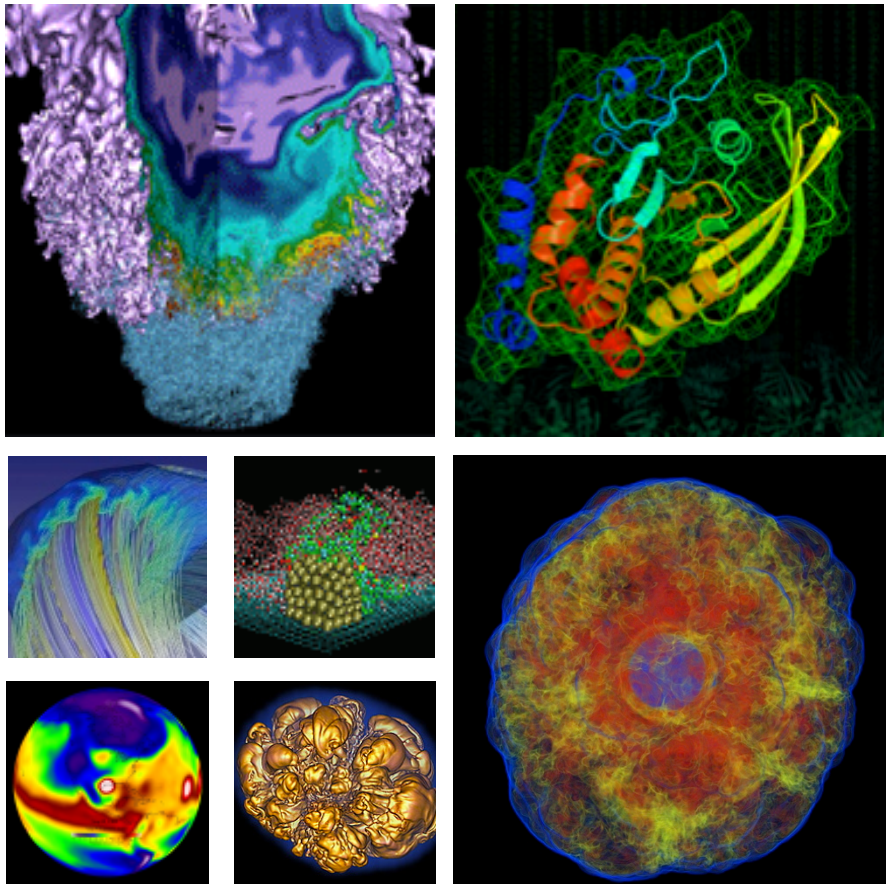
Science Highlights from NERSC's Dirac GPU Testbed



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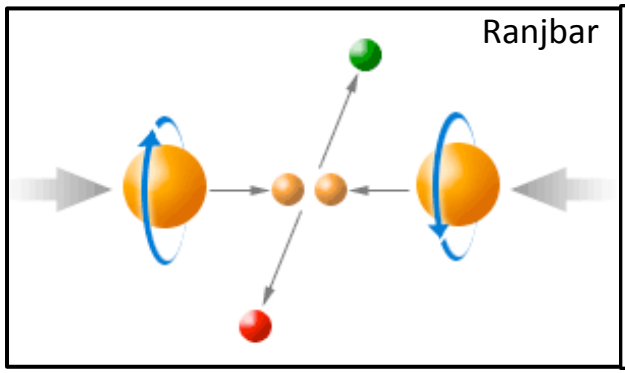
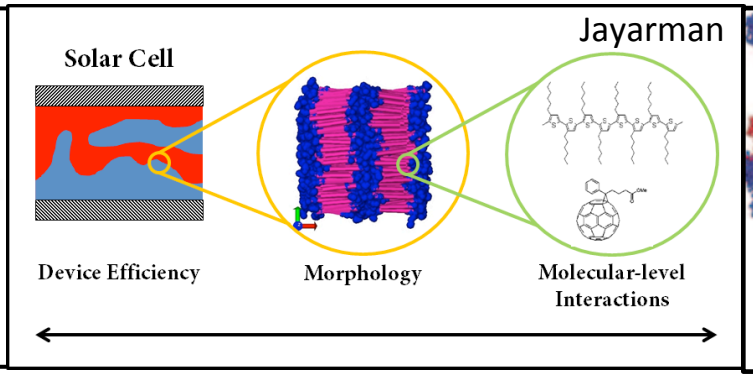
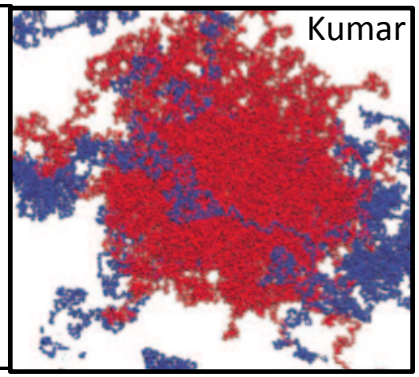
Top Dirac Projects in 2013

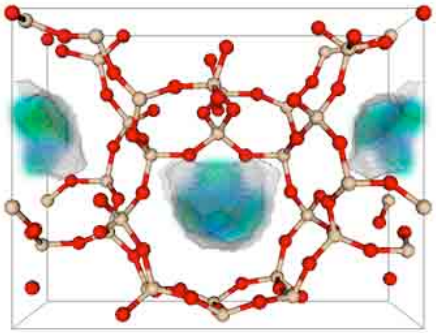
Science Area	Project Title	PI	Node Hours Used	Percent of Total
Nuclear Physics	Polarized Proton Tracking for RHIC and AGS	V. Ranjbar, Brookhaven Nat Lab	24,000	40%
Material Sciences	Molecular Simulations of Conjugated Polymers for Organic Photovoltaics	A. Jayaraman, U. Colorado, Boulder	18,000	30%
Material Sciences	Modeling Nanocomposites and Proteins	S. Kumar, Columbia U.	14,000	24%

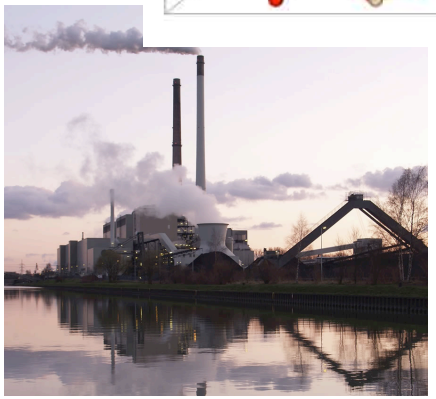






Porous Materials for CO_2 Capture



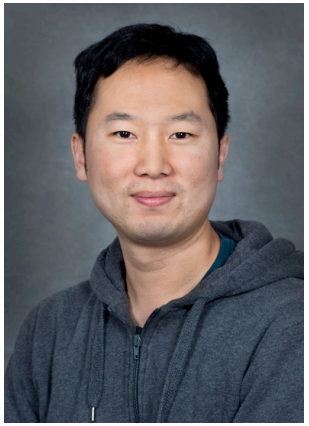


Porous materials can be used to capture CO_2 before it is emitted into the atmosphere.

Many candidate structures must be screened to determine their absorption properties in search of optimal materials.

Berkeley Lab's Jihan Kim developed innovative grid-based Monte Carlo programs from scratch to use GPUs.

Using Dirac, he was able to achieve a 50X speedup over a traditional CPU and screened more than 1 M potential structures. Results have been published in high-impact journals, including Nature Materials, Nature Chemistry, and JACS.



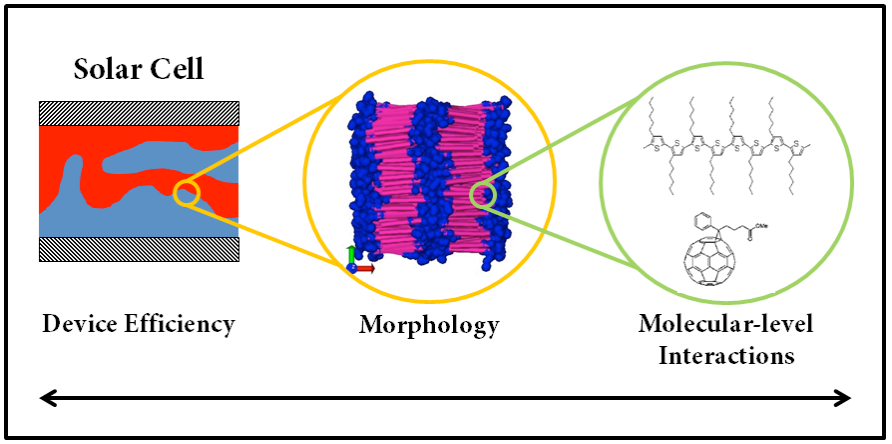
Molecular Simulations of Conjugated Polymers for Organic Photovoltaics

Hilary Marsh, Eric Jankowski, Arthi Jayaraman, U. Colorado – Boulder

Equilibrating a blend of polymers/ fullerenes can take billions of molecular dynamics time steps.

On Dirac, the most computationally intensive runs take ~360 hours on one GPU, allowing sampling of 110 state points in about 2 months.

This broad sampling is crucial for determining trends in how the morphology of blends changes with polymer type and acceptor miscibility at varying temperatures.



The results obtained using Dirac guide experimentalists who are designing polymers for highly efficient organic photovoltaic devices.

Compared to performing the same simulations on multicore nodes with LAMMPS, Dirac is a ~58X more efficient use of core-hours.

Polarized Proton Tracking for RHIC[1] and AGS[2]

Vahid H. Ranjbar, Brookhaven National Laboratory

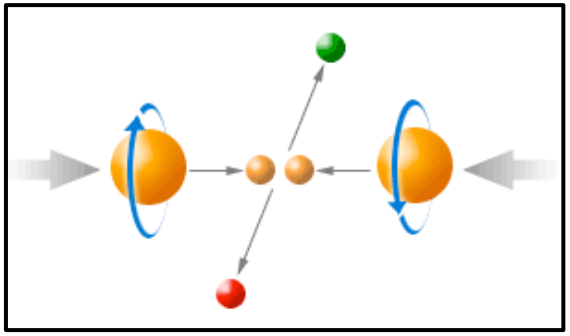
Dirac permits use of 6D particle distributions using 30K particles on a NVIDIA Tesla C2050 GPU.

Equivalent runs on Hopper or Carver would require 30K processors, so usually used few 100s of particles.

Can now study depolarization mechanisms in detail as a function of initial particle phase space coordinates.

This will provide invaluable data for future beam design and analysis.

Keeping beams spin polarized is difficult and demands specialized magnetic structures.



RHIC is the world's only machine capable of colliding and studying high-energy beams of polarized protons.

Experiments have shown that the spins of the proton's constituent quarks (and antiquarks), in some cases accounts for only about 30% of its total spin.

RHIC spin experiments are providing the first information on how much the spin of gluons contributes to the proton's spin.

[1]Relativistic Heavy Ion Collider @ Brookhaven National Lab
[2]Alternating Gradient Synchrotron @ Brookhaven National Lab
Photos from Brookhaven National Laboratory

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