HPC for Discovery and Innovation

Overview of how supercomputers, people, and algorithms solve big challenges.

David Skinner
NERSC Strategic Partnerships Lead
Lawrence Berkeley National Lab
National Lab HPC Drives Scientific Discovery & Tech Innovation
<table>
<thead>
<tr>
<th>System: Joule, 24,192 Cores, 9 Petabytes of storage, Quad Data Infiniband, 76 TB memory</th>
<th>Capabilities: Fluid Dynamics, Materials, Chemistry, MFIX.</th>
</tr>
</thead>
<tbody>
<tr>
<td>System: Vulcan, 24K nodes Power7IBM 1.6 GHz, 393,216 compute cores, 400 TB compute memory</td>
<td>Capabilities: Scaling vendor codes to run on HPC platforms, Expanding software capabilities, algorithm development and multi-physics integration.</td>
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<tr>
<td>System: Trinity, Cray XC30, 19K nodes, Intel Haswell and Intel KNL, 2PB DRAM, unique NVRAM capabilities.</td>
<td>Capabilities: In situ, dynamic measurements, simultaneous imaging and modeling of well-controlled and characterized materials advanced synthesis and characterization in extreme environments.</td>
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</tbody>
</table>

HPC systems and skill sets are important across the national lab system.
NERSC HPC Serves “All of the above” Science for DOE SC

NERSC systems are used by > 7000 scientists

<table>
<thead>
<tr>
<th>Year</th>
<th>System</th>
<th>Platform</th>
<th>TF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>NERSC-5</td>
<td>Franklin</td>
<td>Cray XT4</td>
</tr>
<tr>
<td>2010</td>
<td>NERSC-6</td>
<td>Hopper</td>
<td>Cray XE6</td>
</tr>
<tr>
<td>2014</td>
<td>NERSC-7</td>
<td>Edison</td>
<td>Cray XC30</td>
</tr>
<tr>
<td>2016</td>
<td>NERSC-8</td>
<td>Cori</td>
<td>Cray XC</td>
</tr>
<tr>
<td>2020</td>
<td>NERSC-9</td>
<td>Pelmutter</td>
<td></td>
</tr>
<tr>
<td>2024</td>
<td>NERSC-10</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

LBNL CS staff provide programming, application optimization, and algorithm development so that codes run well.
Over 600 codes run at NERSC using >9B CPU hours/year

- 10 codes make up 50% of the workload
- 25 codes make up 66% of the workload
- DOE SC offices allocate 80% of the computing and storage resources at NERSC
- NERSC Director’s Reserve 10%
- ALCC 10%

- Strong focus on discovery science but...
- HPC4 Energy shows codes can be re-purposed for applied innovations.
- Small business access through SBIR grants.
Industry-led projects at NERSC include principal investigators (PIs) from... and growing. Industry access to NERSC through ALCC, DDR, SBIR, or HPC4EI
Virtually all separation processes rely on thermal energy, i.e. distillation. Reducing this energy footprint is essential to assure the sustainability and global competitiveness of the U.S.-based chemical enterprise.

Solution: NIST and ACS propose survey to map non-cryogenic mass separation agents (MSAs).

Team: Debbie Bard (NERSC) Vincent Shen (NIST) David Constable (ACS) Robert Giraud (Chemours) Nathan Mahynski (NIST)

How to chemically tune MSAs?
Approach: HPC survey of pore-size selective separations

• Use ensemble molecular simulation techniques for thermodynamic behavior of fluid mixtures confined in pores by molecular adsorption.
• Model separation across size/shape of the pore, intra/intermolecular fluid interactions, and fluid-wall interactions, seeking tunable structure-function options in MSA design.
• Use existing MD code with Monte Carlo methods to sample large design phase space.

Impact ➔ HPC simulations yield durable dataset for informatic MSA design.

Fluid selectivity of MSA pores for different chemical species
Demonstrated highly non-monotonic selectivity behavior for certain fluids and pores using > 150M CPU hours
## Lithium-Sulfur Batteries

### Attributes of Battery Technologies

<table>
<thead>
<tr>
<th>Battery Technology</th>
<th>Energy (Wh/kg)</th>
<th>Power (W/kg)</th>
<th>Life (cycles)</th>
<th>Energy Efficiency</th>
<th>Safety</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lithium-ion (current)</td>
<td>80</td>
<td>50 - 1000</td>
<td>&gt; 3,000</td>
<td>&gt; 90%</td>
<td>*Safe</td>
</tr>
<tr>
<td>Lithium-ion (Future*)</td>
<td>200+</td>
<td>2,000</td>
<td>&gt; 3,000</td>
<td>&gt; 90%</td>
<td>--</td>
</tr>
<tr>
<td>Lithium metal polymer</td>
<td>150-200</td>
<td>&lt; 100</td>
<td>~ 1000</td>
<td>85%</td>
<td>Concern</td>
</tr>
<tr>
<td>Lithium metal/Sulfur</td>
<td>250 - 400</td>
<td>~100</td>
<td>&lt;100</td>
<td>85%</td>
<td>Concern</td>
</tr>
<tr>
<td>Lithium metal/Air</td>
<td>400 - 800</td>
<td>Poor</td>
<td>~ 10</td>
<td>&lt; 70%</td>
<td>Concern</td>
</tr>
<tr>
<td>DOE 2020 Goals</td>
<td>250</td>
<td>2,000</td>
<td>&gt;1000</td>
<td>&gt; 90%</td>
<td></td>
</tr>
</tbody>
</table>

**Computed molecular models of Sepion’s polysulfide-blocking polymer membranes cast from polymers of intrinsic microporosity (PIMs).**

Li-S offers 5x energy density but membrane lifetime must be optimized.
HPC methods

MF$^3$ force-field development
- vdW, electrostatics
- polarizability
- charge transfer
Parameters derived ab initio (QChem)

Molecular dynamics simulation (LAMMPS)
- polymer membrane assembly
- annealing
- pore size evaluation
- mechanical properties
- infiltration by solvent/electrolyte

Comparison with performance metrics
- accessibility for solvent/salt/active materials
- conductivity/diffusivity
- mechanical strength/swelling upon infiltration

Revision of chemical design/synthesis

HPC science codes repurposed for product design
Pore size and chemistries simulated for 50K atoms
Membrane designs shaped by modeled chemistries

“Our success suggests a revolution in ion-transporting membranes is within reach.” NanoLett. 15, 9, 5724-5729
In manufacturing settings, paints are frequently applied by an electrostatic rotary bell atomizer.

- Painting consumes 70% of the total energy used in automobile assembly
- 10,000s of gigawatt-hours each year in the U.S. automotive industry alone

3d peta-scale model of surface tension forces, sheeting behavior dependence on film thickness, formation of tendrils and their breakup into droplets. 10K CPUs used.
Method: Multiphase fluid using Discontinuous Galerkin

Quantitative agreement between PPG in-house experiments and computed droplet statistics of ~800 droplets.

In manufacturing settings, paints are frequently applied with a high-throughput electrostatic rotary bell atomizer.

Atomicization behavior (droplet size, uniformity, trajectories) depends on injection rate, rotation speed, paint density, viscosity, surface tension, and cup geometry.

Numerical results from a pilot phase successfully predict a variety of phenomena observed in rotary bell atomization. This figure shows the azimuthal component of velocity as a thin film of paint detaches from cup, breaking up into droplets.

Time-integrated droplet statistics of ~800 droplets

Model indicates 20% higher flow rates can be achieved with insight from this work, representing a saving of 7,400 GJ/year in the US automotive industry alone.
Perlmutter: A System Optimized for Science

- Cray Shasta System providing 3-4x capability of Cori
- GPU-accelerated and CPU-only nodes meet the needs of large scale simulation and data analysis from experimental facilities
  - >4,000 node CPU-only partition provides same capability as all of Cori
  - Support for complex workflows using compute, storage and networking resources
  - Optimized data software stack enabling analytics and ML at scale
- GPU nodes: 4 NVIDIA GPUs each w/Tensor Cores & NVLink-3 and High-BW memory + 1 AMD “Milan” CPU
  - Unified Virtual Memory support improves programmability
- Cray “Slingshot” - High-performance, scalable, low-latency Ethernet- compatible network
  - Capable of Terabit connections to/from the system
- Single-tier All-Flash Lustre based HPC file system
  - 6x Cori’s bandwidth

Delivered in late-2020