties. The computational and storage requirements of these calculations require access to large scale HPC resources.

5.13 Effective Simulation Models for Performance Analysis and Prediction of Parallel Systems

Investigators: Apon (UAF), Dowdy (Vanderbilt), Hoffman (Acxiom Corporation)

The focus of this project is on parallel workload and systems characterization, and on building accurate and effective simulation models of cluster computing systems for performance analysis, capacity planning, and evaluation of fair-share scheduling policies, data placement, and more. Acxiom Corporation has funded this on-going work for several years. The developed tools have been applied to the cluster systems at Acxiom Corporation and to UAF systems to perform workload characterization and to answer various capacity planning questions [z1-z4]. Representative results are shown in Figure 5. The figure illustrates tradeoffs to specific fair-share scheduler parameters as applied to two classes of jobs from the measured UAF supercomputer workload. Access to local computing clusters is used in two ways in this research. First, the simulation calculations are modestly computationally intensive, requiring a few hundred hours for the calculation of all points on each figure above. Secondly, the collected trace measurements of all user jobs on the locally-administrated clusters provides a living laboratory for evaluating the effects of various sharing policies, scheduling, and capacity planning of a large cluster system. The close collaboration with TeraGrid providers in this project creates opportunities for applying the developed workload characterization and performance analysis techniques to the very large Track 1 and Track 2 systems found on TeraGrid.

Figure 5: Effect of Fair Share interval values and decay factor on job queuing time for large (Physics) and small (Chemistry) Jobs



6.0 Diversity Plan

A key objective in the project is to insure that underserved groups are properly represented and that the we increase the representation of these communities at all levels in the project. It is essential that the project is diverse in its institutional, individual, disciplinary, and geographic factors. The Project Director will work closely with the Board of Advisers (BoA) (see Sec 10.0) to monitor and expand diversity efforts and a special subcommittee of the BoA will be configured to focus on this area. At the outset a number of areas have been indentified, with additional areas to be added by the BoA. Those identified to date for focused action are:

- Insure that outreach to high schools will specifically be structured to engage female, underserved, and younger students.
- Insure that undergraduate curricula activities that will help to improve enrollments in computational fields have components that focus on underserved groups.
- Require that IT Campus Champions address the needs of IT professionals, research, educators, and students across the full community, and with particular attention to underserved members
- Make sure that Faculty Campus Champions address the science needs of researchers, including faculty and advanced graduate students, across a range of scientific domains.

- Insure that the needs of the CI-TRAIN partnership's two HBCU's are fully addressed, including providing outreach to minorities on these campuses.
- Project meetings and teleconferences will also have a designated agenda item on diversity to insure that there is a designated forum for discussions about how to further engage underserved groups and increase their representation in HPC activities
- Access to TACC professional consulting will ingest ideas from a national supercomputing center.
- Planned (and funded) travel for a wide range of participants will include participation at SC and TeraGrid conferences and will expose conference participants to the broadest range of cyberinfrastructure. UAF has successfully recruited several women and minority students into the SC Student Volunteer program. The project will extend and continue this effort to recruit and support student volunteers for these events.

7.0 Dissemination and Communications Plan

A large number of communication delivery mechanisms and strategies will be utilized in this project to provide dissemination and communication to and among project participants:

- The project will begin with a Kick Off Meeting in August, 2009.
- Yearly project meetings will be held, proposed to be in conjunction with SC events
- Yearly Project Review meetings will be held, alternating between West Virginia and Arkansas
- The PI, Campus Leads, Project Director in Arkansas, and Project Coordinator in West Virginia will communicate regularly.
- The Project Director will be the Champion of Champions to help communicate and coordinate CI Campus Champions information.
- The CI Campus Champions will hold bi-weekly one hour AccessGrid and teleconferences, and longer monthly CI Training Days sessions
- A mailing list and web site will provide project information dissemination.
- Access Grid, videoconferencing, and "Second Life" meetings will be utilized
- CI Days hosted on each campus at least one time during the project period, will communicate the enabling capability of cyberinfrastructure broadly to the university communities.
- Outreach to high school students in Arkansas and West Virginia will be coordinated by the Outreach Coordinator.

Finally, in addition to internal project communication, the project participants will be aware of emerging trends in cyberinfrastructure. PI Apon has been elected to be the Vice Chair of the Coalition for Academic Scientific Computing for 2009. In this role Apon is in constant communication with cyberinfrastructure architects and leaders at the national level, and she will bring a national perspective on cyberinfrastructure to this project as well as carry project experiences back to the community. Attendance at the annual TeraGrid and SC meetings will provide input to CI Campus Champions at the national level, and will provide another meeting time and location for collaboration opportunities.

8.0 Evaluation and Assessment Plan

A blue ribbon team of external reviewers has been recruited to provide oversight and expert input into the project activities and cyberinfrastructure development in Arkansas and West Virginia. The reviewers, listed below, are the best in the field. A support letter is included from each of them in the supplementary documents:

Dr. Stanley Ahalt, Executive Director, Ohio Supercomputer Center (OSC)

- OSC is arguably the most successful state-supported supercomputing center in the United States. Dr. Ahalt led the deployment of OSCNet, the most advanced statewide research and education network in the nation, serving K-12, colleges and universities, government, hospitals, and public broadcasting. Dr. Ahalt is co-Chair of the Ohio Broadband Council. From these perspectives, Dr. Ahalt can provide guidance about funding mechanisms, the wide range of resources provided by OSC, and also statewide optical networking and broadband access in the state of Ohio and its relevance to high performance computing and state cyberinfrastructure.

Dr. Jay Boisseau, Director, Texas Advanced Computing Center (TACC)

- TACC has emerged as one of the leading supercomputing centers in the world, experiencing rapid growth and success in its seven year history. TACC was awarded and now hosts the first NSF Track2 system, Ranger, as the leading HPC systems in the TeraGrid and world, and also provides the leading remote visualization resources in the TeraGrid and just deployed the largest tiled display in the world. TACC's leadership in HPC and scientific visualization resources is complemented by research and development programs in these areas as well as grid computing (grid portals and job orchestration software), with a new data collections and analysis initiative to be formally initiated in the first quarter of 2009.

Dr. Ralph Roskies, co-Director, Pittsburgh Supercomputing Center (PSC)

- PSC is a multi-agency national supercomputing center. For 22 years it has provided the national research community with leading edge computational, visualization, and storage resources, and will host one of the NSF Track 2 supercomputers. It is renowned for outstanding user support. Currently, most computational research in West Virginia is done through TeraGrid allocations on resources at PSC. The participation of Dr. Roskies in this project brings a level of communication between project researchers and PSC that will provide critical guidance about access and use of national cyberinfrastructure resources.

Collectively, the evaluation team provides insight from three very different perspectives: from the view of a state-supported supercomputing center with state mission, from the view of a University-supported supercomputing center that has grown to have international prominence, and from the view of a national supercomputing center that already provides services to project participants.

A Project Review meeting, held during the late spring or early summer of each year, will be a forum for assessing project performance. The following initial metrics for assessment of project success include:

- Number of researchers who utilize CI-TRAIN and national cyberinfrastructure resources
- Total hours of compute or other resource time utilized on the CI-TRAIN systems and TeraGrid
- Number of new research proposals, amount and number of funded grants, publications, presentations, patents, and other research products that are facilitated through project activities or resources
- Number of participants in CI Training Days, number of distinct topics covered in CI Training Days
- Completion of professional certifications by IT staff facilitated by the CI Campus Champions program
- Participation count of a CI Days event on each participating campus during the project period
- Number of high school students participating in summer programs, short courses and tours

In the first months of the project we plan to review these and expand on them with the assistance of TACC, the external reviewers, and the BoA. An annual assessment document will be prepared by the Project Director (with assistance of PIs and campus leads) and provided to the BoA and External Reviewers. Review comments will be addressed and the final document will be made available to all the participants, campus executives and other interested parties.

Our goal is to increase each year in all assessment metrics, above. Additional yearly milestones are:

Year 1: Deploy into production new clusters (UAF, MU, and ASU) and high-end graphics workstations; add 6 new TeraGrid users; hold 1 CI Days event at UAF; add at least one substantial TeraGrid allocation

Year 2: Deploy all visualization nodes; add 12 new TeraGrid users; hold CI Days events on 3 new campuses; submit 3 competitive MRI/CRI proposals; upgrade data center facilities (MU)

Year 3: Deploy data capture hardware; extend immersive visualization facilities; add 12 new TeraGrid users; hold CI Days events on 4 new campuses; submit 5 competitive MRI/CRI proposals; data center upgrades and deploy new cluster (WVU)

The periodic evaluations of the metrics and milestones mentioned above will be aggregated and annually reviewed by an External Evaluator funded through the WV Higher Education Policy Commission Division of Science and Research as part of their cost share commitment to this project. The Evaluator will prepare an annual report based on his/her findings.

9.0 Sustainability Plan

A key goal of this project is to have an impact on the permanent institutional capability at institutions in Arkansas and West Virginia. The CI Campus Champions program will build institutional expertise and knowledge that will persist over the long term. We have commitment for some staff positions funded through this project to become permanent staff lines at the end of the project from both Arkansas and West Virginia and are seeking further commitment to this from all institutions. (See the supports letters in the supplemental documents.)

The physical resources requested in this proposal are modest, and have an anticipated useful life that is little more than the project period of three years. A single request of this type cannot meet the long term needs for physical cyberinfrastructure resources. Rather, researchers and IT leaders, enabled through the activities of CI Campus Champions, will learn to collaboratively develop proposals during the project period and beyond to include cyberinfrastructure resources to federal programs such as NSF MRI, NSF CRI, NIH, DOD, and other agencies. Through the CI-TRAIN project we do not simply acquire resources for today, but we are enabled to acquire resources for a lifetime.

One projected outcome of this project is a transformational awareness of cyberinfrastructure to executive leadership at the universities. The blue ribbon external review panel can provide critical input to project progress at a level that will be heard by higher education and state leadership.

Over the project period a detailed cyberinfrastructure strategic plan will be developed at each participating institution and within the two states that will create a coherent plan for the long term and guidance to future cyberinfrastructure architecture and acquisition.

10.0 Management and Coordination Plan

The total capability across the two states will be greater than the sum of its parts. This will be achieved by sharing/leveraging best-practices and accrued knowledge of the shared systems and common technology across the partnership. The process of working together on the proposal has already realized significant shared knowledge of cyberinfrastructure and visualization technology.

Amy Apon (UAF), project PI, will provide executive direction for the project. Paul Hill (HEPC Division of Science and Research) will act as Co-PI. A CI-TRAIN Board of Advisors (BoA) will be created which will be composed of the PIs from each state and an individual appointed by the campus chief executive from each participating institution. The CI-TRAIN BoA will meet at least quarterly (via Access Grid) and review the project activities. On an annual basis they will prepare a formal report to be submitted to all the participating campus executives, the Arkansas Science and Technology Authority and the West Virginia Higher Education Policy Commission Division of Science and Research office. The report will also serve as one element in the assessment plan. An overall Project Director, hosted at UAF and funded by this grant, will report to Apon and manage all project activities. This Project Director will provide administrative support to the BoA and will serve as Champion of Champions, ensure that monthly CI Training Days are planned and communicated, help plan yearly meetings and CI Days events, and simultaneously serve as state project director for Arkansas. Similarly, in West Virginia, a state project director will assist with coordination of activities in West Virginia and will help to ensure that related project milestones are met. The quarter-time central-office West Virginia Campus Champion funded by this grant will participate in the professional development activities offered to the project community. By building these skill sets at the central-office level it will be possible to disseminate high performance computing and visualization information resources to, and recruit for participation in future CI-related efforts, those institutions not directly involved in this project.

Fred Limp (UAF), Trevor Harris (WVU), and Tony Szwilski (MU) will co-lead the visualization research components. Apon will lead the high-performance computing research components. Each Campus Lead will oversee the activities and deliverables for that campus. Campus Leads and CI Campus Champions will form a collaboration team to plan specific project activities and priorities. The Cluster Administrator, an addition to UAF HPC operational staff, will be responsible for all server-side HPC and EnVision components. The Visualization Administrators, responsible for management and training of client-side visualization components, and the Outreach Coordinator will report through CAST to the Project Director and PIs.

References Cited

[a1] "The Office of the President-Elect: The Obama-Biden Plan for Technology", December, 2008. http://change.gov/agenda/technology_agenda/

[a2] Stewart, C. et. al., Consensus definition of cyberinfrastructure, Coalition of Academic Scientific Computing (CASC), fall, 2008, http://www.casc.org/

[a3] Arkansas Cyberinfrastructure Strategic Plan, prepared by the Arkansas Cyberinfrastructure Advisory Committee, Arkansas Science and Technology Authority, October, 2008. http://comp.uark.edu/~aapon/CyberinfrastructureStrategicPlan20081024.pdf

[a4] Vision2015, The West Virginia Science and Technology Strategic Plan, prepared by the West Virginia EPSCoR Advisory Council, December, 2005. http://wvepscor.org/

[a5] Arkansas Research and Education Optical Network (ARE-ON), http://www.areon.net/

[a6] Three Rivers Optical Exchange (3ROX), http://www.3rox.net/

[a7] A. Apon, G. Monaco, G. Springer, K. Huxtable, "Great Plains Network: Building the Regional Middleware Infrastructure," NMI-EDIT Identity and Access Management Case Study Series, January, 2006. http://www.nmi-edit.org/case_studies/GPN-Middleware200602.pdf

[a8] M. Baker, A. Apon, C. Ferner, J. Brown, "Emerging Grid Standards," IEEE Computer, 38(4), April 2005, p. 43-50.

[a9] J. Mache, A. Apon, "Teaching Grid Computing: Topics, Exercises, and Experiences," IEEE Transactions on Education, 26 pages, 2007.

[a10] A. Apon, J. Mache, Y. Yara, K. Landrus, "Classroom Exercises for Grid Services," Proceedings of the Linux Cluster Institute International Conference on High Performance Computing, Austin, Texas, May, 2004, 12 pages.

[a11] A. Apon, K. Landrus, J. Mache, K. Huxtable, "Using Shibboleth to Manage Access Control to Remote Cluster Computing Resources," Proceedings of SC2004 - 17th ACM/ IEEE High-Performance Computing, Networking and Storage Conference, November, 2004.

[a12] A. Apon, K. Landrus, "Introduction to Shibboleth," Proceedings of ALAR 2005 Conference on Applied Research in Information Technology, February 18, 2005, 7 pages.

[a13] J. Mache, A. Apon, "Grid Computing in the Undergraduate Classroom: Topics, Exercises and Experiences," Second International Workshop on Collaborative Learning Applications of Grid Technology and Grid Education, Proceedings of the International Conference on Cluster Computing and the Grid, Cardiff, UK, May, 2005.

[a14] B. Taylor, A. Apon, "Architectural Tradeoffs for Unifying Campus Grid Resources," Linux Cluster Institute 2006, May, 2006, 26 pages.

[a15] L. Ngo, A. Apon, "Shibbolized Subversion," International Conference on Information Technology: New Generations, 2007, 8 pages.

[a16] K. Landrus, "Using Shibboleth to Control Access to Remote Cluster Resources," M.S. Thesis, Computer Engineering, University of Arkansas, May, 2005.

[a17] B. Taylor, "Architectural Tradeoffs for Unifying Campus Grid Resources," M.S. Thesis, Computer Engineering, University of Arkansas, December, 2005.

[a18] L. Ngo, "Shibbolized Subversion," M.S. Thesis, Computer Engineering, , University of Arkansas, August, 2006.

[a19] M. Baker, "Methods for Maintaining Local Cluster Resources for Intercampus and Intracampus Grids," M.S. Thesis, CSCE, University of Arkansas, August, 2006.

[a20] A. Apon, “Building the Regional Middleware Infrastructure Across the Great Plains,” PowerPoint presentation at the Educause Extending the Reach Kickoff Meeting, June 30, 2004.

[a21] A. Apon, “Introduction to Grid Security Infrastructure,” PowerPoint presentation to the GPN Middleware Biweekly meeting, September, 2004.

[a22] A. Apon, “Introduction to Shibboleth,” Oklahoma Supercomputing Symposium, Norman, Oklahoma, October 6, 2004.

[a23] Accelerate Arkansas: Building a Knowledge-Based Economy in Arkansas, http://www.acceleratearkansas.com/

[a24] National Science Board Approves Funds for Petascale Computing Systems, Press Release 07-095, 2007. http://www.nsf.gov/news/news_summ.jsp?cntn_id=109850

[a25] Report on the EPSCoR Cyberinfrastructure Assessment Workshop, Lexington, KY. October 15-16, 2007. http://collaboration.greatplains.net/wiki/images/2/2c/CIreportVer4.doc

[a26] Teragrid Campus Champions, 2008. http://www.teragrid.org/eot/campuschamps.html

[a27] Introduction to High Performance Computing UAF Course Home Page, http://comp.uark.edu/~aapon/courses/hpc/index.html

[b1] J. Cothren, F. Limp, A. Payne, J. Herrmann, A. Barnes. 2006. Integrating Terrestrial LIDAR Point Clouds and Independent Close-range Images. *Proceedings of the American Society of Photogrammetry and Remote Sensing National Conference*, Reno, NV

[b2] J. Cothren, F. Limp. 2006. The Application of Long-range, Large-area, High-density Survey for Heritage Site Analysis. Abstracts of the XI International Seminar Forum UNESCO, University and Heritage, Documentation for Conservation and Development, New Strategies for the Future. September 11-15. pp. 127.

[b3] J. Cothren, F. Limp. 2006. The application of long range, large area high density survey for heritage site analysis in Bini, M., S. Bertocci and S. Mecca (eds) *Documentation for conservation and development: New heritage strategy for the future.* Firenze University Press. Firenz IT

[b4] J. Cothren. 2006. Experiments with LIDAR point cloud driven feature extraction in close-range digital photogrammetry applications, Proceedings, ASPRS 2006 Annual Conference and Technology Exhibition, May 1-5, Reno, Nevada, USA.

[b5] J. Cothren, A. Payne, A. Vranich, A., F. Limp. 2006. A Modern Survey of Ancient Ruins. Geoworld. February.

[b6] A. Barnes, J. Cothren. 2007. *Mapping Tiwanaku: using modern photogrammetric methods to analyze an ancient landscape.* Technology and Archaeology Workshop. Dumbarton Oaks. Washington DC. December.

[b7] J. Cothren, A. Barnes, C. Goodmaster, A. Varanich, E. Ernenwein, F. Limp 2007 A*ncient sites in 21st century enviroments: fusion of three-dimensional, multi-scale digital data.* Technology and Archaeology Workshop. Dumbarton Oaks. Washington DC. December.

[b8] C. Goodmaster, A. Payne. 2007 *3D laser scanning at Tiwanaku: potentials for documentation, visualization and analysis.* Technology and Archaeology Workshop. Dumbarton Oaks. Washington DC. December.

[b9] High School Survey of Student Engagement 2007 *Voices of students on engagement.* Indiana University. Accessed Nov 30 2008. http://ceep.indiana.edu/hssse/pdf/HSSSE_2006_Report.pdf

[b10] Committee on increasing high school student’s engagement and motivation to learn 2003 *Engaging Schools.* National Academy Press.

[b11] Committee on Science Learning, Kindergarten through Eighth Grade, Richard A. Duschl, Heidi A. Schweingruber, and Andrew W. Shouse, Editors. 2007 National Academy Press

[b12] J. Tunik, L. Ramsey, A. Simon. *Arkansas Environmental and Spatial Technology Initiative. Statewide Evaluation. Final Report.* Submitted to the Arkansas Department of Education. Accessed on November 30 2008 http://www.eastinitiative.org/howeastworks/downloads/Executive_Summary_EAST_Metisreport.pdf

[b13] J. Cothren, D. Fredrick, W. Limp, T. DeNoble, A. Barnes, C. Goodmaster, C. Stephens. 2008. *Visualizing the roman city: viewing the past through multidisciplinary eyes.* Computer Applications and Quantitative Methods in Archaeology. Budapest, Hungary. April.

[b14] D. Fredrick, T. DeNoble, F. Limp, J. Cothren. 2008. Visualizing the Roman City. Accessed November 30, 2008. http://pompeii.uark.edu/~cast/ostia/

[b15] D. Fredrick. 2008. Digital Pompeii. Accessed November 30, 2009. http://pompeii.uark.edu/classwebsite/Site/Welcome.html

[b16] J. Cothren. 2006. *Managing very large LiDAR point clouds in Oracle 10g spatial*. Mid-America GIS Conference. Kansas City KS. April.

[b17] J. Cothren, W. Limp, A. Payne, J. Herrmann, A. Barnes. 2006. *Integrating terrestrial LiDAR point-cloud and independent close range-images.* American Society for Photogrammetry and Remote Sensing. Reno NV. May.

[b18] F. Limp. 2006. Future developments in 3D GeoWorld. August page 28-31.

[b19] F. Limp. 2006. 3D data and creation *GeoWorld*. June page 28-31.

[b20] F. Limp. 2006. An impending massive 3D mashup. *GeoWorld* April pages 20-25

[b21] Multiple authors, papers. OGC Technical Interoperability Day. 2008. GeoForschungsZentrum Potsdam (GFZ) Potsdam, Germany Accessed November 30 2008 http://www.opengeospatial.org/event/080603techinterop

[b22] U. Quandt, T. Kolbe. 2005. *OGC Discussion Paper OGC 05-019 Web 3D Service*. Accessed November 30 2008 *portal.opengeospatial.org/files/?artifact_id=8869*

[b23] C. Schulte, V. Coors. 2008. Development of a CityGML Application Domain Extension for dynamic flood information. *Proceedings of the 3rd International ISCRAM China Workshop.* Harbin China. Accessed at November 30, 2008. http:// http://www.hft-stuttgart.de/fbv/fbvweb/privhomepages/coors/schulte/docs/Paper_CityGML_ADE_flood.pdf

[b24] EAST on-line tutorials and support. Accessed November 19, 2008 at http://www.eastproject.org/SupportTutorials/

[b25] EAST Short Courses. Accessed November 19, 2008 at http://www.eastproject.org/TrainingEvents/

[c1] C. Thompson. 2004. “Everything is Alive,” IEEE Internet Computing, January-February.

[c2] C. Thompson, P. Parkerson. 2004. “DBMS[me],” IEEE Internet Computing, May-June.

[c3] C. Thompson. 2005. “Smart Devices and Soft Controllers,” IEEE Internet Computing, January-February.

[c4] C. Thompson, Rishikesh Jena. 2005. “Digital Licensing Services,” IEEE Internet Computing, Volume 9, Number 4, July-August.

[c5] C. Thompson, D. Thompson. 2007. “Identity Management,” IEEE Internet Computing, May-June.

[c6] A. Hendaoui, M. Limayem, C. Thompson. 2008. “3D Social Virtual Worlds: Research Issues and Challenges,” IEEE Internet Computing, Jan-Feb.

[c7] C. Bailey. 2008. “Extending Second Life Simulations with Virtual RFID,” Honors College Undergraduate Research Grant, May.

[c8] C. Thompson. 2008. “Modeling Healthcare Logistics in a Virtual World,” IEEE Internet Computing, September-October.

[c9] J. McFarlane. 2008. “Mapping Reality into Virtual Worlds,” BS Honors Thesis, CSCE Dept., August.

[c10] J. Hoag, C. Thompson. 2006. “Architecting RFID Middleware,” IEEE Internet Computing, September-October.

[c11] J. Hoag, R. Phillips, C. Thompson, R. Huetter, J. Veizades. 2007. “SensorConnect Performance and Scalability Experiments,” First IEEE Conference on RFID, Grapevine, TX, March.

[c12] TagCentric RFID Middleware, Open source software released on SourceForge, March 2007, http://tag-centric.sourceforge.net & http://sourceforge.net/projects/tag-centric

[c13] S. Sidhartha. 2007. “RFID Reader Agent Based On Low Level Reader Protocol (LLRP) Standards,” Masters Project, CSCE Dept, August.

[c14] K. Neumeier. 2008. “Smart Device Virtualization: Building an LLRP RFID Reader Emulation Tool,” MS Thesis, CSCE Dept, May.

[c15] S. Barath. 2008. “Message Reliability over UDP,” MS Thesis, CSCE Dept, May.

[c16] J. Patton. 2008. “RFID as Electronic Article Surveillance: Feasibility Assessment,” CSCE Dept., May.

[c17] S. Musunuri. 2008. “Performance and Scalability of TagCentric RFID Middleware,” MS Thesis, CSCE Dept, U Arkansas, August.

[c18] C. Thompson, P. Pazandak, H. Tennant. 2005. “Talk to your Semantic Web,” IEEE Internet Computing, May-June.

[c19] K. Neumeier, C. Thompson. 2006. "Dynamic Composition of Agent Grammars," Proceedings of the Second IASTED International Conference on Computational Intelligence, San Francisco CA, November 20-22.

[c20] N. Lehlou. 2006. “Extending EiA Soft-controllers with a Natural Language Interface,” B.A. Honors Thesis, CSCE Dept, University of Arkansas, August.

[c21] K. Neumeier, C. Thompson. 2007. “Parameterizing Menu Based Natural Language Interfaces with Location Models,”IEEE International Conference on Integration of Knowledge Intensive Multi-Agent Systems (KIMAS-07), Waltham, MA, April.

[c22] V. Reddy. 2007. “Extending Menu-based Natural Language Interfaces with Geospatial Queries,” MS Thesis, CSCE Dept, University of Arkansas, December.

[c23] V. Reddy, K. Neumeier, J. McFarlane, J. Cothren, C. Thompson. 2007. “Extending a Natural Language Interface with Geospatial Queries,” IEEE Internet Computing, November-December.

[c24] Z. Xiao, C. Thompson, W. Li. 2006. “Data Processing Workflow Automation in Grid Architecture,” Fifth International Conference on Grid and Cooperative Computing – Workshops: International Workshop on Workflow Systems in Grid Environments (WSGE06) , Changsha, China, October 21-23, p. 189-195.

[c25] Z. Xiao, C. Thompson, W. Li. 2006. “Automating Workflow for Data Processing in Grid Architecture,” International Conference on Information and Knowledge Engineering (IKE’06), Las Vegas, Nevada, June 26-29, p. 191-195.

[c26] C. Thompson, W. Li, Z. Xiao. 2007. “Workflow Planning on a Grid,” IEEE Internet Computing, January-February.

[c27] J. Eno, C. Thompson, W. Li, W. Deneke. 2008. "Enhanced Workflow Service Modeling,” 2008 Conference Applied Research in Information Technology, Acxiom Laboratory for Applied Research, Conway AR, March 14.

[c28] W. Deneke, J. Eno, W. Li, C. Thompson, J. Talburt, D. Nash, J. Stires, J.Loghry. 2008. “Towards a Domain-Specific Modeling Language for Customer Data Integration Workflow,” Third International Workshop on Workflow Management and Applications in Grid Environments (WaGe08), Kunming, China, May.

[c29] C. Thompson. 2004. “Agents, Grids, and Middleware,” IEEE Internet Computing, September-October.

[c30] C. Thompson. 2006. “Towards a Grid-based DBMS,” IEEE Internet Computing, March-April.

[c31] J. Schisler. 2005. “GRINDEX: Framework and Prototype for a Grid-based Index,” M.S. in Computer Engineering, Computer Science and Computer Engineering Department, U. Arkansas, August.

[c32] Phillips, Reid. 2006. “GRINDEX2: Extensible Indexing in a Grid-Based Relational Database Management System,” M.S. Thesis, CSCE Dept., U. Arkansas, December.

[c33] R. Phillips, J.Allison, C. Thompson. 2007. “Subsetting the Workflow Grid,” Conference on Applied Research in Information Technology, Acxiom Laboratory for Applied Research, Conway AR, March 9.

[c34] E. Kirkconnell. 2008. “GRINDEX3: Extensible Grid Indexing and Query Service,” MS Thesis, CSCE Dept, August.

[c35] K. Jonnalagedda. 2006. “Performance Analysis and Tuning of a Very Large Retail Application implemented on a Grid-based Database Management System,” M.S. Thesis, CSCE Dept., U. Arkansas, August.

[c36 88] J. .Hoag, C. Thompson. 2007. "A Parallel General-Purpose Synthetic Data Generator," SIGMOD Record, March.

[c37 89] J. Eno. 2007. “Generation of Synthetic Data to Conform to Constraints Derived from Data Mining Applications,” MS Thesis, CSCE Dept, December.

[c38 90] J. Hoag. 2008. “Synthetic Data Generation,” Ph.D. Dissertation in Computer Science, Department of Computer Science and Computer Engineering, University of Arkansas, May.

[c39 91] J. Eno, C. Thompson. 2008. “Generating Synthetic Data to Match Data Mining Patterns,” IEEE Internet Computing, May-June.

[c40 92] Modeling Healthcare in a Virtual World Website, http://vw.ddns.uark.edu.

[d1] W. Craig, T. M. Harris, D. Weiner, D. (eds). 2002. Community Participation and Geographic Information Systems, Taylor and Francis, London.

[d2] M. Dodge, M. McDerby, M. Turner, M. (eds) 2008. Geographic visualization: concepts, tools and applications, Wiley, New Jersey.

[d3] J. Dykes, A. MacEachren, M-J. Kraak, (eds), 2005. Exploring geovisualization, Elsevier, Boston.

[d4] P. Fisher, D. Unwin, D. 2002. Virtual reality in geography, Taylor and Francis, New York.

[d5] T.M. Harris, L. J. Rouse, S. Bergeron (forthcoming A) Humanities GIS: adding place, spatial storytelling and immersive visualization into the Humanities, in Geography and the Humanities, Routledge

[d6] Electronic Cultural Atlas Initiative, http://ecai.org/projects/Projectexamples.asp

[d7] T.M. Harris, L.J. Rouse, S. Bergeron, (forthcoming B) The Geospatial Web and Local Geographical Education, International Research in Geographical and Environmental Education.

[d8] T.M. Harris, L.J. Rouse, S. Bergeron, (forthcoming C) The Geospatial Web, Pareto GIS, and the Humanities, in The Spatial Humanities, Indiana University Press.

[d9] L.J. Rouse, S. Bergeron, T.M. Harris. 2007. Participating in the Geospatial Web: Web2.0, social networks and Participatory GIS, in The Geospatial Web: how geo-browsers, social software and the Web 2.0 are shaping the Network Society, eds A. Scharl, K. Tochtermann, Springer Publications.

[e1] G.A. Smolenskii, I.E. Chupis. 1982. ”Ferroelectromagnets,”' Sov. Phys. Usp. 25, 475 (1982).

[e2] P. Fischer, M.Polomskya, I.Sosnowska, M.Szymanksi. 1980. ”Temperature dependence of the crystal and magnetic structures of BiFeO3,” J. Phys. C 13, 1931 (1980).

[e3] V. Kiselev, R. P. Ozerov, G. S. Zhlanov. 1963. “Detection of magnetic order in ferroelectric BiFeO3 by neutron diffractions,” Sov. Phys. Dokl. 7, 742 (1963).

[e4] G. Smolenskii, V. Isupov, A. Agranovskaya, N. Kranik. 1961. ”New ferroelectrics of complex composition,” Sov. Phys. Solid State 2, 2651 (1961).

[e5] J.R. Teague, R. Gerson and W.J. James. 1970. ”Dielectric hysteresis in single crystal BiFeO3,” Solid State Comm. 8, 1073 (1970).

[e6] C. Tabares□Munoz, J.□P. Rivera, A. Bezinges, A. Monnier, H Schmid. 1985. “Measurement of the quadratic magnetoelectric effect on single crystalline BiFeO3,” Jap. Journ. Appl. Phys. 24, 1051 (1985).

[e7] N.A. Hill. 2000. “Why are there so few magnetic multiferroics,” J. Phys. Chem. B 104, 6694 (2000).

[e8] J. Wang, J. B. Neaton, H. Zheng, V. Nagarajan, S. B. Ogale, B. Liu, D. Viehland, V. Vaithyanathan, D. G. Schlom, U. V. Waghmare, N. A. Spaldin, K. M. Rabe, M. Wuttig, R. Ramesh. 2003. “Epitaxial BiFeO3 Multiferroic Thin Film Heterostructures,” Science 299, 1719 (2003).

[e9] J.B. Neaton, C. Ederer, U.V. Waghmare, N.A. Spaldin, K.M. Rabe. 2005. “First-principles study of spontaneous polarization in multiferroic BiFeO3,” Phys. Rev. B 71, 014113 (2005).

[e10] R. Haumont, J. Kreisel, P. Bouvier, F. Hippert. 2006. “Phonon anomalies and the ferroelectric phase transition in multiferroic BiFeO3,” Phys. Rev. B 73, 132101 (2006).

[e11] T. Zhao, A. Scholl, F. Zavaliche, K. Lee, M. Barry, A. Doran, M. P. Cruz, Y. H. Chu, C. Ederer, N. A. Spaldin, R. R. Das, D. M. Kim, S. H. Baek, C. B. Eom, R. Ramesh. 2006. “Electrical control of antiferromagnetic domains in multiferroic BiFeO3 films at room temperature,” Nat. Mater. 5, 823 (2006).

[e12] V.V. Shvartsman, W. Kleeman, R. Haumont and J. Kreisel. 2007. “Large bulk polarization and regular domain structure in ceramic BiFeO3,” Appl. Phys. Lett. 90, 172115 (2007).

[e13] Manoj K Singh, Ram S Katiyar, J F Scott. 2008. “New magnetic phase transitions in BiFeO3,” J. Phys.: Condens. Matter 20, 252203 (2008)

[e14] G. Catalan, H. Bea, S. Fusil, M. Bibes, P. Paruch, A. Barthelemy, J.F. Scott. 2008. “Fractal dimension and size scaling of domains in thin films of multiferroic BiFeO3,” Phys. Rev. Lett. 100, 027602 (2008).

[e15] D. Lebeugle, D. Colson, A. Forget, M. Viret, A.M. Bataille, A. Gukasov. 2008. “Electric-Field-Induced Spin Flop in BiFeO3 Single Crystals at Room Temperature,” Phys. Rev. Lett. 100, 227602 (2008).

[e16] S.K. Streiffer, J.A. Eastmanm D.D. Fong, C. Thompson, A. Munkholm, Murty Raman, O. Auciello, G.R. Baj, G.B. Stephenson. 2002. “Observation of nanoscale 180 degrees stripe domains in ferroelectric PbTiO3 thin films,” Phys. Rev. Lett. 84, 067601 (2002).

[e17] I.A. Kornev, B.-K. Lai, I. Naumov, I. Ponomareva, H. Fu, L. Bellaiche. 2008. “Domains in Ferroelectric Nanostructures from First Principles,” Invited Review Chapter in Handbook of advanced dielectric piezoelectric and ferroelectric materials: Synthesis, properties and applications, edited by Professor Zuo-Guang Ye, Woodhead Publishing Limited.

[e18] S. Prosandeev, L. Bellaiche. 2008. “Controlling double vortex states in low-dimensional dipolar systems,” Phys. Rev. Lett. 101, 097203 (2008).

[e19] S. Prosandeev, I. Ponomareva, I. Kornev, L. Bellaiche . 2008. “Control of vortices by homogeneous fields in asymmetric low-dimensional dipolar systems,” Phys. Rev. Lett. 100, 047201 (2008).

[e20] B-K. Lai, I. Ponomareva, I. I. Naumov, I. A. Kornev, H. Fu, L. Bellaiche, G. J. Salamo. 2006. “Electric-field induced domain evolution in ferroelectric ultrathin films,” Phys. Rev. Lett. 96, 137602 (2006).

[e21] B-K Lai, I. Ponomareva, I. A. Kornev, L. Bellaiche, G. J. Salamo. 2007. “Domain evolution of BaTiO3 ultrathin films under electric field: a first-principles study,” Phys. Rev. B 75, 085412 (2007).

[e22] S. Prosandeev, I. Ponomareva, I. Naumov, I. Kornev, L. Bellaiche. 2008. “Original properties of dipole vortices in zero-dimensional ferroelectrics,” Invited Topical Review, J. Phys.: Condens. Matter 20, 193201 (2008).

[e23] A. Hubert, R. Schafer. 1998. “Magnetic Domains: The analysis of Magnetic Microstructures,” (Springer, Berlin, 1998).

[e24] C. L. Chien, F. Q. Zhu, J-G Zhu. 2007. “Patterned Nanomagnets,” Physics Today 60, 40 (2007).

[e25] J. Rothman, M. Kläui, L. Lopez-Diaz, C. A. F. Vaz, A. Bleloch, J. A. C. Bland, Z. Cui, R. Speaks. 2001. “Observation of a Bi-Domain State and Nucleation Free Switching in Mesoscopic Ring Magnets,” Phys. Rev. Lett. 86, 1098 (2001).

[e26] K. Yu. Guslienko, X. F. Han, D. J. Keavney, R. Divan, S. D. Bader. 2006. “Magnetic Vortex Core Dynamics in Cylindrical Ferromagnetic Dots,” Phys. Rev. Lett. 96, 067205 (2006).

[e27] A. Pimenov, A. Loidl, P. Przyslupski and B. Dabrowski. 2005. “Negative Refraction in Ferromagnet-Superconductor Superlattices,” Phys. Rev. Lett. 95, 247009 (2005).

[e28] L. Peng, L. Ran, H. Chen, H. Zhang, J-A. Kong, T.M. Grzegorczyk. 2007. “Experimental Observation of Left-Handed Behavior in an Array of Standard Dielectric Resonators,” Phys. Rev. Lett. 98, 157403 (2007),

[e29] see, e.g., P. Ball. “Superlenses bring the nanoworld into focus,” http://cmbi.bjmu.edu.cn/news/0703/67.htm

[e30] see, e.g., “Invisibility-Cloak Materials Bend Light "Backward,” http://news.nationalgeographic.com/news/2008/08/080812-invisibility-cloak.html; http://www.youtube.com/watch?v=Y4zwzlnExVU&NR=1

[e31] P. Hohenberg, W. Kohn. 1964. “Inhomogeneous Electron gas,” Phys. Rev. 136, B864 (1964); “Self-consistent equations including exchange and correlation effects,” W. Kohn, L.J. Sham, ibid. 140, A1133 (1965).

[e32] J.P. Perdew, Y. Wang. 1986. “Accurate and simple density functional for the electronic exchange energy: generalized gradient approximation,” Phys. Rev. B 33, 8800 (1986).

[e33] R.D. King-Smith, D. Vanderbilt. 1994. “First-Principles Investigation of Ferroelectricity in Perovskite Compounds,” Phys. Rev. B 49, 5828 (1994).

[e34] L. Bellaiche, D. Vanderbilt. 2000. “Virtual crystal approximation revisited: Application to dielectric and piezoelectric properties of perovskites,” Phys. Rev. B 61, 7877 (2000).

[e35] J.A. Van Vechten. 1969. “Quantum dielectric theory of electronegativity in covalent systems. I. Electronic dielectric constant,” Phys. Rev. A 182, 891 (1969).

[e36] N.J. Ramer, A.M. Rappe. 2000. “Application of a new virtual crystal approach for the study of disordered perovskites,” J. Phys. Chem. Solids 61, 315-320 (2000).

[e37] L. Bellaiche, A. Garcia, D. Vanderbilt. 2000. “Finite-temperature properties of Pb(Zr1-xTix)O3 alloys from first-principles,” Phys. Rev. Lett 84, 5427 (2000).

[e38] R. Hemphill, L. Bellaiche, A. Garcia, D. Vanderbilt. 2000. “Finite-temperature properties of disordered and ordered Pb(Sc0.5Nb0.5)O3 alloys,” Appl. Phys. Letters 77, 3642 (2000).

[e39] A. Al-Barakaty, L. Bellaiche. 2002. “Global and secondary ferroelectric minima in ordered Pb(Sc 0.25Nb0.25Ti0.50)O3 alloys,” Appl. Phys. Letters 81, 2442 (2002).

[e40] R. Haumont, B. Dkhill, J.M. Kiat, A. Al-Barakaty, L. Bellaiche. 2003. “Cationic competition induces monoclinic phase in high piezoelectric PSN-PT compounds,” Phys. Rev. B 68, 014114 (2003).

[e41] X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, P. Ghosez, J.Y. Raty, D.C. Allan. 2002. “First-principles computation of material properties: the ABINIT software project,” Computational Materials Science 25, 478 (2002).

[e42] V. Ranjan, S. Bin-Omran, D Sichuga, R. S. Nichols, L. Bellaiche, A. Alsaad. 2005. “Properties of GaN/ScN and InN/ScN superlattices from first principles,” Phys. Rev. B 72, 085315 (2005).

[e43] V. Ranjan, L. Bellaiche, E.J. Walter. 2003. “Strained hexagonal ScN: A material with unusual structural and optical properties,” Phys. Rev. Lett. 90, 257602 (2003).

[e44] I. Kornev, P. Bouvier, P.-E. Janolin, B. Dkhil, J. Kreisel, L. Bellaiche. 2005. “Ferroelectricity of perovskites under pressure,” Phys. Rev. Lett. 95, 196804 (2005).

[e45] I. A. Kornev, L. Bellaiche. 2007. “The nature of ferroelectricity under pressure,” Phase Transitions 80, 385 (2007); Invited Review.

[e46] I. A. Kornev, S. Lisenkov, R. Haumont, B. Dkhil, L. Bellaiche. 2007. “Finite-temperature properties of multiferroic BiFeO3,” Phys. Rev. Lett. 99, 227602 (2007).

[e47] S. Baroni, A. Dal Corso, S. de Gironcoli, P. Giannozzi, C. Cavazzoni, G. Ballabio, S. Scandolo, G. Chiarotti, P. Focher, A. Pasquarello, K. Laasonen, A. Trave, R. Car, N. Marzari, A. Kokalj, (www.pwscf.org).

[e48] G. Kresse, J. Hafner. 1996. “Ab initio molecular dynamics for liquid metals,” Phys. Rev. B 47, 558 (R) (1993); G. Kresse, J. Furthmuller. 1996. “Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set,” Phys. Rev. B 54, 11169 (1996).

[e49] V.I. Anisimov, F. Aryasetiawan, A.I. Lichtenstein. 1997. “First-principles calculations of the electronic structure and spectra of strongly correlated systems: the LDA+U method,” J. Phys: Condens. Matter 9, 767 (1997)

[e50] D. Vanderbilt. 1997. “First-principles based modeling of ferroelectrics,” Curr. Opin. Solid State Mater. Sci. 2, 701 (1997).

[e51] W. Zhong, D. Vanderbilt, K.M. Rabe. 1995. “First-Principles theory of ferroelectric phase transitions for perovskites: the case of BaTiO3,” Phys. Rev. B 52, 6301 (1995); W. Zhong, D. Vanderbilt, K.M. Rabe. 1994. “Phase transition in BaTiO3 from first principles,” Phys. Rev. Lett. 73, 1861 (1994).

[e52] U. V. Waghmare, K. M. Rabe. 1997. “Ab initio statistical mechanics of the ferroelectric phase transition in PbTiO3,” Phys. Rev. B 55, 6161 (1997).

[e53] A. Garcia, D. Vanderbilt. 1998. “Electromechanical behavior of BaTiO3 from first principles,” Appl. Phys. Letters 72, 2981 (1998).

[e54] L. Walizer, S. Lisenkov, L. Bellaiche. 2006. “Finite-temperature properties of (Ba,Sr)TiO3 systems from atomistic simulations,“ Phys. Rev. B 73, 144105 (2006).

[e55] I. A. Kornev, L. Bellaiche, P.-E. Janolin, B. Dkhil, E. Suard. 2006. “Phase diagram of Pb(Zr,Ti)O3 solid solutions from first principles,” Phys. Rev. Lett. 97, 157601 (2006).

[e56] L. Bellaiche, J. Iniguez, E. Cockayne, B.P. Burton. 2007. “Effects of Vacancies on Properties of Relaxor Ferroelectrics: a First-Principles Study,” Phys. Rev. B 75, 014111 (2007).

[e57] I. Ponomareva, I.I. Naumov, I. Kornev, H. Fu, L. Bellaiche. 2005. “Atomistic treatment of depolarizing energy and field in ferroelectric nanostructures,” Phys. Rev. B 72, 140102(R) (2005).

[e58] I. Ponomareva, I.I. Naumov, L. Bellaiche. 2005. “Low-dimensional ferroelectrics under different electrical and mechanical boundary conditions,” Phys. Rev. B 72, 214118 (2005).

[e59] S. Prosandeev, L. Bellaiche. 2006. “Properties of ferroelectric nanodots embedded in a polarizable medium: Atomistic simulations,” Phys. Rev. Lett. 97, 167601 (2006).

[e60] I. Ponomareva, L. Bellaiche. 2006. "Influence of the growth direction on properties of ferroelectric ultrathin films," Phys. Rev. B 74, 064102 (2006).

[e61] I. Kornev, H. Fu, L. Bellaiche. 2004. "Ultrathin films of ferroelectric solid solutions under residual depolarizing field," Phys. Rev. Lett. 93, 196104 (2004).

[e62] I. I. Naumov, L. Bellaiche, H. Fu. 2004. "Unusual phase transitions in ferroelectric nanodisks and nanorods", Nature (London) 432, 737 (2004).

[e63] E. Almahmoud, Y. Navtsenya, I. Kornev, H. Fu, L. Bellaiche. 2004. "Properties of Pb(Zr,Ti)O3 ultrathin films under stress-free and open-circuit electrical boundary conditions," Phys. Rev. B 70, 220102(R) (2004).

[e64] A. R. Akbarzadeh, L. Bellaiche, J. Iniguez, D. Vanderbilt. 2007. "Theoretical phase diagram of ultrathin films of incipient ferroelectrics," Appl. Phys. Lett. 90, 242918 (2007).

[e65] S. Prosandeev, I. Kornev, L. Bellaiche. 2007. "Tensors in ferroelectric nanoparticles: First-principles-based simulations," Phys. Rev. B 76, 012101 (2007).

[e66] B-K. Lai, I.A. Kornev, L. Bellaiche, G. J. Salamo. 2005. "Phase Diagrams of Epitaxial BaTiO3 Ultrathin Films From First Principles," Appl. Phys. Lett. 86, 132904 (2005).

[e67] B-K. Lai, I. Ponomareva, I.A. Kornev, L. Bellaiche, G.J. Salamo. 2007. "Thickness dependency of 180 degrees stripe domains in ferroelectric ultrathin films: a first-principles-based study," Appl. Phys. Lett. 91, 152909 (2007).

[e68] L. Bellaiche, A. Garcia, D. Vanderbilt. 2001. "Electric-field induced polarization paths in Pb(Zr1-xTi x)O3 alloys," Phys. Rev. B 64, 060103(R) (2001).

[e69] J. Hlinka, T. Ostapchuk, D. Nuzhnyj, J. Petzelt, P. Kuzel, C. Kadlec, P. Vanek, I. Ponomareva, L. Bellaiche. 2008. "Coexistence of the Phonon and Relaxation Soft Modes in the Terahertz Dielectric Response of Tetragonal BaTiO3," Phys. Rev. Lett 101, 167402 (2008).

[e70] T. Ostapchuk, J. Petzelt, P. Kuzel, S. Veljko, A. Tkach, P. Vilarinho, I. Ponomareva, L. Bellaiche, E. Smirnova, V. Lemanov, A. Sotnikov, M. Weihnacht. 2008. "Infrared and THz soft-mode spectroscopy of (Ba,Sr)TiO3 ceramics," Ferroelectrics 367, 1-10 (2008).

[e71] I. Ponomareva, L. Bellaiche, T. Ostapchuk, J. Hlinka, J. Petzelt. 2008. "Terahertz dielectric response of cubic BaTiO3," Phys. Rev. B 77, 012102 (2008).

[e72] S. Prosandeev, I. Ponomareva, L. Bellaiche. 2008. "Electrocaloric effect in bulk and low-dimensional ferroelectrics from first principles," Phys. Rev. B 78, 052103 (2008).

[e73] S. Prosandeev, L. Bellaiche. 2008. "Order parameter in complex dipolar structures: Microscopic modeling," Phys. Rev. B 77, 060101(R)(2008).

[e74] J. Iniguez, L. Bellaiche. 2001. "Ab-initio design of perovskite alloys with prefixed properties: The case of Pb(Sc0.5Nb0.5)O3," Phys. Rev. Lett 87, 095503 (2001).

[e75] See A. Franceschetti, A. Zunger. 1999. "The inverse band-structure problem of finding an atomic configuration with given electronic properties," Nature 402, 60 (1999); and W. Schweika. 1998. Disordered Alloys (Springer-Verlag, Berlin Heidelberg 1998) for a more general discussion.

[e76] I. Sosnowska, M. Lowenhaupt, W.I.F. David, R.M. Ibberson. 1992. "Investigation of the unusual magnetic spiral arrangement in BiFeO3," Physica B 180, 117 (1992).

[e77] A. M. Kadomtseva, Yu. F. Popov, A. P. Pyatakov, G. P. Vorob'ev, A. K. Zvezdin, D. Viehland. 2006. "Phase Transitions in Multiferroic BiFeO3 Crystals, Thin-Layers, and Ceramics. Enduring Potential for a Single Phase, Room-Temperature Magnetoelectric Holy Grail," Phase Transitions 79, 1019 (2006).

[e78] T. Atou, H. Chiba, K. Ohoyama, Y. Yamaguchi, Y. Syono. 1999. "Structure Determination of Ferromagnetic Perovskite BiMnO3," Journal of Solid State Chemistry 145, 639 (1999).

[e79] A. Dos Santos Moreira, K.A. Cheethama, T. Atou, Y. Syono, Y. Yamaguchi, K. Ohoyama, H. Chiba, C.N.R. Rao. 2002. “Orbital ordering as the determinant for ferromagnetism in biferroic BiMnO3,” Phys. Rev. B 66, 064425 (2002).

[e80] T. Kimura, S. Kawamoto, I. Yamada, M. Azuma, M. Takano, Y. Tokura. 2003. “Magnetocapacitance effect in multiferroic BiMnO3,” Phys. Rev. B 67, 180401 (2003).

[e81] R. V. Shpanchenko, V. V. Chernaya, A. A. Tsirlin, P. V. Chizhov, D. E. Sklovsky, E. V. Antipov, E. P. Khlybov, V. Pomjakushin, A. M. Balagurov, J. E. Medvedeva, E. E. Kaul, C. Geibel. 2004. “Synthesis, Structure, and Properties of New Perovskite PbVO3,” Chem. Mater. 16, 3267 (2004).

[e82] A. A. Belik, M. Azuma, T. Saito, Y. Shimakawa, M. Takano. 2005. “Crystallographic Features and Tetragonal Phase Stability of PbVO3, a New Member of PbTiO3 Family,” Chem. Mater. 17, 269 (2005).

[e83] D. J. Singh. 2006. “Electronic structure and bond competition in the polar magnet PbVO3,” Phys. Rev. B 73, 094102 (2006).

[e84] L.D. Landau, E.M. Lifshitz, L.P. Pitaevskii. 1984. “Electrodynamics of Continuous Media,” (Butterworth Heinemann, Oxford, 1984).

[e85] H. W. Jang, S. H. Baek, D. Ortiz, C. M. Folkman, R. R. Das, Y. H. Chu, P. Shafer, J. X. Zhang, S. Choudhury, V. Vaithyanathan, Y. B. Chen, D. A. Felker, M. D. Biegalski, M. S. Rzchowski, X. Q. Pan, D. G. Schlom, L. Q. Chen, R. Ramesh, C. B. Eom. 2008. “Strain-Induced Polarization Rotation in Epitaxial (001) BiFeO3 Thin Films,” Phys. Rev. Lett. 101, 107602 (2008)

[e86] L. Landau and E. Lifshitz. 1935. “On the theory of the dispersion of magnetic permeability in ferromagnetic bodies,” Phys. Z. Sowjetunion 8, 153 (1935).

[e87] C. Kittel. 1946. “Theory of the Structure of Ferromagnetic Domains in Films and Small Particles,” Phys. Rev. 70, 965 (1946).

[e88] S. Prosandeev and L. Bellaiche. 2007. “Influence of crystallographic steps on properties of ferroelectric ultrathin films: an Ab-initio study,” Appl. Phys. Lett. 91, 072901 (2007).

[f1] D.E. Spearot, K.I. Jacob, D.L. McDowell. 2005. Nucleation of dislocations from [001] bicrystal interfaces in aluminum, Acta Materialia, 53, 3579-3589.

[f2] D.E. Spearot, K.I. Jacob, D.L. McDowell. 2007. Dislocation Nucleation from Bicrystal Interfaces with Dissociated Structure, International Journal of Plasticity, 23, 143-160.

[f3] D.E. Spearot, M.A. Tschopp, D.L. McDowell, K.I. Jacob. 2007. Tensile Strength of <100> and <110> Tilt Interfaces in Copper, Acta Materialia, 55, 705-714.

[f4] R. Rajgarhia, D.E. Spearot, A. Saxena. 2008. Interatomic potential for copper-antimony in dilute solid-solution alloys and application to single crystal dislocation nucleation, Computational Materials Science, in press.

[f5] R. Rajgarhia, D.E. Spearot, A. Saxena. 2008. Microstructural Stability and Plastic Deformation Behavior of Nanocrystalline Copper-Antimony Alloys, presented at: MRS Fall 2008 Meeting, Boston, MA.

[f6] C.L. Kelchner, S.J. Plimpton, J.C. Hamilton. 1998. Dislocation nucleation and defect structure during surface indentation, Physical Review B, 58, 11085.

[g1] A.P. Alivisatos. 1996. Semiconductor clusters, nanocrystals, and quantum dots. Science (Washington, D. C.) 271, 933-7 (1996).

[g2] W. Kohn, L.J. Sham. 1965. Self-consistent equations including exchange and correlation effects. Phys. Rev. 140, A1133 (1965).

[g3] K. Uchino. 1996. Piezoelectric actuators and ultrasonic motors (Kluwer Academic, Boston, 1996).

[g4] M.E. Lines, A. M. Glass. 1979. Principles and applications of ferroelectrics and related materials (Clarendon, Oxford, 1979).

[g5] J.F. Scott. 2000. Ferroelectric memories (Springer Verlag, 2000).

[g6] R.D. King-Smith, D. Vanderbilt. 1993. Theory of polarization of crystalline solids. Physical Review B: Condensed Matter and Materials Physics 47, 1651-4 (1993).

[g7] R. Resta. 1994. Macroscopic polarization in crystalline dielectrics: the geometric phase approach. Reviews of Modern Physics 66, 899-915 (1994).

[g8] R. M. Martin, G. Ortiz. 1997. Functional theory of extended Coulomb systems. Phys. Rev. B 56, 1124-1140 (1997).

[g9] X. Gonze, P. Ghosez, R.W. Godby. 1997. Density-functional theory of polar insulators. Physical Review Letters 78, 294-297 (1997).

[g10] J. Junquera, P. Ghosez. 2003. Critical thickness for ferroelectricity in perovskite ultrathin films. Nature 422, 506-509 (2003).

[g11] P. Ghosez, K.M. Rabe. 2000. Microscopic model of ferroelectricity in stress-free PbTiO3 ultrathin films. Applied Physics Letters 76, 2767-2769 (2000).

[g12] C.H. Ahn et al. 1997. Local, nonvolatile electronic writing of epitaxial Pb(Zr0.52Ti0.48)O3/SrRuO3 heterostructures. Science 276, 1100-1103 (1997).

[g13] I.I. Naumov, L. Bellaiche, H. Fu. 2004. Unusual phase transitions in ferroelectric nanodisks and nanorods. Nature (London, United Kingdom) 432, 737-740 (2004).

[g14] W. Zhong, D. Vanderbilt, K.M. Rabe. 1994. Phase transitions in BaTiO3 from first principles. Physical Review Letters 73, 1861-4 (1994).

[g15] L. Bellaiche, A. Garcia, D. Vanderbilt. 2000. Finite-Temperature Properties of Pb(Zr1-xTix)O3 Alloys from First Principles. Physical Review Letters 84, 5427-5430 (2000).

[g16] H. Fu, O. Gulseren. 2002. Piezoelectric Pb(Zr0.5Ti0.5)O3: interplay of atomic ordering, ferroelectric soft modes, and pressure. Physical Review B: Condensed Matter and Materials Physics 66, 214114/1-214114/7 (2002).

[g17] A. Nazzal, H. Fu. 2005. Organic-inorganic hybrid semiconductor ZnSe(C2H8N2)1/2 under hydrostatic pressure. Physical Review B: Condensed Matter and Materials Physics 72, 075202/1-075202/6 (2005).

[g18] H. Fu, L. Bellaiche. 2003. First-Principles Determination of Electromechanical Responses of Solids under Finite Electric Fields. Physical Review Letters 91, 057601/1-057601/4 (2003).

[g19] H. Fu. 2002. Band-edge states and optical properties of ordered Pb(Zr0.5Ti0.5)O3 from first principles. AIP Conference Proceedings 626, 17-25 (2002).

[g20] R.E. Cohen, E. Heifets, H. Fu. 2001. First-principles computation of elasticity of Pb(Zr,Ti)O3: The importance of elasticity in piezoelectrics. AIP Conference Proceedings 582, 11-22 (2001).

[g21] D. Karanth, H. Fu. 2005. Large electromechanical response in ZnO and its microscopic origin. Physical Review B: Condensed Matter and Materials Physics 72, 064116/1-064116/6 (2005).

[g22] W. Su, X. Huang, J. Li, H. Fu. 2002. Crystal of Semiconducting Quantum Dots Built on Covalently Bonded T5 [In28Cd6S54]-12: The Largest Supertetrahedral Cluster in Solid State. Journal of the American Chemical Society 124, 12944-12945 (2002).

[g23] H. Fu. 2002. Stark shifts, band-edge transitions, and intrinsic optical dipoles in spherical InP quantum dots under electric fields. Physical Review B: Condensed Matter and Materials Physics 65, 045320/1-045320/5 (2002).

[g24] H. Fu, A. Zunger. 1998. Quantum-Size Effects on the Pressure-Induced Direct-to-Indirect Band-Gap Transition in InP Quantum Dots. Physical Review Letters 80, 5397-5400 (1998).

[g25] H. Fu, A. Zunger. 1997. Local-density-derived semiempirical nonlocal pseudopotentials for InP with applications to large quantum dots. Physical Review B: Condensed Matter 55, 1642-1653 (1997).

[h1] M. Austin-Seymour, G.T.Y. Chen, J. Rosenman, J. Michalski, K. Lindsley, M. Goitein. 1995. Tumor and target delineation: Current research and future challenges. Int J Radiat Oncol Biol Phys 33 (1995), pp. 1041–1052.

[h2] M. Austin-Seymour, I. Kalet, J. McDonald et al. 1995. Three dimensional planning target volumes: A model and a software tool. Int J Radiat Oncol Biol Phys 33 (1995), pp. 1073–1080

[h3] M. Goitein, M. Abrams. 1983. Multi-dimensional treatment planning: I. Delineation of anatomy. Int J Radiat Oncol Biol Phys 9 (1983), pp. 777–787.

[h4] C.H. Ketting, M. Austin-Seymour, I. Kalet, J. Unger, S. Hummel, J. Jacky. 1997. Consistency of three-dimensional planning target volumes across physicians and institutions. Int J Radiat Oncol Biol Phys 37 (1997), pp. 445–453.

[h5] G. Shafirstein, L. Hennings, Y. Kaufmann, et al. 2007. Conductive interstitial thermal therapy (CITT) device evaluation in VX2 rabbit model. Technol Cancer Res Treat. 2007;6:235-246.

[h6] G. Shafirstein, P. Novak, E.G. Moros, et al. 2007. Conductive interstitial thermal therapy device for surgical margin ablation: in vivo verification of a theoretical model. Int J Hyperthermia. 2007;23:477-492.

[h7] U. Topaloglu, E.D. Bearden, Y. Yan, P. Novak, P. Spring, J. Suen, G. Shafirstein. 2008. “A New Computer Simulation Method for Improved Treatment Planning of Thermal Ablation in the Head and Neck”, ICHO 2008 Germany

[h8] R.G. Belleman, J.A. Kaandorp, D. Dijkman, P.M.A. Sloot. 1999. GEOPROVE: Geometric Probes for Virtual Environments, in P.M.A. Sloot; M.T. Bubak; A.G. Hoekstra and L.O. Hertzberger, editors, High-Performance Computing and Networking (HPCN Europe '99), Amsterdam, The Netherlands, in series Lecture Notes in Computer Science, nr 1593 pp. 817-827. Springer-Verlag, Berlin, April 1999.

[h9] N. Graf, C. Desmedt, A. Hoppe, M. Tsiknakis, D. Dionysiou, G. Stamatakos. 2007. Clinical requirements of “In Silico Oncology” as part of the integrated project ACGT (Advancing Clinico-Genomic Trials on Cancer), European Journal of Cancer Supplements, Vol5 No 4, p. 83andECCO Conference September 2007, Barcelona

[j1] A. Yildiz, P.R.Selvin. 2005. Fluorescence Imaging with One Nanometer Accuracy (FIONA): Application to Molecular Motors. *Accounts of Chemical Research*,38(7), 574-82 (2005).

[k1] B. Zhang. 1998. ZPC 1.0.1: a parton cascade for ultrarelativistic heavy ion collisions, *Computer Physics Communications,* 1998*, 109*, 193-206.

[k2] M.P. Allen, D. Frenkel, J. Talbot. 1989. Molecular dynamics simulation using hard particles. *Comput. Phys. Rep*, 9:301–353, 1989.

[k3] B. D. Lubachevsky. 1991. How to simulate billiards and similar systems, *Journal of Computational Physics,* 1991*, 94*, 255-283.

[k4] M. Marin, D. Risso, P. Cordero. 1993. Efficient algorithms for many-body hard particle moledular dynamics, *Journal of Computational Physics,* 1993*, 109*, 306-317.

[k5] H. Jiang, H.-C. Su, B. Zhang. 2007. Toward Optimizing Particle-Simulation Systems, *Proceedings of International Conference on Computational Science,* 2007, 286-293.

[k6] R. Li, H. Jiang, H.-C. Su, B. Zhang, J. Jenness. 2007. Speculative and Distributed Simulation of Many-Particle Collision Systems, In *Proceedings of the 13th International Conference on Parallel and Distributed Systems*, 2007.

[k7] R. Li, H. Jiang, H.-C. Su, J. Jenness, B. Zhang. 2008. Adaptive and Fault Tolerant Simulation of Relativistic Particle Transport with Data-level Checkpointing, In *Proceedings of the 11th IEEE International Conference on Computational Science and Engineering* , 2008.

[k8] M. Isobe. 1999. Simple and efficient algorithm for large scale molecular dynamics simulation in hard disk system, *International Journal of Modern Physics,* 1999*, C*, 1281-1293.

[k9] A. Donev, S. Rorquato, F. Stillinger. 2005. Neighbor list collision-driven molecular dynamics simulation for nonspherical hard particles. I. Algorithmic details, *Journal of Computational Physics,* 2005*, 202*, 737-76.

[k10] A. Donev, S. Rorquato, F. Stillinger. 2005. Neighbor list collision-driven molecular dynamics simulation for nonspherical hard particles. II. Algorithmic details, *Journal of Computational Physics,* 2005*, 202*, 765-793.

[k11] S. Miller, S. Luding. 2004. Event-driven molecular dynamics in parallel, *Journal of Computational Physics,* 2004*, 193*, 306-31.

[k12] B. D. Lubachevsky. 1991. How to simulate billiards and similar systems, *Journal of Computational Physics,* 1991*, 94*, 255-283.

[k13] M. Mu. 2002. A multiple-heaps algorithm for parallel simulation of collision systems, *Journal of Computational Physics,* 2002*, 179*, 539-556.

[k14] H. Sigurgeirsson, A. Stuart, W.-L. Wan. 2002. Algorithms for particle-field simulations with collisions, *Journal of Computational Physics,* 2002*, 172*, 766-807.

[m1] H. Byelas, A. Telea. 2008. Texture-based visualization of metrics on software architectures. In SoftVis '08: Proceedings of the 4th ACM symposium on Software visualization, pp 205–206, New York, NY, USA, 2008. ACM.

[m2] J.A. Cottam, J. Hursey, A. Lumsdaine. 2008. Representing unit test data for large scale software development. In SoftVis '08: Proceedings of the 4th ACM symposium on Software visualization, pp 57–66, New York, NY, USA, 2008. ACM.

[m3] G.F. Carneiro, R. Magnavita, M. Mendonc. 2008. Combining software visualization paradigms to support software comprehension activities. In SoftVis '08: Proceedings of the 4th ACM symposium on Software visualization, pp 201–202, New York, NY, USA, 2008. ACM.

[m4] J. Dietrich, V. Yakovlev, C. McCartin, G. Jenson, M. Duchrow. 2008. Cluster analysis of java dependency graphs. In Soft-Vis '08: Proceedings of the 4th ACM symposium on Software visuallization, pp 91–94, New York, NY, USA, 2008. ACM.

[m5] D. Harel, I,. Segall. 2008. Visualizing inter-dependencies between scenarios. In SoftVis '08: Proceedings of the 4th ACM symposium on Software visualization, pp 145–153, New York, NY, USA, 2008. ACM.

[m6] A. Jermakovics, R. Moser, A. Sillitti, G. Succi. 2008. Visualizing software evolution with lagrein. In OOPSLA Companion '08: Companion to the 23rd ACM SIGPLAN conference on Object oriented programming systems languages and applications, pp 749–750, New York, NY, USA, 2008. ACM.

[m7] A. Jermakovics, M. Scotto, G. Succi. 2007. Visual identification of software evolution patterns. In IWPSE '07: Ninth international workshop on Principles of software evolution, pp 27–30, New York, NY, USA, 2007. ACM.

[m8] A. Marcus, X. Xie, D. Poshyvanyk. 2005. When and how to visualize traceability links? In TEFSE '05: Proceedings of the 3rd international workshop on Traceability in emerging forms of software engineering, pp 56–61, New York, NY, USA, 2005. ACM.

[m9] A.A. Martınez, J.J.D. Cosın, C.P. Garcia. 2008. A metro map metaphor for visualization of software projects. In SoftVis '08: Proceedings of the 4th ACM symposium on Software visualization, pp 199–200, New York, NY, USA, 2008. ACM.

[m10] A. Noack, C. Lewerentz. 2005. A space of layout styles for hierarchical graph models of software systems. In SoftVis ’05: Proceedings of the 2005 ACM symposium on Software visualization, pp 155–164, New York, NY, USA, 2005. ACM.

[m11] C. Parnin, C. Gorg, O. Nnadi. 2008. A catalogue of lightweight visualizations to support code smell inspection. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pp 77–86, New York, NY, USA, 2008. ACM.

[m12] B. Ploeger, C. Tankink. 2008. Improving an interactive visualization of transition systems. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pp 115–124, New York, NY, USA, 2008. ACM.

[m13] H. Shah, C. Gorg, M.J. Harrold. 2008. Visualization of exception handling constructs to support program understanding. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pp 19–28, New York, NY, USA, 2008. ACM.

[m14] J. Sundararaman, G. Back. 2008. Hdpv: interactive, faithful, invivo runtime state visualization for c/c++ and java. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pp 47–56, New York, NY, USA, 2008. ACM.

[m15] S. Tangsripairoj, M. H. Samadzadeh. 2005. Organizing and visualizing software repositories using the growing hierarchical self-organizing map. In SAC ’05: Proceedings of the 2005 ACM symposium on Applied computing, pp 1539–1545, New York, NY, USA, 2005. ACM.

[m16] A. Telea, L. Voinea. 2008. An interactive reverse engineering environment for large-scale c++ code. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pp 67–76, New York, NY, USA, 2008. ACM.

[m17] R. Theron, A. Gonzalez, F.J. Garcia. 2008. Supporting the understanding of the evolution of software items. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pp 189–192, New York, NY, USA, 2008. ACM.

[m18] D. Zeckzer, R. Kalcklosch, L. Schroder, H. Hagen, T. Klein. 2008. Analyzing the reliability of communication between software entities using a 3d visualization of clustered graphs. In SoftVis ’08: Proceedings of the 4th ACM symposium on Software visualization, pages 37–46, New York, NY, USA, 2008. ACM.

[n1] E.E. Hood, R. Love, J. Lane, J. Bray, R. Clough, K. Pappu, C. Drees, K.R. Hood, S. Yoon, A. Ahmad, J.A. Howard. 2007. Subcellular targeting is a key condition for high-level accumulation of cellulase protein in transgenic maize seed. Plant Biotechnol J 5, 709-719.

[n2] K.R. Hood, R.A. Baasiri, S.E. Fritz, E.E. Hood. 1991. Biochemical and tissue print analyses of hydroxyproline-rich glycoproteins in cell walls of sporophytic maize tissues. Plant Physiol 96, 1214-1219.

[q1] A. Akbarzadeh et Al. 2006. “Towards Urban 3D Reconstruction From Video,” in Proceedings of the Third International Symposium on 3D Data Processing, Visualization, and Transmission, 2006, pp. 1-8.

[q2] S. Se, P. Jasiobedzki. 2008. “Stereo-Vision Based 3D Modeling and Localization for Unmanned Vehicles,” International Journal of Intelligent Control and Systems, Special Issue on Field Robotics and Intelligent Systems, vol. 13, no. 1, pp. 47-58, 2008.

[q3] S. Teller. 1998. “Automated urban model acquisition: Project rationale and status,” in Image Understanding Workshop, 1998, pp. 455–462.

[q4] G. M. Hegde, C. Ye. 2008. “SwissRanger SR-3000 range images enhancement by a singular value decomposition filter,” in Proceedings of IEEE International Conference on Information and Automation, 2008, pp. 1626-1631.

[q5] G. M. Hegde, C. Ye. 2008. “Singular value decomposition filter: an effective method to enhance the SwissRanger SR-3000’s range images,” submitted to the International Journal of Information Acquisition (invited paper), 2008.

[q6] C. Ye, G. M. Hegde. 2009. “Robust edge extraction for SwissRanger SR-3000 range images,” submitted to 2009 IEEE International Conference on Robotics and Automation.

[s1] A. Szwilski, J. Smith, M. Lewis, T. Buckland. 2008. “Mine Safety Training: Advantage of Collaborative and Interactive Web-based Virtual Technology”, proceedings of the 17th International Symposium on Mine Planning and Equipment Selection, Beijing, China, October 20-22, 2008.

[s2] S. Li, W. K. Liu. 2002. “Meshfree and particle methods and applications”, Appl Mech Rev vol 55, no 1, January 2002.

[s3] W. Roush. 2007. “Second Earth”, Technology Review, July/August 2007. https://www.technologyreview.com/Infotech/18911

[s4] R. Begley (PI), A.B. Szwilski (Co-PI). 2000-2009. Developing an Integrated Track Stability Assessment and Monitoring System for Railway Track; Intelligent Transportation Systems for Railroads. Total funding $5.37 million. Federal Rail Administration funding.

[s5] A.B. Szwilski, R.D. Begley, P. Dailey, Z. Sheng. 2003. Multi-Sensor Mobile System to Monitor Rail Track Superstructure and Substructure: Initial Studies with Non-Invasive Technologies, American Railway Engineers (AREMA) Conference, Chicago, October.

[s6] A.B. Szwilski, R.D. Begley. 2003. Developing an Integrated Rail Track Stability Assessment and Monitoring System Using Non-Invasive Technologies, Transportation Research Board 82nd Annual Meeting, Washington, D.C., January.

[s7] A.B. Szwilski, H.M. Lees Jr, R.D. Begley, P. Dailey, Z. Sheng. 2006. Employing High Accuracy DGPS to Monitor Track Shift, 7th World Congress on Railway Research, Montreal, Canada, June.

[s8] A.B. Szwilski, W.B. Kerchof, J. Tomlin, P. Dailey, Z. Sheng, R.D. Begley. 2005. Rapid Surveying of a Classification Yard Employing High Accuracy DGPS (RTK), American Railway Engineers (AREMA) Conference, Chicago, October.

[s9] A.B. Szwilski, P. Dailey, , Z. Sheng, R.D. Begley. 2005. “Employing HADGPS to Survey Track and Monitor Movement at Curves”, Railway Engineering 2005: 8th International Conference and Exhibition, London, June.

[s10] A.B. Szwilski, R.D. Begley, P. Dailey, Z. Sheng. 2003. Determining Rail Track Movement Trajectories and Alignment Using HADGPS, American Railway Engineers (AREMA) Conference, Chicago, October 2003.

[s11] A.B. Szwilski, J. Ball, T. Cook, L. Tulley. 2002. Rock Fall Hazard Evaluation and Data Management System for Highway and Railway Rock Slopes”, Seventh International Symposium on Environmental Issues and Waste Management in Energy and Mineral Production, Cagliary, Sardinia, Italy, October 2002.

[s12] Appalachian Consortium for Geohazards in Transportation, sponsored by the Rahall Transportation Insitutute http://www.marshall.edu/cegas/geohazards/

[y1] The RCSB Protein Databank. http://www.rcsb.org/pdb/home/home.do

[z1] B. Lu, A. Apon, L. Dowdy, F. Robinson, D. Hoffman, and D. Brewer, “A Case Study on Grid Performance Modeling,” International Conference on Parallel and Distributed Computing Systems, November 13, 2006, 9 pages.

[z2] B. Lu, A. Apon, L. Ngo, H. Bui, L. Dowdy, N. Hamm, D. Hoffman, "Capacity Planning of Supercomputing Resources in an Academic Environment: A Case Study", LCI International Conference on High-Performance Clustered Computing, April, 2008.

[z3] D. Hoffman, A. Apon, L. Dowdy, B. Lu, L. Ngo, H. Bui, N. Hamm, "Performance Modeling of Grid Systems," book chapter accepted, to appear, 2009.

[z4] B. Lu, L. Ngo, H. Bui, A. Apon, N. Hamm, L. Dowdy, D. Hoffman, D. Brewer, "Workload Modeling for Performance Management," Computer Measurement Group '08, December, 2008.

[z5] A. Apon, P. Wolinski, D. Reed, D. Amerson, and P. Gorjala. "Massive Data Processing on the Acxiom Cluster Testbed," Conference on Commercial Applications for High Performance Computing, held as a part of SPIE 2001, Denver, Colorado, August 19-23, 2001, p. 147-158.

[z6] A. Apon, P. Wolinski, G. Amerson, "Sensitivity of Cluster File System Access to I/O Server Selection," Proceedings of CCGrid 2002, May, 2002, pp. 183-192.

[z7] M. Ibrahim, A. Apon, "Sorting using MPI on workstation clusters," Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications, Las Vegas, Nevada, June, 2003, pp. 151-156.

[z8] Y. Zhang, A. Apon, P. Pulay, "Array Files for Out-of-Core Computations" Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications, Las Vegas, Nevada, June, 2003, 7 pages.

[z9] Y. Zhang and A. Apon, "Implementation Tradeoffs of the Array Files Library for Out-of-Core Computations," International Conference on Cluster Computing (Cluster 2006), Barcelona, September 26, 2006, 8 pages.

[z10] G. Amerson, and A. Apon, "Implementation and Design Analysis of a Network Messaging Module Using Virtual Interface Architecture," International Conference on Cluster Computing (Cluster 2004), San Diego, September, 2004, 11 pages.

[z11] B. Lu, M. Tinker, A. Apon, D. Hoffman, and L. Dowdy. "Adaptive Automatic Grid Reconfiguration Using Workload Phase Identification," Proceedings of EScience 2005, December, 2005, 9 pages.

[z12] L. Ngo, B. Lu, H. Bui, A. Apon, N. Hamm, L. Dowdy, D. Hoffman, D. Brewer. "Application of Empirical Mode Decomposition to the Arrival Time Characterization of a Parallel Batch System Using System Logs," (submitted).

[z13] D.V. Foster, L.W. Dowdy, and J.E. Ames, "File assignment in a computer network," Computer Networks 5, (September, 1981), 341-349.

[z14] A. Perez-Davila and L.W. Dowdy, "Parameter interdependencies of file placement models in a Unix system," (Award Paper) Proceedings of the Conference on Measurement and Modeling of Computer Systems. Also, Performance Evaluation Review 12, 3 (1984), 15-26.

[z15] L.W. Dowdy and D.V. Foster, "Comparative models of the file assignment problem," Computing Surveys 14, (June, 1982), 287-313. Reprinted in Tutorial: Distributed Database Management, (J.A. Larson and S. Rahimi, eds.), IEEE Computer Society Press, (1985), 95-121.

[z16] K.H. Park and L.W. Dowdy, "Dynamic partitioning of multiprocessor systems," International Journal of Parallel Programming, 18, 2 (April, 1989), 91-120.

[z17] E. Rosti, E. Smirni, T. D. Wagner, A. Apon, and L. W. Dowdy. "The KSR1: Experimentation and Modeling of Poststore," ACM Sigmetrics Conference on Measurement and Modeling of Computer Systems, 1993, pp. 74-85.

[z18] L.W. Dowdy and M.R. Leuze, "On modeling partitioned multiprocessor systems," International Journal of High Speed Computing, 6, 1 (1994), 31-53.

[z19] T. D. Wagner, E. Smirni, A. Apon, M Madhukar, and L. W. Dowdy. "Measuring the Effects of Thread Placement on the Kendall Square KSR1," Eighth International Parallel Processing Symposium, 1994.

[z20] E. Rosti, E. Smirni, L.W. Dowdy, G. Serazzi, and K.C. Sevcik, "Processor saving scheduling policies for multiprocessor systems," IEEE Trans. On Computers, 47, 2 (February, 1998), 178-189.

[z21] A. Apon, T. D. Wagner, and L. W. Dowdy. "A Learning Approach to Processor Allocation in Parallel Systems," Eighth International Conference on Information and Knowledge Management CIKM99, November, 1999, p. 531--537.

[z22] P.R. Chintamaneni and L.W. Dowdy, "Workload characterization and synthetic work load generation: an application study," Computer Systems Science and Engineering, 4, 4 (October, 1989), 205-215.

[z23] A. Apon and L. W. Dowdy. "The Circulating Processor Model of Parallel Systems," IEEE Transactions on Computers, 46(5), May, 1997, p. 572-587.

[z24] K.H. Park and L.W. Dowdy, "Execution signatures, a parallel characterization, and its properties," Intl. Journal of Computers and Applications, 19, 3, (1997), 123-129.

[z25] D.A. Menasce, V.A.F. Almeida, and L.W. Dowdy, Capacity Planning and Performance Modeling: From Mainframes to Client-Server Systems, Prentice-Hall, 1994.

[z26] D.A. Menasce, V.A.F. Almeida, and L.W. Dowdy, Performance by Design, Prentice-Hall, 2004.