# FY05 Innovations in Teaching with Technology Awards: A Computer Lab That Is Also a Super-computing Cluster for Students

## FY05 Innovations in Teaching with Technology Awards

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<th>Proposal Title:</th>
<th>A Computer Lab That Is Also a Super-computing Cluster for Students</th>
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| Investigators: | Claudio Margulis  
|                | Jeffrey Miller |
| Org Unit:      | College of Liberal Arts & Sciences |
| Department(s): | Chemistry |
| Funding Awarded: | $29,500 |

### What do you intend to do?

We intend to develop a functional cluster out of a lab of computer to harness off-use idle cycle time by using a novel approach. Specifically, the intent is to use VMware to provide Microsoft applications for chemistry students over a Linux base Operating System. At the same time we wish to develop a computational cluster in order to expose our undergraduate students to software that is not currently available for student use at the University of Iowa.

Currently the Undergraduate Computing facility located in CB235 is running only the Windows Operating System on 10 PC computers. Specialized software allows our students to visualize and manipulate complicated molecular species, perform sophisticated theoretical calculations, create scientifically sound papers, and process and plot data from laboratory experiments. However, much of the computation and modeling software currently being developed for chemistry are being streamlined for clusters of Linux computers. We are intending to create a Linux cluster from an existing lab of machines by shifting the Microsoft Windows to a virtual system running inside of VMware on top of the Linux system.

Testing of this concept thus far has shown that the current lab applications perform acceptably within a VMware virtual machine. The next logical step of the process is to scale this up to a lab of ten systems. We can then determine the impact of this type of a setup in a lab environment subjected to the use and abuse of the student users. We believe that with the read only image inside of the VMware Virtual Machines the performance of the lab will be enhanced since any changes that a student might do on the windows side will be wiped out upon logout. In addition, in today’s virus and spyware ridden world, if a student does happen to infect a system, as soon as it is
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| turned off those changes are lost as well. Access for students storage in the local machines is not needed since information is currently stored on zip disks, CDRoms, or in the Chemistry Department file server that is dedicated for this purpose.  

Currently in the department, we have a Linux cluster of 22 Pentium original systems purchased in 1996 to provide access to computational chemistry programs to undergraduate students. Due to the severe limitations of the hardware, we are only able to run a couple of programs on this cluster, mainly GAMESS. By creating a “Lab Cluster”, we can run other programs that are needed for instruction without impacting this current cluster. Possible programs to be used on the Lab Cluster are Gromacs, VMD, Tinker, Amber, QChem, NWChem, and NAMD. The addition of these programs will allow students to get hands on experience with top of the line software that is being used not only for teaching purposes but also in active research.  

If this approach succeeds, it would be possible to scale this up to other labs increasing the amount of computational power available. |
| What resources will you need? |
| We will need to purchase the following items:  
  - A dedicated head node to manage the system  
  - Hardware upgrades for the 10 systems for creating the cluster such as an extra NIC card, extra memory, Ethernet cabling, and GigaBit Switch.  
  - 10 copies of VMware  
  - Compilers for creation, customization, and acceleration of software package for the systems in the cluster  
  - Licenses for QChem and Amber. |
| Rough estimate of costs |
| Currently the Department is seeking the replacement of computers in CB235 through student computer fees. If they are replaced with the requested dual processor systems, we can create a 22 processor cluster that will be able to function both as windows workstations and compute nodes with following cost:  
  - Head Node: $5700.00  
  - Computer Upgrades: $15,595.00  
  - VMware: $1129.90  
  - Compilers: $6348.90  
  - QChem: $1500.00  
  - Amber: $400.00  

...for a total of: $30,674.70. If the requested systems are not purchased or different systems are purchased, the cost of the upgrades would most likely go down but the other components will remain similar. |