# Research Computing Status Report, April 2009 Executive Summary

# Services Provided by Research Computing

- Administration of High Performance Computing (HPC) resources for USF
- Excess computational power from grant funded systems harvested for the USF research community
- Over 30 scientific software packages licensed, installed and maintained
- Over 100 researchers from over 20 departments
- Over 200 student researchers supported
- Researchers supported responsible for over \$90 million in grants from 2002-2007 and over \$7.8 million in 2008-2009
- Consulting and programming assistance
- Grant support activities
- Gateway to national supercomputing centers
- Support faculty in the delivery of High Performance Computing instruction
- Online and classroom HPC training
- Administration of Unix/Linux platforms for instruction and other student services
- Support services for the College of Marine Sciences

# <u>Budget</u>

- Budget for maintaining current service levels has traditionally come from nonrecurring funds
- Budget needed to maintain current service levels would be \$1,060,445
- Current budget of \$527,139 represents a deficit of \$533,306 and will result in reduction of services and HPC resources
  - Reduction in computational resources for instruction and research
  - o Elimination of some software packages
  - Inability to participate at national level for collaboration and to influence policy
  - No training or conference participation to maintain expertise on cutting edge technologies
  - No improvements in infrastructure needed to expand computational resources
  - Disk systems remain too small for current levels of research and instruction
  - o No funding to move systems from inadequate server room
  - Cluster network infrastructure is at end of life and will become unstable
  - No hardware replacement for systems providing some student services
- Current HPC services and resources at USF are insufficient for a major research university. Service improvements needed include:
  - o Visualization
  - o Staff Scientist and scientific programming
  - o Increased computational resources
  - Budget for new services and resources
    - Non-recurring \$521,000
    - Recurring \$457,000

# Letters of support from faculty members

# Research Computing Status Report April 2009

# Introduction

In spring 2001, a review of the research computing facilities at USF was conducted to determine if these facilities were sufficient for a major research university. It was concluded that the facilities were inadequate. As a result of that review, Research Computing was formed later that year with a mandate to improve the availability of high performance hardware, research software, instructional facilities, and to provide support for these areas.

This report will provide an overview of the status of the Research Computing department. Specifically, the report will detail the services provided by Research Computing, provide a review of the budget situation, outline the reduction of services and resources that are inevitable without increased funding and describe the resources needed for a major research university, resources that are not currently available at USF.

#### <u>Services</u>

# HPC Administration

Research Computing administers the hardware and software for a 264 node computational cluster with 1364 processors and a large memory SMP system for the USF research community. A prototype visualization cluster was built to explore the possibility of providing large scale visualization facilities. These systems are available for all faculty and students involved in research.

Most of the resources of the cluster have been purchased through grant funds by researchers. This service frees the researchers from having to perform administrative tasks. Having these systems maintained by experienced administrators in an existing facility is more efficient and less expensive for the University. Research Computing is currently administering systems for seven research groups and will be adding systems for another researcher this summer. These systems are not used to capacity by the research groups that funded them. This allows Research Computing to share the excess capacity with the rest of the USF research community. Due to substantial demand, The current systems are oversubscribed, resulting in increasing wait time in the queue.

The systems administered by Research Computing are used by over 100 researchers from over 20 departments. The researchers supported by Research Computing were PIs on \$40 million in grants and CoPIs on an additional \$50 million in grants in the period from 2002 to 2007. Although the 2008-2009 year is incomplete, these researchers accounted for \$4.4 million in grants as PIs, and a separate \$3.4 million as CoPIs.

#### Software Administration

Research Computing administers over 30 scientific software packages on the central cluster. These packages are often not commercial quality, and require experienced administrators for installation, maintenance and optimization. In addition, Research Computing licenses and administers commercial software packages necessary for research and advanced instruction. These packages serve an estimated 200 researchers and numerous classes.

#### Consulting and Administration Services

Research Computing offers hardware consulting services for those systems that are included in the central cluster, as well as, for specialty workstations for researchers. These consulting services include hardware specification, design review, and vendor negotiations. Research computing also offers programming and software support services to researchers who need to develop new codes. In addition, the staff of Research Computing also provides services for helping researchers acquire computing resources at the national supercomputing centers when their tasks become too large for local resources.

Research Computing has partnered with several research groups on large (> \$300K) grant proposals. In addition, Research Computing is often listed as a University resource on grant proposals. In the past three years, Research Computing staff and services have been listed as resources on grant proposals that resulted in \$1 million in awards.

## HPC Training

Research Computing also supports instruction by making resources available for faculty teaching High Performance Computing (HPC) oriented courses. This often requires software installation and other system modifications to satisfy the pedagogical needs of the instructor. Many of the software packages licensed by research computing are used for class work.

Beyond for credit classes, Research Computing has developed several on-line courses for HPC instruction. These courses are tutorial in nature and cover both introductory and advanced topics. Research Computing has also developed an HPC "Boot Camp". This week long seminar is intended to give new researchers the tools necessary to begin using the HPC resources.

#### Unix Systems Administration for Student Systems

Research Computing is responsible for maintaining the UNIX systems that provide services to students and those that provide resources for classes. The services provided include student web pages, and student blogs. The class resources provided include programming environments and software that are not available on other operating systems. These systems also provide some specialized support to various faculty members. The staff of Research Computing is currently in the process of centralizing these systems for increased efficiency of administration.

# <u>Budget</u>

#### Historical Perspective

As part of the founding of Research Computing, an initial budget was developed. The salaries of the staff, OPS staff, and some of the software packages were funded through the budget of Academic Computing. Additional funds were proposed to act as an operational budget for the center. The initial budget called for a total budget that averaged \$600,000 for the first six years and a recurring budget of over \$450,000 for years seven and on. The first year's budget (\$332,500) was transferred to the department. After the first year, the budget was cut, and beyond the salaries of the staff and funding for some software package maintenance, there was no recurring funding. There were non-recurring funds made available, and those amounts are listed in Table 1.

Year	Amount
2001-2002	\$ 332,500
2002-2003	\$200,000
2003-2004	\$0
2004-2005	\$200,000
2005-2006	\$200,000
2006-2007	\$500,000
2007-2008	0

#### Table 1. Non-Recurring Funding for Research Computing

Due to the lack of recurring funding, these one-time funds have been used to pay for recurring costs that include salary for a staff scientist (position eliminated due to lack of funding), Internet 2 (2006-2007), hardware replacement, software maintenance, shipping, telecommunications costs, dues and memberships, travel, cluster infrastructure improvements (needed to expand cluster), and training.

#### Budget Requirements Needed To Maintain Current Service and Resource Levels

To maintain the current service and HPC resource levels Research Computing has requested a budget of \$1,060,445. A summary of this budget is given in Table 2. This budget reflects not only the needs of Research Computing, but also the funds needed to support UNIX services for students (web space, blogs, and support for instruction) and support services provide by IT for the College of Marine Sciences.

#### **Table 2 Budget Request**

Description	Budget Request	Current Budget	Difference
Salary and Benefits	\$490,000	\$425,000	\$65,000
OPS	\$36,090	\$36,090	\$0
Expenses	\$146,755	\$56,049	\$90,706
000	\$387,600	\$10,000	\$377,600
Total	\$1,060,445	\$527,139	\$533,306

#### Service Reductions

Based on the budget shortfall outlined above, certain services and resources will be made unavailable. These are outlined in this section.

# Large Memory Resources

Certain research computations will only run on nodes with a large amount of main memory. The cluster relied on three of these large memory SMP nodes to provide this resource for USF. Two of these nodes are already out of service, and the third is beginning to experience memory errors. This system is end-of-life and repairs are not possible. When this system becomes unusable, there will be no central resource for this type of computation.

# Other Computational Resources

Within the last six months, 44 nodes have been removed from service because of problems due to the age of the equipment. The loss of these nodes has reduced researcher and student ability to run jobs and reduces resources available for instruction. There are currently 77 nodes in the cluster that are end-of-life, which will become unusable in the next 12 to 24 months. Without recurring funding, it is estimated that within three years the central cluster will be unavailable for computations. These nodes represent the last of the equipment that is available for general use, which includes use in classes and graduate student research.

# Infrastructure Supporting Research Group Purchases

There are currently no recurring funds to provide central infrastructure for additional HPC hardware, without which researchers will revert to a distributed, less cost effective computing model by installing equipment in their own areas. There is a researcher who wishes to add nodes to the cluster. However, there are not currently sufficient infrastructure resources to add these nodes to the central facility. A decentralized model requires researchers to operate their own HPC resources. This leads to more expensive funding for distributed AC, electricity and personnel.

#### Disk Systems

Over half of the high-speed disk systems used for computations on the cluster are end-of life and will not remain in service more than six months due to hardware failures. This resource within the cluster is already undersized for the amount of computing required by the research faculty at USF. If this resource is not replaced, it will represent a serious bottleneck for research computations. In addition, the local storage (not high speed) for the cluster is undersized for the volume of computations that are supported. This results in wasted time, because researchers must continually transfer files off of the cluster to make room for new computations. Planned upgrades to this system will not be possible without additional funding.

## UPS Systems

The current cluster setup includes systems that use individual UPS battery backup in the Library server room. The current UPS are end-of-life. Possible solutions include, relocating systems to another server room or replacing the UPS systems, but either will require some investment. Unless one of the solutions is implemented, a significant part of the cluster resources may become unstable or unusable.

## Cluster Network Infrastructure

Renewal of the maintenance contract on approximately 30% of the cluster's network infrastructure will not be possible within the current budget. This will leave the cluster vulnerable to a network outage. In addition, another 30% of the network infrastructure equipment is end-of-life, and will start experiencing outages over the next 12 to 24 months if it is not replaced.

#### Software

Several software packages that are used for research and instruction are licensed through Research Computing. These packages were purchased and maintained with one time funds that have been exhausted. It will not be possible, under the current budget, to be renew these packages in the next fiscal year. This will negatively impact the ability to do research and to use the software in classroom settings. Software maintenance is not a static cost. Each year the increase in maintenance costs have been absorbed by the Research Computing budget. Without additional funds, this will result in the loss of more software packages, including ones that are used for instruction.

# UNIX Systems Supporting Classes and Student Services

Most of the UNIX systems used for classes, student research, student web pages, student blogs, and other services provided to students and faculty are end-of-life, or will be within the next 12 to 24 months. These systems are being centralized into a cluster of systems to provide redundancy, greater ease of use and a cost savings in simplified administration. Sustaining these advantages will be possible only if the systems can be replaced as they become unusable. This will not be possible with the current funding levels.

# Training and Collaboration

Without the recurring funding, Research Computing will not be able to remain active in the national groups that provide collaborative opportunities and influence policy decisions. There also will be no funds for training and to attend conferences which provide opportunities to remain at the forefront of the technology needed for high performance computing.

## Services and Resources Unavailable at USF

There are some services and resources that are either undersized or unavailable at USF that are needed to fully support a major research university. The different areas are described below. Budget increases needed to support these improvements are given in Table 3.

Description	Non-Recurring	Recurring
Visualization	\$107,000	\$120,000
Staff Scientist and Scientific Programming Support	\$14,000	\$204,000
Increased Computational Resources	\$400,000	\$133,000
Total	\$521,000	\$457,000

#### Table 3 Budget for Needed Research Computing Improvements

#### Visualization

The amount of data collected by modern sensor grids and produced by large-scale computations surpasses the ability of humans to interpret without the aid of advanced computer visualization. This usually takes the form of a large scale 3D display.

The addition of visualization hardware would be insufficient without the addition of a visualization specialist. Producing large-scale and 3D simulations is not a skill that most researchers have developed. To make the systems usable, a visualization specialist would aid researchers in the production of data visualization. This position would become a resource for the instruction of students.

#### Staff Scientist and Scientific Programming Support

There are many faculty members who could benefit from the use of advanced computing, but do not have the training to use these resources. The addition of a scientific programmer would allow any faculty member to make use of these systems. In addition, this programmer would allow USF faculty to develop custom codes to solve new computational problems. A staff scientist would act as a consultant on grants and in the design and implementation of new projects. In many institutions, these positions have dual appointments with academic departments. This arrangement allows for enhanced interaction between computing centers and the various academic departments.

#### Increased Computational Resources

The resources that are available to the research community of USF are significantly undersized. The majority of the resources that are managed by Research Computing have been purchased through the grant activities of faculty members. These resources are available to the USF community on a time available basis. The result is that many students and new faculty are often waiting for jobs to run.

It is possible that, if there were sufficient resources available to the USF community at large, that new computational faculty could receive grants of time rather than money for new equipment. This could result in savings for the University. Without increases in the resources, this type of cost saving program would not be available.

There are new technologies becoming available in the HPC market. For example, many programs are significantly faster when run on a Graphic Processing Unit (GPU) based system. USF currently does not support any of this type of resource.



February 10, 2009

Research Computing (RC) at USF is a critical resource to my research. Specifically, it has allowed a group of us faculty members to compete for the NSF-MRI program to acquire funding for a large computer cluster (\$500,000 from NSF, plus matching funds from SUN Microsystems to at least the NSF-level). This cluster, in turn, has helped me compete for, and win 2 other NSF grants that are current. Computation on these resources is made extremely easy for me and students by RC. As one interesting example, one of my senior Ph.D. students working on a NSF-funded project is located at Harvard University in Boston. It has been totally transparent for us to do computational work on RC-supported clusters, utilizing the internet, phone and email. I must emphasize that the productivity of this student is equal to that of what it would have been if she were here at USF!

In particular, I would like to mention the enormous help provided by Dan Majchrzak and Brian Smith of RC, who have helped with writing the MRI proposal, have helped with setting up the cluster, and have helped with keeping the clusters working as well as can be done here at USF over the years. I also would like to take this opportunity to thank Tony Llewellyn (the past Director of Academic Computing) for having the vision to support RC much before we have had significant resources. Finally, I get the impression that Mike Pearce has every intention of supporting research computing at a high-performance level. All this support for high performance computing in general is critical for USF to attain research excellence. Computation and theoretical work and infrastructure are necessary and complement experimental efforts and resources, in the pursuit of research excellence. We must continue to invest in them.

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Venkat R. Bhethanabotla Professor



Wayne C. Guida, Ph. D. Department of Chemistry, CHE205 University of South Florida 4202 E. Fowler Avenue Tampa, FL 33620-5250 Email: wquida@cas.usf.edu

Dear Colleagues:

My research, which involves computer-aided drug discovery and design and which is funded through the National Institutes of Health, relies extensively on the CIRCE Computer Cluster. I am a co-PI (along with several other USF colleagues) on a \$500,000 National Science Foundation Major Research Instrument grant awarded to USF, with Dr. Venkat Bhethanabotla in Chemical Engineering as the PI. This grant has contributed significantly to the current capabilities of the CIRCE Cluster. Such a cluster is absolutely essential for my work since my students (both at the graduate and undergraduate level) rely heavily on CIRCE for the large scale protein computer simulations that is absolutely essential to our work.

I very strongly advocate that the university continue to support high-performance computing. A central high performance computing facility is absolutely necessary, in my opinion, for a major research university like USF to retain and attract top caliber research scientists. In my own case, I joined the Department of Chemistry at USF in August, 2007. Since my work is entirely theoretical and computational, a major reason that I was attracted to join USF was the very presence of a significant computational cluster. I would have had to have asked for significantly higher start-up funds to establish my lab at USF had a high performance computational cluster not existed. I, in fact, had no interest in acquiring and maintaining my own computational cluster since my student's time is much more effectively spent performing computer simulations as opposed to maintaining hardware and the massive software packages we require that are designed to run on machines with tens to hundreds of processors. Even in economically challenging times, I believe it is essential for USF to continue to invest in centralized high performance computing.

Finally, I would like thank Dan Majchrzak and Brian Smith of Research Computing at USF, who have been extremely helpful in getting my research operation up and running in short order, and to Mike Pearce for his support of high performance computing.

Sincerely. Wayne C. Guida

# USF UNIVERSITY OF SOUTH FLORIDA

Department of Computer Science and Engineering 4202 E. Fowler Ave, ENB 118 University of South Florida Tampa, Fl. 33620

February 9, 2009

Colleagues University of South Florida

Dear Colleagues:

The Computer Science and Engineering Department strongly supports the maintenance of a highperformance computing facility (CIRCE) at the University of South Florida. We have several faculty who currently do research work that requires high-performance computing. This includes grid computing research done by Dr. Iamnitchi, who is also teaching a course on parallel and distributed computing which uses multiple processors. Professor Ken Christensen uses it for running large-scale simulation models of computer networks. Our computer vision group does biometric recognition research which requires significant computing resources. In particular, they want to recognize people in streaming video and track them. This is very computationally expensive.

There is a recent set of articles in IEEE computer Society publications on cloud computing, which is the utilization of many computers to obtain high performance. High-performance computing is becoming more necessary for mainstream research. This can be seen in our effort to recruit a bioinformatics faculty member. They have asked for access to a high-performance cluster computing facility to enable the complicated genomic analysis their research entails. Also, from my own work in bioinformatics we find that doing gene selection from microarrays can take many days even when run on a high-performance computer cluster (we use one in Hawaii). We have also used the DOE ASC supercomputers to do high-performance simulation analysis through learning.

So, to summarize much of the ongoing and future research and Computer Science and Engineering will be facilitated by high-performance computing facilities. In particular, much of the funding available will depend on the ability to utilize high-performance computing. Hence, it is critical for the universe is South Florida to maintain a high-performance computing facility to facilitate faculty research and the ability to receive external funding in many areas. Thank you for your

consideration.

Sincerely,

Lawrence O. Hall Professor and Chair



February 2, 2009

Dear Colleagues,

I am writing to express my strong support for maintaining and enriching the Research Computing resources and activities at USF.

I am using CIRCE's capabilities in teaching a course this semester in the Department of Computer Science and Engineering. The course, entitled "Basics of Parallel and Distributed Processing" (http://www.csee.usf.edu/~anda/PDS) is addressed to both graduates and undergraduate students interested in high performance computing and distributed systems. On the theoretical realm, the course presents the basic principles that are at the foundation of parallel programming and distributed systems. On the practical realm, the course applies the theoretical foundations in developing programming projects in different parallel and distributed environments. This course component is accompanied by hands-on mini-projects that introduce students to the practice of parallel programming with POSIX threads, Java threads, MPI, and Google's MapReduce.

We are using CIRCE this semester for experimenting with Google's MapReduce framework for large-scale data processing. As you are probably aware, the big computational challenge of our time is managing and processing the tremendous amount of data produced by research groups and their sophisticated instruments (such as the CERN's Large Hadron Collider), by digitizing vast libraries, and by the data produced everyday by web users through blogging and media sharing. Google's MapReduce framework has been used successfully by Google for processing web documents and has been made available through an implementation called Hadoop. It is now in use by multiple academic and corporate efforts clustered under the name of "cloud computing".

This new data processing paradigm promoted by MapReduce/Hadoop is likely to revolutionize the practice of parallel programming for a particular but important class of applications. The framework runs on a large cluster of independent computers part of CIRCE. Similar or appropriate resources are not available for teaching in the Department of Computer Science and Engineering. Through its large cluster and extremely supportive technical staff, CIRCE proved an invaluable resource for teaching cutting edge technologies.

Sincerely,

Adriana Iamnitchi Assistant Professor anda@cse.usf.edu

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February 2, 2009

То

Dr. David Rabson Professor Physics, USF, Tampa

Subject: CIRCE

Dear Dr. Rabson,

I am writing to express my unequivocal support for CIRCE and the important service that it is providing for the research community.

This Center is providing is in direct support of the University's Strategic Plan and Goals. In particular it is aligned with Goal 1: **Expanding world-class interdisciplinary research**, creative, and scholarly endeavors. In particular,

- Promote nationally and internationally distinctive and prominent research and graduate programs, and
- Strengthen and support integrated and synergistic interdisciplinary research across disciplinary, departmental, college and campus boundaries.

As such the Center plays a crucial role in supporting the research computing needs of faculty from a variety of disciplines and will probably form the core research infrastructure support for a Cluster of faculty and scholars involved in Computationally oriented research to be located in the IDRB building according to current plans.

In addition to providing support for research, CIRCE is also providing the capability for faculty to use state of the art software in their offerings of graduate and upper level courses.

I have been involved in a number of federally and state funded projects that have utilized the high performance computing. I can say without a doubt that this would not be possible without the continued support of CIRCE.

Yours sincerely,

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Babu Joseph Professor and Chairman



February 5, 2009

Dr. David Rabson Professor Department of Physics, University of South Florida, Tampa, FL 33620.

Dear Professor Rahson:

After a ton-year biatus, I am cautiously venturing back into modeling that requires large computational times. Two of my students are running finite element models to solve diverse problems such as simulation of

micromechanical experimental testing of composite materials, and

assembly procedure of fulcrums of bascule bridges.

These computer programs take up to 18 hours to run on a PC, but now take only a couple of hours of running time on the cluster. The problem would have been time-prohibitive to solve because we need to make hundreds of runs to complete these studies based on the concepts of design of experiments.

I have been at USF for 22 years and I started as a heavy computer user to conduct my research. Between 1991-99, for research funded by Air Force Office of Scientific Research, I would use the spare time on the USF IBM machine and also remotely use the FSU supercomputing facility. But this was not enough, as these computational facilities were much less competitive than my peers in other universities.

Unwillingly, in 1998, I had to make a decision - look for other research opportunities that did not involve large-scale computing.

With the formation of the cluster in the last few years, and getting encouraged by finding more of my colleagues conducting heavy computational research, I have ventured back into large-scale computing. I do not want to regret having made this decision if every year or so the Damoeles' sword is over the research computing group and its infrastructure (although Damoeles was treated with high indulgence before the end of his meal).

A university desiring to be invited to join AAU needs to shows consistency in the support of critical infrastructure such as the research computing facilities. The fear of

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whether the facilities will be here or not in the future does not bode well for the university that continues to make new strides in education. training and development of new knowledge.

Let's not lose our edge in spite of the current tough economie times.

Sincerely.

Autar K. Kaw Professor, Mechanical Engineering Department. Fellow, American Society of Mechanical Engineers University of South Florida 4202 E Fowler Ave ENB(18, Tampa FL 33620-5350).

Numerical methods for STEM undergraduates: http://mmericalmethods.eng.usf.edu/ A Blog for Numerical Methods: http://autarkaw.wo<u>glpress.com</u> Videos for Numerical Methods: http://w<u>ww.youtube.com/mmericalmethodsguy</u> Office: (813) 974-5626 | Fax: (813) 974-3539 |K-mail: <u>kaw@eng.ust.edu</u> February 5, 2006



Department of Mathematics, 4202 E. Fowler Ave., PHY114 Tampa, FL 33620

Dear Colleagues:

I am a member of a research team that will be using large-scale computing in the near future.

Our project is to design novel crystalline materials with new and useful properties. During the last two years, USF chemists have synthesized two crystals with (graphical) topologies new to science. Such innovations are currently quite rare, so USF chemists are at the forefront of synthesizing novel crystals. But our greatest goal is to develop the tools that will make such innovations routine, and that will require a systematic method for generating designs of novel crystals to synthesize.

We have under development a demonstration version of a computer program that enumerates designs of highly symmetric graphical topologies of crystals, and underlying the underlying theory strongly suggests that it can be generalized to a program that enumerates graphical designs of *all* possible such designs – provided that the computational power is available. The current little demonstration program can severely overtax a desktop computer, so the more ambitious programs will require more powerful machines.

Our projected need is not unique, for there is a growing trend in material science for heavy duty computations in analysis and design. External funding agencies are aware of this need, and will review the resources of grant applicants when evaluating proposals; proposals from institutions with perceptibly inadequate computational facilities will be at a competitive disadvantage.

Therefore, I strongly recommend that the university increase its support of the research computing facilities at the University of South Florida.

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Gregory McColm Associate Professor of Mathematics mccolm@cas.usf.edu

February 12, 2009

Dear Colleagues,

I am writing this to request an increase in support for high-performance computing (HPC) in USF. In justification of my request I would like to list the following reasons why HPC is essential for USF leadership in research and education:

- 1. Many faculty members (such as myself) working in the area of computational physics, chemistry, biology, computer science and others entirely depend on the on-campus HPC resources in their research. The continued support and increase of HPC resources at USF is crucial to successfully compete for the leading positions in the important area of computational sciences.
- 2. Computational research is a well-funded area. All the major research agencies currently have programs in computational sciences and award millions of dollars every year to support such research. Increase in the HPC resources will result in greatly increasing the amount of external funds brought to the USF.
- 3. Students heavily use on-campus HPC resources for both their education and research. For example, the course on Computational Physics offered in the Physics Department is possible only due to the existence of such resources. This course is very popular with students and essential for their careers. Education in the area of HPC is a must component of student's curriculum in the computer-dominated era. The skills in HPC will contribute to the competitiveness of USF graduates on the job market.
- 4. Shared HPC resources is the best way to efficiently use and manage such resources. All leading research universities in the US have such shared facility and are working hard to increase such resources to support high-demand computational research as well as to attract students.

I would also like to mention that I am a new faculty member in the Physics Department working in the frontier area of computational nanoscience. My decision to join USF was based on both the excellence of USF in research and the existence of HPC resources. In the early stages of my career, it is crucial to have such resources available to generate high-quality publications, attract external funds and to educate students.

Sincerely,

Inna Ponomareva, Ph.D. Assistant Professor



28 January 2009

Dear Colleagues:

As you know, Research-Computing at USF has, over the last seven years, grown from nothing to a group managing over one thousand computer processors and providing software licensing and support for heavily-used packages such as Matlab and Maple. My own research effort, which has brought in several external grants, depends on the CIRCE computing cluster, and I know that many of my colleagues are in the same position.

I am PI on a current \$500,000 grant from the National Science Foundation to support undergraduate students in the area of computational science. The grant is tied explicitly to CIRCE, with students learning techniques of parallel computing applied to their majors, and two of the staff of Research Computing were co-investigators on this grant. Many of the scholarship students have also used CIRCE in their undergraduate research. In addition, I am a co-PI on a \$499,999 equipment grant, led by Venkat Bhethanabotla in Chemical Engineering, that has doubled CIRCE's capabilities. Three of my proposals pending with the NSF rely on CIRCE.

By supporting high-performance computing, the university also saves money on startup costs for new faculty, who can use the central facility instead of having to buy their own, find space for it, and arrange for necessary electrical and air-conditioning upgrades. In addition, these faculty and their students are freed from the substantial time drain of having to maintain their own hardware. At universities without such central support, scores of faculty members end up duplicating efforts in acquiring, installing, documenting, and managing large software packages, often at the cost of graduate-student careers. Because of this, my department has used the existence of the Research-Computing group as a recruiting tool when hiring new faculty.

I and my colleagues in computational science recognize the difficult financial position of the university. It is precisely because Research Computing has a track record of high return on investment and the potential to generate new revenue in terms of external funding that the university should increase its support.

David A. Rabson, Ph.D. Associate Professor of Physics davidra@ewald.cas.usf.edu



Civil and Environmental Engineering University of South Florida 4202 East Fowler Avenue, ENB 118 Tampa, Florida 33620-5350 (813) 974-2275

February 13, 2009

Dear Colleagues,

I have been a user of the CIRCE cluster for the three years I have been at USF. As a code developer, rather than code user, my projects do not typically require the same level of CPU time or other computer resources as the larger users of the CIRCE cluster. However, the access to a large cluster is crucial for my work as I must develop codes to work on such large systems so that users of my codes can make effective use of modern computational capabilities. My work is currently funded by the Boeing Company, and CIRCE has played a major role in my ability to fulfill the research objectives of this research. The CIRCE cluster and usage model fulfills my needs perfectly. When I accepted a position at USF, I negotiated a startup package that included my own small cluster for my work. With the current CIRCE computing model in place, such startup costs can, and should, be eliminated, ultimately saving the University a significant amount of money.

The research benefits of the CIRCE go beyond the accountants argument on cost savings and grant money received. CIRCE is a focal point for computational engineering and science researchers from across campus. As the interested parties across campus have met, sometimes for the very first time, to discuss and plan for the future of CIRCE, a variety of research interests and efforts have been poured into a mixing bowl of academic discourse. The outcome of this mixture has already led to the First Symposium on High Performance Computing at USF, held this past January, that attracted a world-class scholar as a speaker. In our quest for AAU eligibility and emphasis on multi-disciplinary research, such venues are essential. This mixture has already sprouted a collaboration with a colleague from across campus and myself, a collaboration that would never have occurred otherwise.

Dan Simkins Assistant Professor Civil and Environmental Engineering



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6<sup>th</sup> February 2009

Dear Colleagues:

Research Computing at USF is and has been an essential resource in supporting ongoing research activities and in fostering new opportunities. The value of the resource far out performs its cost and the department of chemistry fully supports it. The facility generates funds through grant proposals and attracts talented faculty at a reduced rate – clearly a bargain. They are efficient, professional and cost effective; they deserve continued support.

Professor and Associate Chair Brian Space



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# Amy L. Stuart, Ph.D.

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February 13, 2009

To whom it may concern,

I am writing this letter to request you continued support of the research computing cluster and staff at USF. My group's research involves the study of interactions of multi-scale process related to air pollution and its human health effects. My main tool of research is numerical modeling, for which access to a supercomputing cluster and staff knowledgeable in it's technical administration is essential. For that reason, the USF Research computing center has been very instrumental to me, even before I accepted a position at USF. Indeed, the existence of a supercomputing center to house and administer the \$40K supercomputer that I would be purchasing with my start up funds was a very important component of my acceptance of USF's faculty offer in fall 2004.

Since arriving at USF in January 2005, I have been building a research group that heavily uses the Research computing cluster CIRCE (within which my original cluster is now integrated) and its expert staff. Successes include 7 published or in-press manuscripts in respected peer-reviewed journals (in addition to numerous abstracts and presentations national, and local conferences), all which relied on Research Computing. In the past four years, the center has been necessary to our projects supported by a USF New Researcher Grant (\$8K), a multi-investigator USF Sustainable Healthy Communities Grant (\$392K), and a Florida Department of Environmental Protection contract (\$116K). Recently, I was also awarded a National Science Foundation five-year CAREER grant (\$400K) for which the supercomputing center was an essential element to the success of the proposal and will be required for the success of the research. I'm also the PI and co-PI, respectively, on two pending contracts from the Florida Department of Transportation (for \$100K each) that will also rely upon the Research Computing center.

Regarding research training, my core research group currently includes 7 graduate students pursuing thesis or dissertations and 1 undergraduate honor's student. The group is multidisciplinary, with students pursuing degrees in both Public Health and Engineering. Additionally, I am involved in mentoring other students from Geography, Anthropology, and Engineering through interdisciplinary grants and committees. Group graduates include 2 MPH students, 1 ME student, 1 undergraduate honor's student, a few GAs, and two visiting scholars pursuing MS degrees from a collaborating university in Thailand.

In closing, I want to reiterate that the Research computing center at USF is essential to the research work that I do. I hope that you will continue to support it and the funding of qualified staff.

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Dear Colleagues,

Research Computing at USF has grown tremendously over the past several years. Many researchers, such as faculty, students, and postdocs, have experienced its benefits.

My own research strongly depends on the existing of state of the art local computing facilities and qualified personnel to support the relevant hardware and software. I had a Petroleum Research Fund grant and a current Department of Energy grant which heavily rely on the CIRCE computer cluster. Currently, I have three pending grants which also rely on the USF parallel computers.

I would like to express in the strongest possible terms that Research Computing at USF is a necessity for us to perform cutting edge research as well as to have leverage when applying for external grants. Having computing facilities at USF also saves faculty and students time from maintaining their own hardware. Having personnel maintaining the computer cluster saves faculty and students time from installing and supporting complicated research software. Usually such tasks are given to graduate students who devote large amounts of time instead of focusing on research problems. At the same time, the USF parallel computer cluster serves as a tool for students and postdocs to learn how to use such facilities. Such knowledge is necessary for their further carriers at other universities or research establishments.

Therefore, I hope the university leadership will recognize how important it is for a research university to have a state of the art computing facilities and it will increase its financial support for the CIRCE cluster. Having such facilities saves money from start-up funds for new faculty, saves time from maintaining smaller clusters, and provides tremendous opportunities for research efforts.

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