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SDSC Graduate Student Awarded NVIDIA Graduate Fellowship

\$25,000 Scholarship Granted for GPU-accelerated Molecular Dynamics Research



Madej

A graduate student working in the Walker Molecular Dynamics laboratory at the San Diego Supercomputer Center (SDSC) at the University of California, San Diego is a recipient of the 2012-2013 [NVIDIA Graduate Fellowship Program](#) award for his innovative molecular dynamics research using GPU (graphics processing unit) computing.

Benjamin Madej, a chemistry and biochemistry Ph.D. student at UC San Diego, will receive a \$25,000 scholarship to further his research. Madej received his Bachelor of Science in biomedical engineering from

Washington University in St. Louis, Missouri, and is currently working on new methods for developing force fields used in molecular dynamics software, specifically the [AMBER MD](#) package.

Madej's research proposal focused on not only improving the AMBER Molecular Dynamics GPU engine, but extending the use of GPUs to multiple facets of molecular dynamics development and workflow for new drug discovery.

"We are proud of Ben's achievement in being awarded this prestigious scholarship and recognition," said SDSC Director Michael Norman. "It is very gratifying to see such a high level of accomplishment in computational science as Ben pursues his doctorate here at UC San Diego."

“This fellowship is a testimony to Ben’s past work, the importance of GPUs at the frontiers of molecular dynamics and drug discovery, and recognition of the future potential of his contributions to science. The GPU revolution is transforming the field and this fellowship provides vital support for us to continue this cutting-edge research,” said Ross C. Walker, an assistant research professor with SDSC and head of the [Walker Molecular Dynamics laboratory](#). Walker also is an adjunct assistant professor in UC San Diego’s Department of Chemistry and Biochemistry, as well as an NVIDIA CUDA Fellow.

The NVIDIA Graduate Fellowship Program provides funding to Ph.D. students who are researching topics that will lead to major advances in the graphics and high-performance computing industries, and are investigating innovative ways of leveraging the power of GPUs. Recipients not only receive crucial funding for their research, but are provided access to NVIDIA products, technology, and expertise.

“This year the NVIDIA Foundation joined in our search for top Ph.D. students who are investigating innovative ways to leverage the power of the GPU, especially those that will ultimately benefit humanity,” said Chandra Cheij, NVIDIA’s research program manager. “Congratulations to Ben and SDSC for this significant achievement.”

SDSC’s Walker Molecular Dynamics lab is focused on computational chemistry, molecular biology, and high-performance computing. The lab is particularly interested in the development of efficient algorithms for parallel computation of Quantum Mechanical and hybrid Quantum/Molecular Mechanical (QM/MM) techniques, as well as improvements in the computational efficiency and accuracy of classical MM dynamics simulations.

Practical applications of the techniques developed in the WMD lab include the development of next-generation viral inhibitors, improvements in bio-ethanol production, drug discovery, and advanced algorithms for high performance of scientific application on supercomputers. The lab is also closely involved with the development of the AMBER molecular dynamics software.

The WMD lab is funded through a combination of grants from the National Science Foundation (NSF), the University of California, NVIDIA, Microsoft, and the UK Foreign and Commonwealth Office, Department for Business, Innovation and Skills.

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