Case Study

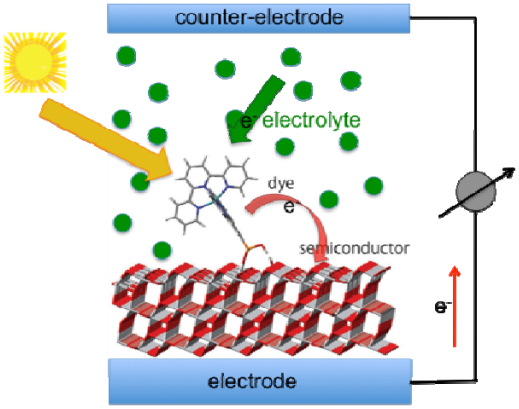
"Murgas" 240 Core HPC Cluster from Ace

"The system we purchased from Ace Computers is an ideal setup for quantum chemistry calculations using a variety of commercial as well as custom-made codes. Some of the codes we use can only run as shared-memory parallel programs, while others ran across the nodes. Our calculations are often memory-bound and some create large temporary files on the compute nodes, making a lot of memory and a large disk a necessity. Having a rack cluster with several nodes, high density of cores per node, 2GB RAM/core and at least 1TB disk on each compute node, gives us the flexibility we need in our research."

Elena Jakubikova
Assistant Professor
Computational Chemistry

Ace provides North Carolina State with a Linux Cluster for Quantum Chemistry.

Customer Challenge



The overall theme of our research at N. C. State is to use the tools of computational chemistry to uncover structure-function-property relationships in molecules and materials and to use this understanding for the rational design of new materials and molecular systems with desired properties. Our current focus revolves around the photovoltaic solar cells, dye-sensitized solar cells more specifically. We aim to obtain a deeper understanding of how structural features of various chromophores used in the dye-sensitized solar cells influence their light-harvesting capabilities and develop strategies for their improvement.

Solution Overview

When researching the system, Dr. Jakubikova requested quotes from several companies, but found communication was somewhat difficult, as other companies were often not responsive to her needs. After weeks of frustration, a colleague at North Carolina State (an existing customer of Ace high performance workstations) recommended she contact Marc Fertik (Ace Director Eastern Region) to obtain a quotation. Ace recommended a 6U Linux Cluster based on Quad CPU Nodes, built around the AMD Opteron 6164HE (12 Core CPU's), consisting of a 2U Head Node, and four (4) 1U Compute Nodes. "The quoted system was up to my specifications and included exactly what I wanted within only a few days." Dr. Jakubikova was very impressed with how Ace handled the process, "making it very easy for me and I felt like they actually cared about providing the best solution for my needs."

What issues were key to making this project successful?

- Tight budget and quick delivery were very important, as research was ongoing, and the new cluster was a vital asset.
- Future expandability with the easy addition of additional nodes was critical, *"One great thing about our cluster is that it gives us a lot of room to grow. Our next addition will likely be some form of DAS to expand the disk space available to the users and we plan on adding nodes to the system as well."*
- Cluster Management with ROCKS+ was required, and Ace had the experience to pre-install and configure the solution
- Onsite Installation and knowledge transfer was handled by Daniel Arendt, Engineering Director for Ace

Background on Elena Jakubikova:

Leads the *Jakubikova Research Group* at N.C.State, focused on Computational Chemistry and Photochemistry of Coordination Compounds

"We use the tools of computational chemistry to study ground and excited state properties of molecular compounds with potential application as light-harvesting molecules in solar cells or photocatalytic systems."
http://www4.ncsu.edu/~ejakubi/Welcome.html

Postdoctoral, Los Alamos National Laboratory, 2007-2010
Ph.D. in Chemistry, Colorado State University, 2007
M.S. in Mathematics, Colorado State University, 2005
Magister (M.S.) in Physics, Comenius University, (Bratislava, Slovakia), 2000

Detailed Tech Specs:

2U Head Node

- Quad 6164HE CPUs
- 96GB of Memory, with 16 Open slots for future expansion!
- 6x 1TB Enterprise SATA HDD
- Dual 1400W 80+ GOLD PS
- 2x Gigabit NIC plus IPMI 2.0 KVM over LAN

1U Compute Nodes (Variable HDD)

- Quad 6164HE CPUs
- 96GB of Memory, with 16 Open slots for future expansion!
- 3x 2TB Enterprise SATA HDD or 1x 1TB Enterprise SATA HDD (2 Open Drive Bays)
- 1400W 80+ GOLD PS
- 2x Gigabit NIC plus IPMI 2.0 KVM over LAN

Peripherals

- APC NetShelter SX 42U with APC PDU
- NetGear 24 Port L2 Managed Ethernet Switch with 2x Mini-GBIC Uplink Ports
- IOGear GCL1816 Integrated LCD / 16 port KVM

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