Classroom Computing

Challenge

A professor at The Ohio State University wanted to help more scientists access high performance computing (HPC) resources.

Approach

The scientist developed a course, "Computational Chemistry," to teach graduate-level students how to use HPC in their research.

Solution

Over 40 student HPC research projects have been published in different academic journals, including top chemistry journals.

Any Device, Anywhere

"The idea I've always had was essentially to help develop expertise in different research groups on how they can use computational methods as a benefit to their experimental studies."

— *Chris Hadad, Ohio State professor*
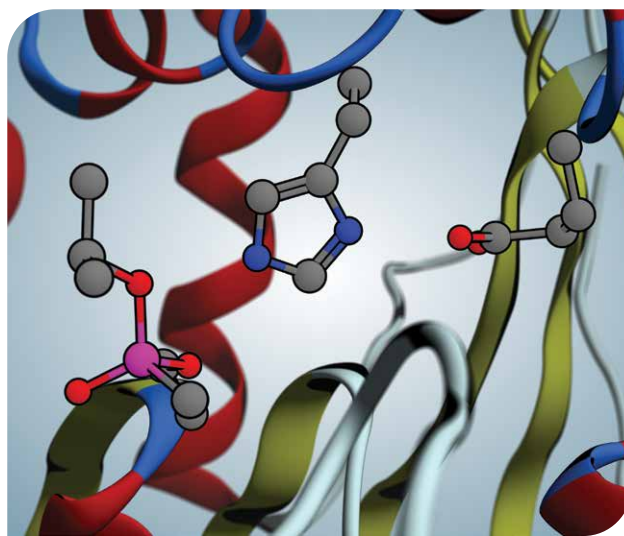
Ohio State course helps students use HPC in chemistry research

Chris Hadad has been a client of the Ohio Supercomputer Center (OSC) for over two decades and leads one of the most active accounts.

A professor of organic chemistry at The Ohio State University, Hadad is currently developing medical countermeasures against organophosphorus chemical nerve agents used in chemical warfare and as pesticides in agriculture.

More than 20 years ago, Hadad was inspired by the impact of OSC on his research to help others in the scientific community learn about and access high performance computing (HPC) resources.

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how they can use computational methods as a benefit to their experimental studies," he said.

To accomplish this goal, in 1996 Hadad developed a course at Ohio State, "Computational Chemistry," that teaches graduate-level students how to use HPC within their various fields of research.

Today Hadad has taught the course 16 times and has made a significant impact on students' education and careers. "Computational Chemistry" introduces students to real-world research using the HPC resources provided by OSC. The students choose their projects based on what interests them, and Hadad helps them tailor their use of OSC to find the answers they are seeking.

When Hadad began teaching this course, some students encountered difficulty using OSC, as they first needed to learn Unix commands to interface with the systems, the professor recalled. With the development of OSC's online portal Open OnDemand, much of this complexity has been eliminated, as OnDemand integrates software familiar to the students.

Not only are Hadad's students highly engaged in the classroom, but they also complete research that later may become the basis for their theses.

"Over 40 student projects have actually been published in different journals, many of them in some of the best journals in chemistry," Hadad said.

Hadad's integration of OSC within the classroom has caused a domino effect, disseminating HPC skills throughout educational and research communities.

"I've even had faculty take my class, including some faculty who have then gone on to other institutions to teach a computational chemistry class there," Hadad said.

openondemand.org/hadad

Try Open OnDemand

It is simple to set up a live demo of Open OnDemand for evaluation. Just follow the directions at **openondemand.org/demo**. Once the steps are complete, explore Open OnDemand's documentation and core applications—Files, Editor and Job Composer—for more information.
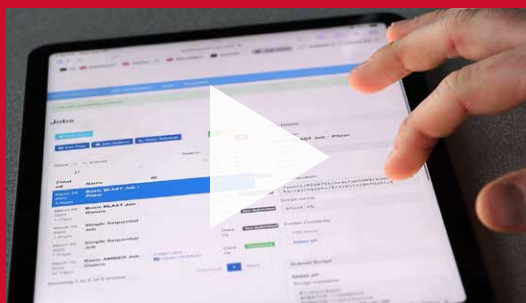
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