

## HPC Annual Report 2009-2010

November 1, 2010

### Accomplishments and Activities

To carry out our mission of providing HPC-based services to UF research faculty, the HPC Center undertook the following activities during 2009-2010:

1. **Website:** The HPC Center web site was completely redesigned to make information more easily available and more clear and compact and it went live on June 15, 2010;
2. **Service Offerings:** A new, richer slate of offerings of services is now available so that more faculty members may find that the HPC Center meets their HPC needs.
3. **Reliability/Availability:**
  - a. **Login Server:** Redundant login servers (head nodes) were implemented as a load-balanced server farm to ensure that the failure of a single server does not result in (apparent) down time for our users.
  - b. **Home Storage Areas:** User home directories are now deployed as NFS mounted file systems on top of hardware-based, RAID-6, storage volumes. Additionally, a redundant, standby server is updated nightly with a backup copy of users' home directories.
  - c. **Scratch Storage Areas:** The HPC Center staff has designed and is currently building a more affordable, highly available storage platform for use within the HPC Center. This platform is based on commodity hardware and open-source software.
4. **Industry Partnership:** The HPC Center staff, under an NDA, has been working with, and providing expertise to, a major storage industry partner as they develop their next generation storage platform. The HPC Center will be provided with evaluation units as the development progresses.
5. **Ease of Use:** A web-based interface to the Gaussian computational chemistry application was developed and deployed allowing users to run Gaussian with no exposure to the Linux command line. Additional interfaces for bioinformatics applications are in development.

These activities are in addition to our daily work of maintaining the facilities and providing support to our users.

### Budget Overview

Faculty investments for the next equipment purchase generated \$148,000 for the year. These funds are being used to enhance storage and add additional, faster cores. We invite any researcher who has a need for HPC services to contact the HPC Center for further information. We welcome broad participation in this vital faculty-led initiative.

The HPC Center operates on a very small annual budget for operations, but it manages a significant amount of assets and funds. A brief overview is presented in the table below.

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In the first part of the table, each row represents the entity that contributed funds towards the HPC Center operation. Faculty members contribute funds to buy equipment, individually or in small groups. Departments and Colleges and the Office of IT contribute funds for staff and facilities.

<b>Description</b>	<b>2004-2005</b>	<b>2005-2006</b>	<b>2006-2007</b>	<b>2007-2008</b>	<b>2008-2009</b>	<b>2009-2010</b>
Faculty	\$1,092,000	\$0	\$620,000	\$480,000	\$113,000	\$306,000
Dept/Inst	\$213,000	\$25,000	\$67,000	\$389,000	\$25,000	\$37,000
College	\$463,000	\$130,000	\$182,000	\$238,000	\$169,000	\$168,000
OIT	\$301,000	\$110,000	\$336,000	\$607,000	\$137,000	\$137,000
<b>TOTAL IN</b>	<b>\$2,069,000</b>	<b>\$265,000</b>	<b>\$1,205,000</b>	<b>\$1,714,000</b>	<b>\$444,000</b>	<b>\$623,000</b>
Staff	\$171,000	\$244,000	\$263,000	\$300,000	\$306,000	\$306,000
Facilities	\$0	\$0	\$158,000	\$340,000	\$0	\$0
Equipment	\$1,667,000	\$0	\$760,000	\$872,000	\$0	\$326,000
Operation	\$10,000	\$10,000	\$61,000	\$45,000	\$46,000	\$48,000
<b>TOTAL OUT</b>	<b>\$1,848,000</b>	<b>\$254,000</b>	<b>\$1,242,000</b>	<b>\$1,557,000</b>	<b>\$352,000</b>	<b>\$680,000</b>

### List of investors

Some investors are investing as head of a college or department, some as individual faculty, and some as both.

Archer D. L., Associate Dean, IFAS  
Avery P., Professor, Physics  
Balachandar S., Chair, Mechanical and Aerospace Engineering  
Beck H. W., Professor, Agricultural and Biological Engineering  
Casella G., Professor, Statistics/IFAS  
Cheng H.-P., Professor, Physics QTP  
Curtis J., Chair, Chemical Engineering  
D'Anieri P., Dean, College of Liberal Arts and Sciences  
Deumens E., Director, Chemistry QTP  
Emond J.P., Professor, Agricultural and Biological Engineering  
Eyler J., Professor, Chemistry  
Frazier C., Interim CIO, Office of Information Technology  
Gao B., Professor, Agricultural and Biological Engineering  
Graham W., Professor, Agricultural and Biological Engineering  
Guo J, Professor, Electrical and Computer Engineering  
Ford E., Professor, Astronomy  
Fortes J., Professor, Electrical and Computer Engineering  
Haman D.Z., Chair, Agricultural and Biological Engineering  
Haselbacher A., Professor, Mechanical and Aerospace Engineering  
Hoit M., Interim CIO, Office of Information Technology  
Humphrey S., Professor, Natural Resources and Environment  
Jones J., Professor, Agricultural and Biological Engineering  
Khargonekar P., Dean, College of Engineering  
Kiker G. A., Professor, Agricultural and Biological Engineering  
Law M., Chair, Electrical and Computer Engineering  
Martinez C., Professor, Agricultural and Biological Engineering

McLellan M., Dean of Research, IFAS  
Meng, Professor, Materials Science and Engineering  
Merz K, Professor, Chemistry QTP  
Munoz-Carpena R., Professor, Agricultural and Biological Engineering  
Philpott S., Professor, Materials Science and Engineering  
Roitberg A., Professor, Chemistry  
Shea J., Professor, Electrical and Computer Engineering  
Sinnott S., Professor, Materials Science and Engineering  
Soltis P, Professor, Florida Museum of Natural History  
Tao L., Professor, Electrical and Computer Engineering

An additional group of investors consists of the principal investigators of the NSF-MRI 2004 grant that created the Campus Research Network and provided the InfiniBand switch network for the Phase II cluster with a matching grant from Cisco, Inc.

Ranka S., Professor, Computer Science and Engineering  
George A. D., Professor, Electrical and Computer Engineering  
Avery P., Professor, Physics  
Trickey S. B., Professor, Physics  
Sheng P., Professor, Coastal Engineering

### **HPC Center Staffing**

The HPC Center reports to the office of the CIO, similar to CNS and AT, and has three full-time staff members:

1. Charles Taylor, IT senior, and associate director of the HPC Center,
2. Craig Prescott, IT senior,
3. Jon Akers, IT engineer

The part time position of program director is currently held by Dr. Erik Deumens, scientist in the Department of Chemistry and in the Department of Physics. In addition, the center has had several students working part-time.

### **Usage Statistics**

The HPC Center website provides a wide range of information, including live data about system utilization: <http://www.hpc.ufl.edu/sysinfo>.

The table with the total hours used during fiscal year 2009-2010 organized by college, department, and research group identified by the sponsoring faculty member is shown below. Sums per department, and per college are listed, as well as the percentage of the total used by each college. The UF HPC Center provided over 21 million CPU hours to its users. This represents a **53%** increase over the number of hours provided in the 2008-2009 academic year.

<b>College</b>	<b>Department</b>	<b>Investigator</b>	<b>Jobs</b>	<b>Hours</b>	<b>(%)</b>
<b>CLAS</b>	Physics	Alan Dorsey	91	45	
		Christopher Stanton	287	1,226	
		David Tanner	10	3,165	
		Ho-Bun Chan	20	196	
		Hai-Ping Cheng	20,193	2,759,540	
		James Fry	68	4	
		David Micha	641	25,927	
		John Sabin	17,185	283,293	
		Kevin Ingersent	5,661	50,306	
		Paul Avery	2,166,515	5,534,915	
		Sam Trickey	152	62	
		Peter Hirschfeld	6,845	113,938	
		Pierre Sikivie	101	386	
		Robert Buchler	1,278	30,526	
		<b>Total</b>	<b>2,219,047</b>	<b>8,803,529</b>	<b>40.60%</b>
	Zoology	Ben Bolker	8,288	35,422	
		Charles Baer	36	474	
		Michael Miyamoto	513	4,272	
		<b>Total</b>	<b>8,837</b>	<b>40,168</b>	<b>0.19%</b>
	Chemistry	George Christou	292	13,671	
		John Eyler	204	5,589	
		John Reynolds	4	0	
		Martin Vala	171	6,019	
		Mike Scott	401	60,154	
		Nick Polfer	32,572	106,980	
		Erik Deumens	47,069	1,000,566	
		Ken Merz	66,581	2,429,270	
		Rodney Bartlett	9,572	67,957	
		Nicole Horenstein	165	1,335	
		Richard Yost	6	65	
		So Hirata	6,667	29,479	
		Adrian Roitberg	31,786	862,965	
Nigel Richards	1,258	192,698			

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	Ronald Castellano	22	52	
	William Dolbier	261	22,964	
	<b>Total</b>	<b>197,031</b>	<b>4,799,767</b>	<b>22.14%</b>
Astronomy	Eric Ford	513,926	872,455	
	Jonathan Tan	153	3,658	
	<b>Total</b>	<b>514,079</b>	<b>876,113</b>	<b>4.04%</b>
Anthropology	Connie Mulligan	513	24,077	0.11%
FLMNH	Matt Gizendanner	17	1,098	0.01%
Math	John Klauder	4,766	101,602	0.47%
	Christopher			
Biology	Baraloto	12	133	0.00%
Statistics	George Casella	291	1,489	0.01%
<b>COE</b>	Arnoldo Valle-Levinson	1,567	55,348	
Coastal	Peter Sheng	355	5,135	
	<b>Total</b>	<b>1,922</b>	<b>60,483</b>	<b>0.28%</b>
ISE	Jean-Philippe Richard	279	4,454	
	Timothy Middelkoop	359	3,150	
	Yongpei Guan	3	0	
	<b>Total</b>	<b>641</b>	<b>7,604</b>	<b>0.04%</b>
CISE	Anand Rangarajan	184	3,921	
	Arunava Banerjee	1,672	7,327	
	Jih-Kwon Peir	25	0	
	Paul Gader	1	0	
	Sanjay Ranka	36	3	
	Tamer Kaveci	413	45,331	
	<b>Total</b>	<b>2,331</b>	<b>56,583</b>	<b>0.26%</b>
ECE	Jing Guo	6,996	126,518	
	John Shea	46,742	613,716	
	Jose Fortes	17,660	146,759	
	Tao Li	541,172	135,538	
	Toshikazu Nishida	1,181	532	
	<b>Total</b>	<b>613,751</b>	<b>1,023,063</b>	<b>4.72%</b>
MAE	Bhavani Sankar	146	269	
	Carl Crane	1,511	11,746	

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		Curtis Taylor	2	1	
		Ghatu Subhash	5	0	
		James Klausner	4	1	
		Prabir Barooah	23,040	20,084	
		S. Balachandar	11,926	1,995,918	
		Subrata Roy	3,271	100,380	
		Youping Chen	21,213	1,292,756	
		<b>Total</b>	<b>61,118</b>	<b>3,421,155</b>	<b>15.78%</b>
	<b>MSE</b>	Brij Moudgil	537	93,464	
		John Mecholsky	965	2,409	
		Shirley Meng	4,199	232,115	
		Simon Phillpot	17,409	872,128	
		Susan Sinnott	3,460	243,089	
		<b>Total</b>	<b>26,570</b>	<b>1,443,205</b>	<b>6.66%</b>
	<b>CHME</b>	Aravind Asthagiri	1,838	248,771	
		Jennifer Curtis	1,276	140,880	
		Tim Anderson	187	187	
		<b>Total</b>	<b>3,301</b>	<b>389,838</b>	<b>1.80%</b>
	<b>BME</b>	Huabei Jiang	3,406	132,042	
		Mingzhou Ding	49	1,596	
		<b>Total</b>	<b>3,455</b>	<b>133,638</b>	<b>0.62%</b>
	<b>EES</b>	Ben Koopman	20	44	0.00%
	<b>SNRE</b>	Stephen Humphrey	1,021	1,512	0.01%
<b>IFAS</b>	<b>IFAS</b>	Byung-Ho Kang	17	0	
		Daniel Hahn	60	396	
		Donald McCarty	2,582	4,926	
		James Jones	124	2,511	
		Jasmeet Judge	810,676	201,821	
		Rafael Munoz-Carpena	13,907	116,036	
		Sabine Grunwald	23	2	
		Wendy Graham	382	30,843	
		<b>Total</b>	<b>827,771</b>	<b>356,536</b>	<b>1.64%</b>
<b>COM</b>	<b>ICBR</b>	William Farmerie	100,882	112,193	0.52%
	<b>ICHP</b>	June Nogle	754	4,021	0.02%
	<b>Pathology</b>	David Ostrov	95	9,383	0.04%

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MDPHD	Stephen Hsu	1,609	3,230	0.01%
PHHP	Ning Li	6	307	0.00%
MGM	Lei Zhou	21	7,909	0.04%
EHPR	Yueh-Yun Chi	157	2,866	0.01%
Pharmacology	Stephen Baker	18	774	0.00%
EPI	David Smith	103	157	0.00%
	<b>Total</b>	<b>103,645</b>	<b>140,842</b>	

<b>Grand Total</b>		<b>4,590,139</b>	<b>21,682,478</b>	<b>99.35%</b>
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