MSU INVESTMENT PROPOSAL FOR INSTITUTIONAL PRIORITIES

PROPOSAL OVERVIEW

Title	Computational Facility for Molecular Sciences	**Request Date**	December 16, 2011
Department	Chemistry and Biochemistry	**Email**	szilagyi@montana.edu
Requestor	Robert K. Szilagyi	**Phone**	X4263

STRATEGIC ALIGNMENT

Core Themes and Objectives (check all that apply)

Educate Students

☒ Our graduates will have achieved mastery in their major disciplines

☒ Our graduates will become active citizens and leaders

☒ Our graduates will have a multicultural and global perspective

☒ Our graduates will understand the ways that knowledge & art are created and applied in a variety of disciplines

☒ Our graduates are prepared for careers in their field

☒ We will provide increased access to our educational programs

☒ Communities and external stake holders benefit from broadly defined education partnerships with MSU

Create Knowledge and Art

☒ Students, faculty, and staff will create knowledge and art that is communicated widely

Serve Communities

☐ We help meet a fundamental need of the citizens of Montana by providing degree programs for our students

☒ We help meet the educational needs of the citizens of Montana by providing a wide range of educational opportunities to a variety of students

☒ Our students, faculty, staff, and administrators reach out to engage and serve communities

☐ Our students, faculty, staff, and administrator reach in to build the university community

Integrate Learning, Discovery, and Engagement

☒ Each graduate will have had experiences that integrate learning, discovery and engagement

☐ Outreach activities will educate students and address the needs of the communities we serve

☒ Students, faculty, and staff will create knowledge and art that addresses societal needs

☒ MSU is a community that will be characterized by synergy within and across disciplines, roles and functions.

Stewardship

☒ The public trusts the institution to operate openly and use resources wisely

☒ The faculty and staff are well-qualified and supported

☒ MSU will support Native American students, programs, and communities

☐ MSU will be an inclusive community, supporting and encouraging diversity

☒ Our publicly provided resources are used efficiently and effectively

☐ Natural resources are used efficiently and sustainable

☐ MSU nurtures a culture of resource conservation and ecological literacy among students, faculty and staff

☒ Our physical infrastructure (e.g., building, equipment, open spaces) will be well-maintained and useful

INSITUTIONAL BENEFIT						
Campuses	☒ Bozeman ☒ Billings ☒ Havre ☐ Great Falls ☐ FSTS ☐ Extension ☐ MAES					
Cross Depts	Chemistry&Biochemistry, Physics, Chem&Biol Engineering, Plant Sciences, Microbiology, Mathematics					
TIMEFRAME						
Proposed Dates	Start: June 1, 2012 End: May 30, 2015					
COST AND REQUIREMENTS						
Funding Type	One-Time ($)	Multi-Year ($)			Base ($)	FTE
		Year 1	Year 2	Year 3		
Personnel (*w/benefits*)						
Materials & Supplies		$ 25,000	$ 25,000	$ 25,000		
Travel						
Contracted Services						
Capital		$125,000	$125,000	$125,000		
Other Operations		$75,000				
TOTAL		$225,000	$150,000	$150,000		

Please comment, if necessary, regarding cost and requirements.

The main item of the proposed budget is computational hardware installation of a top-of-the-line multi-processor and multi-compute unit configuration (Blade Server) with appropriate computational interconnect (Infiniband) and 10Gbs internet for user access and maintenance.

Each 'blade' is proposed to be composed of two computational units with 64 nodes altogether (16 core 2.6GHz Opteron G34 6282SE) and 64 Gbyte RAM per unit (2 Gbyte per node). The temporary file storage would be on two 600 Gbyte 10,000 RPM, 6Gbs drives. A single 19" industry standard enclosure would hold two of these blades (TwinBlades) and thus would reduce the server footprint. Power, cooling and networking devices are aggregated in the rear of the chassis which optimizes the required amount of space. This proposed configuration would allow for a gradual development of a computational powerhouse in three years providing computational resources for molecular scientific simulations with close to 2000 computational nodes, 4 terrabyte of memory, and more than 70 terrabyte fast access harddisk drive.
To my best knowledge, this scale of computational facility is unprecedented in Montana and even in the entire Northern Rockies region.

The materials and supplies are requested for hardware and software maintenance, duplicate long- and short-term file backup systems, optical storage media and related office supplies.

The computational server room 254 in Chemistry and Biochemistry Building has already adequate air-conditioning (two A/C units), shelving, and expandable power connection to house the blade servers. There is already an approximately 200 node, heterogeneous server park being operated and maintained in the same room.

The $75,000 other operational cost is requested for the Facilities (Loras O'Toole and co) to assure that the server room has adequate power by installing additional lines to accommodate all the 60 servers with individual power supplies in each of them.

Due to the dedicated application environment, already existing expertise with similar hardware and software there is no immediate need for creation of a new FTE line for operating the hardware.
The requestor would be in charge of maximizing resource utilization by working with a group of administrators/superuser from various disciplines to provide balanced access to an expected diverse group of users with research, coursework, and outreach related tasks.

PROPOSAL SCOPE

Describe the Proposal

Rational and Justification: An investment is proposed over the next three years in modernizing MSU computational facilities for education, research & discovery, and outreach activities related to molecular sciences. Top-of-the line computational servers would create a modular and versatile system to serve the needs of multiple undergraduate and graduate courses from various disciplines (physics, chemistry, biology) and a diverse set of scientific research labs (see next page) at MSU and beyond. In addition, the combined computational power would undoubtedly generate interest from other academic entities from Montana, including Tribal Colleges and high schools with advanced science programs. These would be ideal targets for outreach activities in both educational and research activities. The Spring 2011 meeting of the Montana Section of the American Chemical Society has already discussed the need for organizing hands-on modeling workshops in molecular sciences even for professors, instructors, and educators in order to modernize their physics, chemistry, and biology curriculum at their home institutes.

There are flagship centers and programs at MSU that have the words “molecular science” in their descriptions or at least in their mission statements. This parallels that the main focus of the early 21st century in scientific discovery and engineering is the molecular understanding and manipulation of matter. The concept of molecules/molecular processes is no longer limited to chemistry, but over the past century this world became a trademark for interdisciplinarity. From physicists to biologist and even to ecologist and nutritional scientists, the molecular level details of physical, chemical, or biological processes are of essential interest.
Our students and their instructors need to be comfortable with the related terminology and familiar with recent developments in molecular sciences in order to stay competitive among their peers. The advancement of experimental techniques that many MSU researchers routinely can access within their research programs enables so much data to be produced that often scientists and engineers turn to computational modeling and simulation. Having a top-of-the line, dedicated computational facility for molecular sciences (as broadly defined in physics, chemistry, and biology) would allow our undergraduate and graduate students to get the training they will need for successfully landing in their first jobs in industry or academia, enable new scientific opportunities for our researchers, contribute to more successful recruiting efforts for college, graduate school, and even postgraduate training.
In addition to student recruiting, the existence of a dedicated infrastructure to theoretical molecular scientific research would also be very attractive for recruiting top notch faculty with likely well-funded research program in the next couple of years. Transparent access to the proposed close to 2000 node computational cluster could be a notable in-kind value of about half million dollar as part of a startup package.

It is now common sense to say that computers are everywhere in our lives. Studies indicate how smart technology-enabled tools change the way we interact with each other, how we learn, and how we carry out daily tasks. It is still anecdotal and somewhat controversial to bring up the positive effects of computer-enabled games. Leading game research scientists (Dr. Jane McGonigal, for example) started to promote the benefit of harnessing the power of games to solve real-world problems. There are now statistics showing that about 174 million Americans are gamers and the average young person, our college students, in the US spends ten thousands hours gaming by their mid-twenties. Perhaps it is not too far fetched to assume that several MSU faculty members have also experienced that when a course assignment is delivered and evaluated online in a user-friendly environment without computer crashes, long wait times, and ‘blue-screens of death’ the student participation and involvement are considerably better and more instantaneous that using traditional, photocopier-enabled methods. The requestor could demonstrate in a separate document how creating computer technology-enabled hybrid courses first WebCT and now the D2L already enhanced his teaching efficiency in the past five years. The power of involving students in manipulating atoms, orbitals, electron spins, molecules, nanoparticles in real time with instantaneous response would be very rewarding for both the students and their instructors. The proposed investment into creating a dedicated computational facility would tremendously enhance our ability to integrate learning, discovery, and engagement in molecular sciences.

Background and Pre-existing Facilities: A recent initiative by the Provost and VP of Research has brought together a group of faculty members at the Center for Computational Biology (CBB) to discuss the past, present, and future of computational sciences at MSU. For the specific details I would like to refer to the envisioning committee's final report. In brief, these discussions have identified a considerable interest and formulated plans for further enhancing our current computational facilities to better serve both the student body and faculty needs. The Faculty Leadership Committee of the CBB has already started working toward developing campus-wide data management, mining, storage, and utilization strategies. The given investment proposal plans to complement their effort by also emphasizing the identified need for focusing on computational power-hungry applications in molecular sciences, which is beyond the current scope of the CBB activities.

In the past decade, the research foci at many departments, cross colleges moved toward molecular level probing of physical, chemical, and biological processes that require theoretical simulations at the molecular level. A representative example here is the activities of the Department of Chemistry and Biochemistry. Practically every research program has a need for theoretical simulations of molecular scale processes that are either addressed by collaborations within the department or outside MSU. Due to the limited computational resources and the related know-how, these needs are often set aside and thus limiting scientific impact and student experience. Again a similar situation is expected for other departments on campus with molecular science foci or interests.

As part of the activities of the above mentioned envisioning committee, it was estimated that about a dozen of small size computational clusters exist campus-wide in Bozeman. However, there is only one facility operated by the requestor's research laboratory; which has been providing resources to undergraduate students (Honors General Chemistry, Advanced Inorganic Chemistry, Physical Chemistry, Organic Chemistry courses; independent studies; REU summer research programs) or in collaboration to various research labs from the Department of Chemistry and Biochemistry (Broderick, Peters, Douglas, Minton, Lawrence), Chemical and Biological Engineering (Peyton, Gerlach), Plant Sciences (Young), Physics (Craig). The current limitation in extending these collaborative efforts and involving additional courses is the availability of computer hardware. The main objective of the proposal is to overcome this limitation by installing the proposed server park. By establishing a dedicated facility additional research labs would benefit from the Chemistry and Biochemistry (Bothner, Callis, Copie, Dratz, Kohler, Rainey, Teintze, Walker), Physics (Idzerda, Avci, Longscope, Rebane), Chemical and Biological Engineering (Carlson, Heys, Larsen, Seymour), Cell Biology and Neuroscience (Miller, Jacobs), Microbiology (Dlakic, Geesey), Mathematical Sciences (Gedeon). This list is far from being complete due to lack of a campus wide survey about the interests, facilities, and specific needs of heavy computation demanding molecular science applications. Additional potential benefactors (and also potential 'customers') of a MSU Bozeman centered facility beyond the borders of Gallatin County would be from MSU Billings (Dillman, Lewis, Marlow, Wiles), MSU Havre (Towne), University of Missoula (Rosenberg, McGuirl, Xi, Bowler, Earle), Caroll College (Strode, Thomas), Flathead Community College (Alexander), MT Tech (Klem).

The most essential software packages for molecular scientific simulations, such as Gaussian suite of programs, Amsterdam Density Functional, Tinker molecular mechanical and dynamics packages, a large set of semi-empirical software package, high performance Fortran and C-compilers, mathematical libraries, and scientific software are already available with site licenses for some of them. Using the 'roll'-based automatic installations (rockscluster.org) software updates, new scientific applications can be straightforwardly deployed to each node without any human interaction. This would practically eliminate the need for a dedicated hardware support personnel. As has been done in the past in the requestor's research lab, the materials and supplies budget would allow for purchase of parts to build in modest redundancy. There would not be any troubleshooting, just swap out of the faulty part and mail that back to the manufacturer for warranty replacement.

A group of selected users with administrative/superuser privileges would be able to maintain both the software and the hardware as has been done for the last 8 years by the requestor's research group. In the case of considerable interested from outside of the field of molecular sciences (new applications and software) as well as interest in using the facility beyond MSU campuses (new users) the facility will need to have a dedicated software and hardware personnel. This is beyond the current scope of the proposal and to be developed upon the hiring the chief-information technology officer for MSU.

PROPOSAL SCOPE
Describe the broader impacts and benefits of this proposal

Educate Students A computational facility geared toward serving a larger community than isolated, single research labs. Direct hands-on experience for our students would enable training a more versatile group of graduates who master both experimental and theoretical aspects of their major discipline. Access to top of the line technology sets up a good example for modern educational facilities and boosts our students as well as faculty's chances to become leaders of their respective community. Given the competitive work environment in industry and even in academia, larger scale facilities such as the proposed one give a cutting-edge advantage to our students and faculty to become successful in their careers, and continue attracting extramural funding from federal research organizations. The installation of close to 2000 compute nodes is notable and expected to attract national and international collaborative projects and unavoidable extramural funding. Bringing visiting faculty, exchange students would create opportunities for our faculty and students to work in a multicultural environment with international perspective.

It is important to emphasize that computer-enabled simulations and visualizations have the potential to bring the abstract world of molecules and atoms closer to our students and provide them with a first-hand experience in theoretical modeling. Timely generation of course materials with the above content would require the existence of the proposed facility. With modest effort, the resources to be provided by the computational facility can be integrated with online educational programs and thus increasing the state-wide access. The MSU Extended University has already the expertise and personnel to take the crude animations that are based on accurate theoretical models and elevate the presentation quality that could meet the requirement of a professional production studio. Also course materials generated and distributed electronically from the research activities of faculty and students utilizing the proposed facility can feed into online courses. A notable outreach activity would involve the community, high schools, community colleges, and tribal colleges via demonstrations, hands on activities, multimedia presentations. The requestor has successfully experimented with showing examples of molecular science to a group of home schooled children, Native American high school students (AIRO MAP), a group of middle and high school teachers (summer MSSE courses). One of the popular Science Saturday events (spearheaded by Prof. Trevor Douglas) was organized around the molecular world of carbon, biology, inorganic complexes, and minerals.

Create Knowledge and Art The computational facility has the potential to greatly to enhance the scientific publication (peer reviewed papers, oral presentations and posters at meetings and conference) activity of any involved faculty members and students. The combined computational power would allow them to stretch their research focus to larger and more complex molecular structures without the compromise of structural truncation that often hold the key to fine tuning a given process. In addition to the spatial dimension, the possibility for modeling time-dependent processes would be possible by molecular dynamics, Monte Carlo, and/or genetic algorithm-based simulations executed for experimentally relevant millisecond time scale. In addition to producing a large tables of 'numbers', the fast compute nodes would also allow for enhancing the documentation of scientific results by generating informative and educational graphics and animations. The latter would have a direct impact on teaching abstract scientific concepts in lower classes as well as outreach to the general public and K-12 schools.

Serve Communities The given focus of the proposed computational facility would be solely the molecular sciences. A decade long expertise exists in how to set up, maintain, operate, and develop such a facility in house. No new FTE line is required, no new software is needed. Thus, with the proposed investment MSU would be able to show the viability of such a facility by building on already successful research programs and educational activities. Building on success stories in molecular sciences, the scope of the facility could be straightforwardly extended to meet a broader need of our students enrolled in our degree programs. For example, instead of a costly set up a new computational facility (Whitman College, Walla Walla, WA), Willamette University in Salem, OR decided to leave their computational servers in the requestor's lab for operation. The free CPU hours are traded with Willamette faculty for accessing some

of the software that they would have not been able to purchase. The cost of future diversification (additional hardware and software and personnel) could then be covered from extramural funding sources. One of the attraction of future growth beyond just the initial 3 year period is being able create an engaging and stimulating learning environment to a variety of students state wide including outreach to serve communities that would not have the financial means and expertise to operate and utilize such a facility. Recent meeting of the American Chemical Society, Montana Section brought up the interest in organizing traveling demonstrations of molecular and structural chemistry, which would nicely couple of the activities of the proposed facility.

Integrate Learning, Discovery, and Engagement In general, the hallmark of computational sciences is by definition that they provide an efficient platform for integration of learning, discovery, and engagement. This is especially true for molecular sciences. Breaking down a complex macroscopic physical, chemical, or biological system by modeling to its microscopic and molecular essential elements and then reassembling into a functional model are powerful methods for learning natural sciences. The possibility of scientific discovery within this process is nearly guaranteed, since even the most detailed scientific study can be revisited and approached from alternative angles to obtain new insights. However, the skills the students acquire are perhaps even more valuable than the specific molecular scientific problem they solve. Students and faculty empowered by the knowledge and skills of what computational molecular science can provide would enable to extend the notion of "engagement" beyond traditional outreach activities of sharing knowledge and create opportunities to serve society in a more direct and efficient manner.

The list of potential courses that could benefit from the existence of the proposed facility would unnecessarily burden the size of this proposal. However, it is notable that the words "computational molecular science" do not even show up on MSU website search; while there are about 272,000 hits if searched on the web from Institutes (Temple University), Centers (Georgia Tech), books, professional organizations, conferences, etc. MSU is missing out on something that is practically resource limited. The nationally and internationally recognized faculty and teaching staff with already some experience with scientific computations are standing by to expand the type and breath of problems that they can tackle given sufficient resources are available. The same is true for graduate students and postdocs, who may become our best messengers to spread the news about the quality of education and research MSU represents and stands for.

Specifically in the science discovery process, the relevant topics are that would directly benefit from the availability of the proposed facility would be the design of alternative energy sources, storage, and utilization; metal toxicity to environmental and human health, carbon sequestration, drug design, cancer research to name a few currently undergoing research activities that already utilize computational facilities with molecular science focus. The proposed facility has definitely the potential to catalyze the formation of user groups and foster synergy in an interdisciplinary environment among involved faculty members, graduate and undergraduate student as well as representatives of the broader community.

Stewardship The close to half million dollar investment over the next three years would be a considerable step toward enhancing MSU's reputation of thriving to provide state-of-the-art facilities for their students and faculty. A series of recent discussions by the envisioning committee of the future for computational sciences at MSU concluded that there is a considerable interest in research and teaching resources for computation-intense applications. This is paralleled with the availability and well-qualified faculty and staff. Currently, numerous small efforts are undergoing at various departments for building up mini computational facilities. These are important for code/algorithm development and pilot projects; however, for using and operating resources wisely the community of computational scientist would greatly benefit from a dedicated facility for production jobs. The requestor has already started to involve Native American high school and tribal college students (MAP, IMSD programs at AIRO) in learning and research activities related to the world of chemistry. One of the elements of these successful activities was that the students were provided with visual demonstrations and hands-on-activities vs. 'dry' text-book-based memorization activities. Last but not least, it is also important to be able to highlight that MSU has the means and skills to set up, maintain, and utilize a flagship resource that is not available within Montana anywhere else or even in the neighboring states.

ADDITIONAL INFORMATION

Implementation Plan *(Please describe with timelines)*

Summer 2012: bidding, purchase, and installation of the first TwinBlade server
Fall 2012: development of course materials and activities, training of researchers and instructors
Winter 2012: development of outreach activities, creation of case studies, How-to-s, manuals
Spring 2013: deployment of course materials, outreach activities, evaluation of progress

Summer 2013: installation of the second TwinBlade server
Fall 2013: training students to update and generate new course materials, opening the resource to state wide users
Winter 2013: training the teachers - courses for community college and high school teachers, student helpers
Spring 2014: aggressive application for extramural funding for sustainable operations and broadening participation

Summer 2014: installation of the third TwinBlade server
Fall 2014: extending educational activities beyond MSU to local high schools, graduate student teachers
Winter 2014: interdisciplinary scientific research conference, formal user group formations, funding opportunities
Spring 2015: continued aggressive application for extramural funding for sustainable operations and new installations

Assessment Plan *(Please describe with indicators)*

The direct return on the investment of MSU into the proposed facility would be assessed by utilization in course work (number of courses and students, student evaluations), independent studies (undergraduate and graduate), research metrics (student, staff, and faculty presentations, acknowledgements in publications), outreach activities (targeted groups, size, exit interviews/evaluations). The direct use can be readily tracked by user access accounting systems that is available in most computational operating system (rockscluster.org). The utilization by course work can be tracked through the Registrar's office. The research-related metrics will be solicited monthly and followed up with automated searches in publication databases, such as Web of Knowledge.

The indirect return would be estimated from increase in external funding (even for grants without a direct computational focus, but capitalizing on the existence of the facility as possible support), visiting professors and scientists, exchange students using the facility, increased success in recruiting graduate students and attracting new faculty who were attracted by the facility. These indirect information could be obtained from the MSU Office of Sponsored Programs, annual activity reports of departments.

In addition, the facility's dedicated website would be organized by a content management system (WordPress for example) to allow instantaneous interaction of the general users and a selected group of administrators/superusers representing various disciplines and research interests.

If assessed objectives are not met in the timeframe outlined, what is the plan to sunset this proposal?

The proposal request funding for computer hardware, materials and supplies, which can be readily distributed and reutilized by ITC or other central MSU organization without much loss in value. However, it is highly unlikely that the objectives will not be met in the above outlined timeframe due to the ongoing activities toward these goals.

The main role of the proposed facility would be to catalyze all these efforts, create synergistic activities and enhance the efficiency of already undergoing educational and research activities.

Computational Facility for Molecular Sciences C&B

SIGNATURES		
Department Head *(please print)*	**Signature** *(required)*	**Date**
Bern Kohler	Bern Kohler	**12-21-2011**
Dept Head Priority *(please circle one):* Very High High Medium (Low) Very Low		
Dean/Director *(please print)*	**Signature** *(required)*	**Date**
Paula Lutz	Paula Lutz	1-3-12
Dean/Director Priority *(please circle one):* Very High High Medium (Low) Very Low		
Executive/VP *(please print)*	**Signatures** *(required)*	**Date**
Executive/VP Priority *(please circle one):* Very High High Medium Low Very Low		