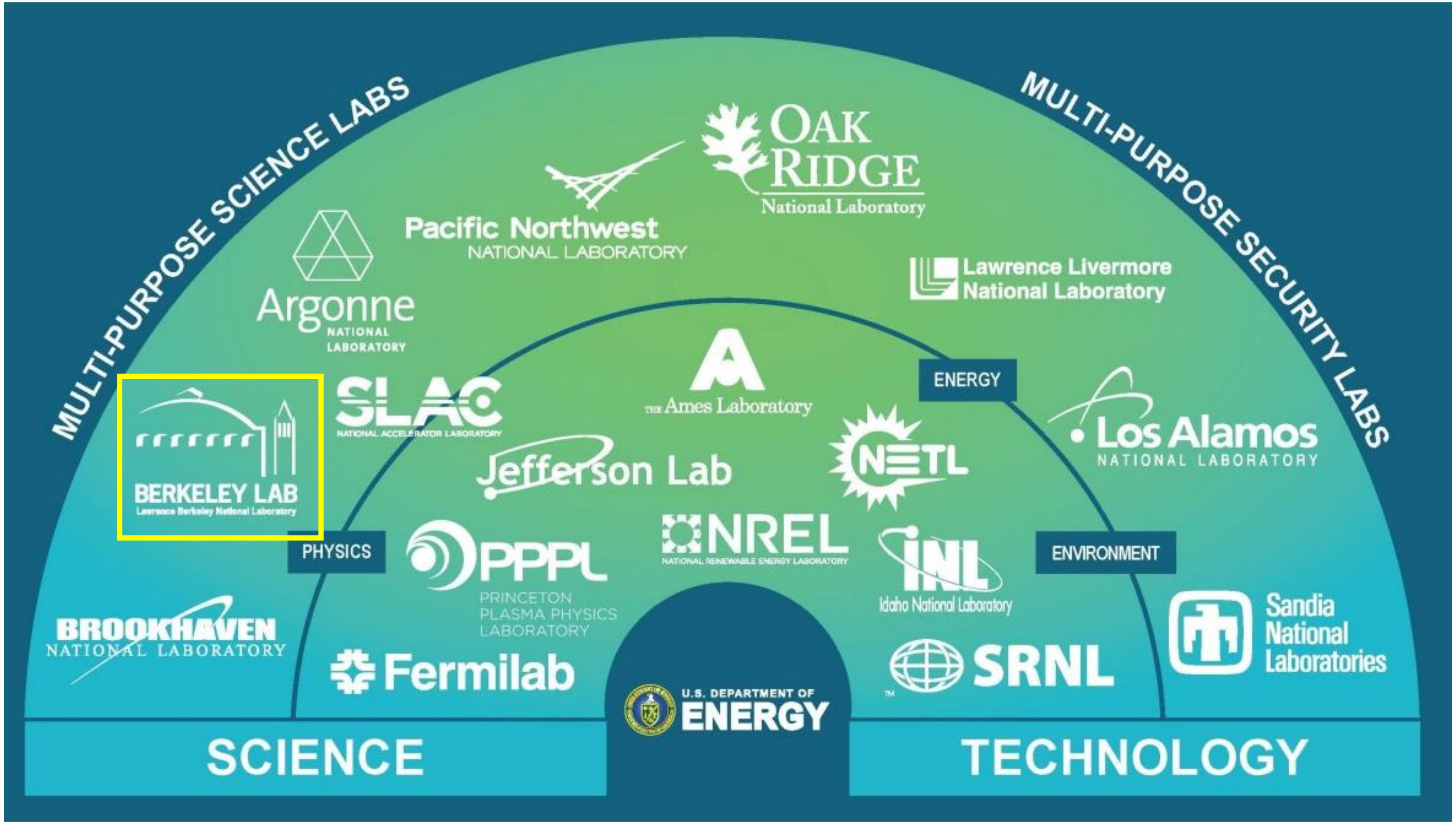
HPC for Discovery and Innovation

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

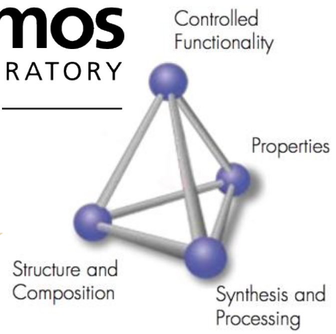
National Energy Research Scientific Computing Center

David Skinner
NERSC Strategic Partnerships Lead
Lawrence Berkeley National Lab

National Lab HPC Drives Scientific Discovery & Tech Innovation



System: Joule, 24,192 Cores, 9 Petabytes of storage, Quad Data Infiniband, 76 TB memory	Capabilities: Fluid Dynamics, Materials, Chemistry, MFIX.
System: Titan, Cray XK7, 18K nodes, 300K CPUs, 18K GPUS,	Capabilities: Computational Biology, Chemistry, Engineering, Earth, Energy, GIS, Technology and Matierials.
System: Vulcan, 24K nodes Power7IBM 1.6 GHz, 393,216 compute cores, 400 TB compute memory	Capabilities: Scaling vendor codes to run on HPC platforms, Expanding software capabilities, algorithm development and multi-physics integration.
System: Trinity, Cray XC30, 19K nodes, Intel Haswell and Intel KNL, 2PB DRAM, unique NVRAM capabilitiles.	Capabilities: In situ, dynamic measurements ,simultaneous imaging and modeling of well-controlled and characterized materials advanced synthesis and characterization in extreme environments.

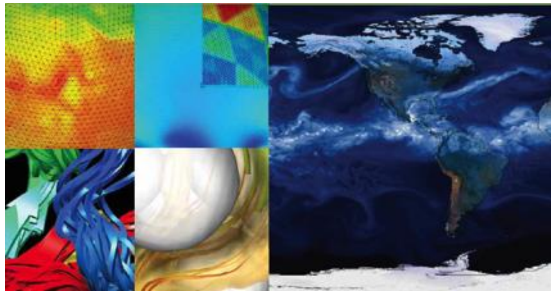


HPC systems and skill sets are important across the national lab system

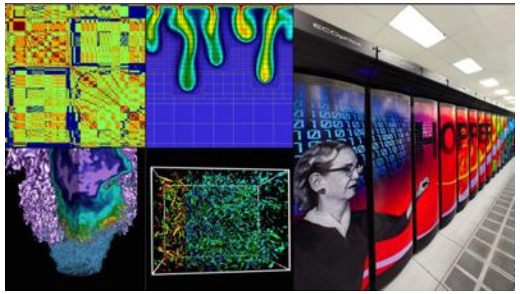
NERSC HPC Serves “All of the above” Science for DOE SC

U.S. DEPARTMENT OF ENERGY | Office of Science

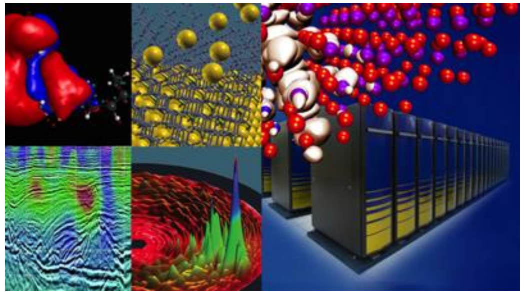
Largest funder of physical science research in U.S.



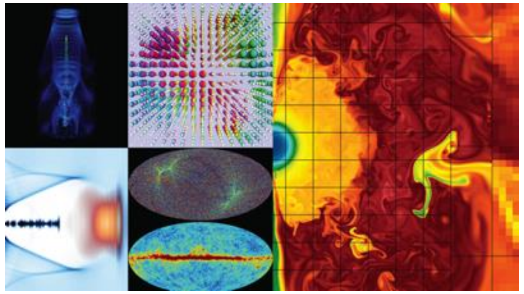
Biology, Environment



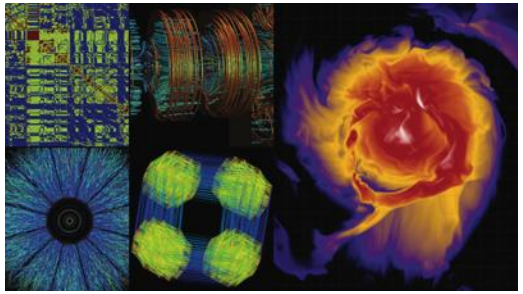
Computing



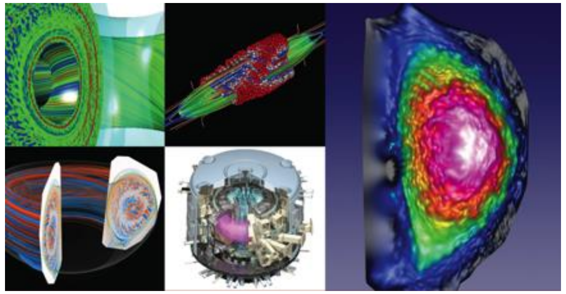
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



Nuclear Physics

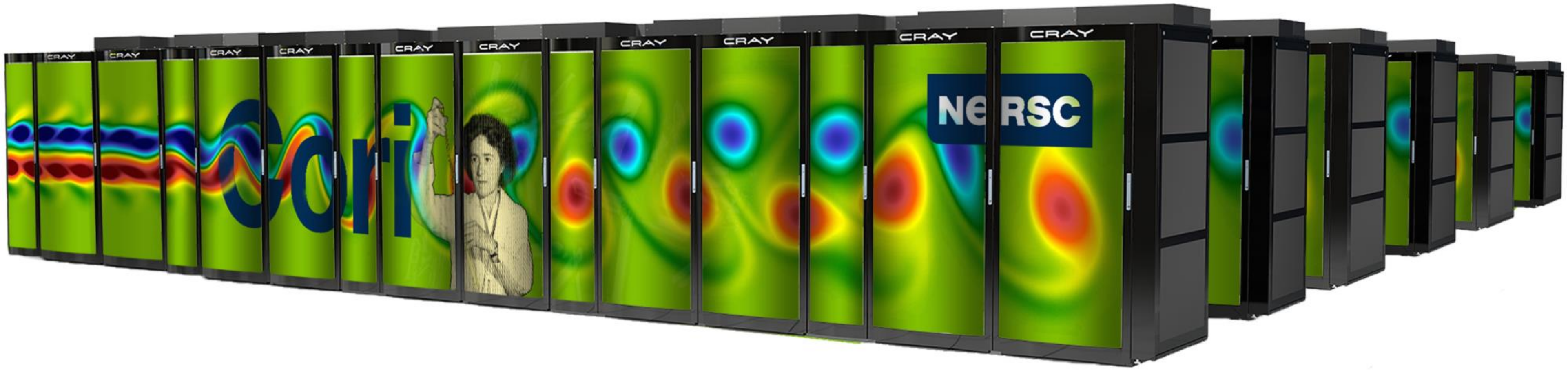


Fusion Energy, Plasma Physics

NERSC is the National Energy Research Scientific Computing Center, Founded in 1974, Focused on open science
Located at Lawrence Berkeley National Laboratory, Operated for the U.S. Department of Energy (DOE) Office of Science

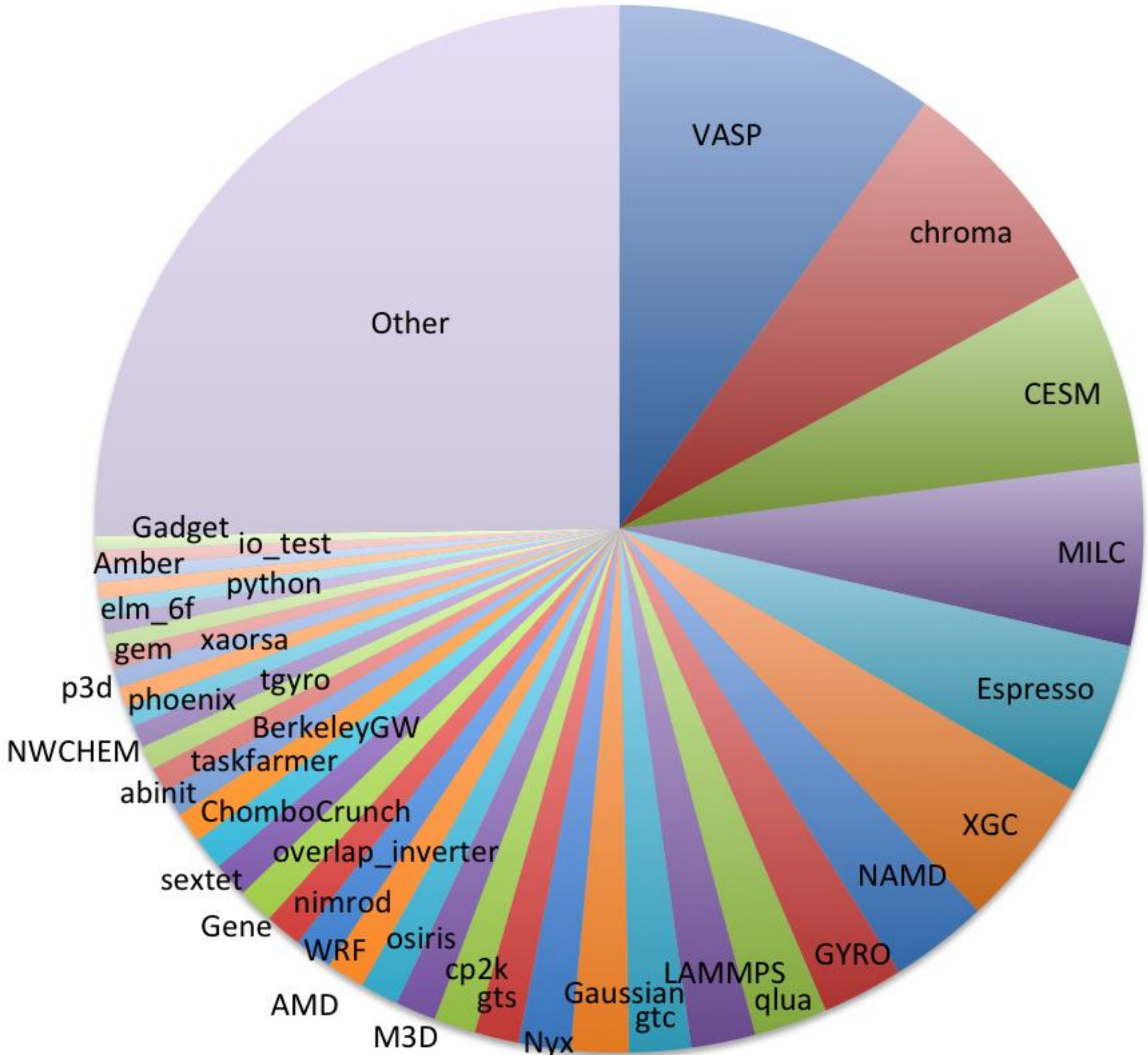
NERSC systems are used by > 7000 scientists

2007/2009	NERSC-5	Franklin	Cray XT4	102/352 TF
2010	NERSC-6	Hopper	Cray XE6	1.28 PF
2014	NERSC-7	Edison	Cray XC30	2.57 PF
2016	NERSC-8	Cori	Cray XC	30 PF
2020	NERSC-9	Pelmutter		100PF-300PF
2024	NERSC-10			1EF



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.

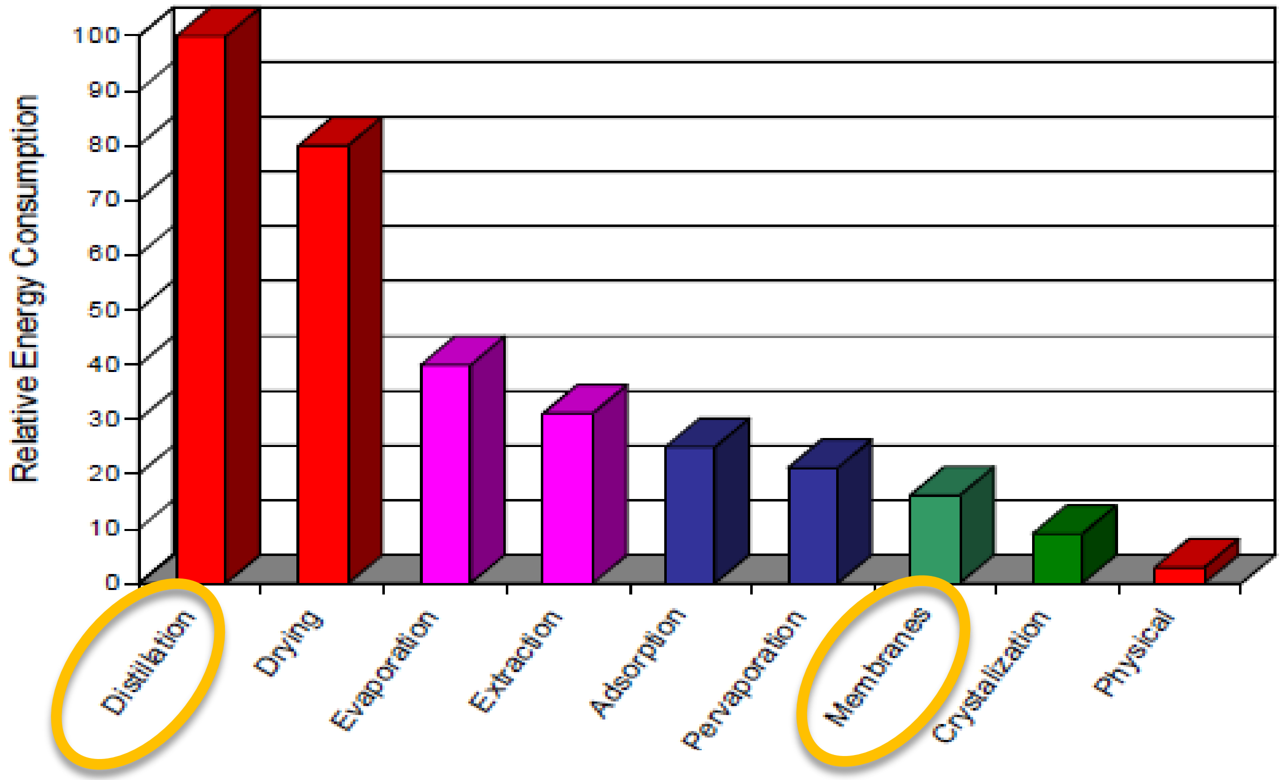
Industry-led projects at NERSC include principal investigators (PIs) from...

QuantumScape
Q-CHEM
A Quantum Leap Into the Future of Chemistry
GENERAL ATOMICS
SIEMENS
SciberQuest
LODESTAR
ADVISORY PARTNERS
ROGUE WAVE
SOFTWARE
VertumPartners
VorCat
ParaTools
Muons, Inc.
Innovation in Research
TECH-X
SIMULATIONS EMPOWERING YOUR INNOVATIONS
WOODRUFF • SCIENTIFIC
LIFE CYCLE MANAGEMENT SOLUTIONS
FOR THE ELECTRICITY INDUSTRY
KINECTRICS
nanoPrecision
products
United Technologies
Research Center
MELIOR Innovations
Delivering Material Value
Chemical Semantics
radiasoft
Kitware

and growing. Industry access to NERSC through ALCC, DDR, SBIR, or HPC4EI

Distillation: Cryo-separations > 10% of U.S. energy consumption

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.*



140 T BTU/year in Alkane-Alkene separation alone

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

BERKELEY LAB

ACS Green Chemistry Institute®

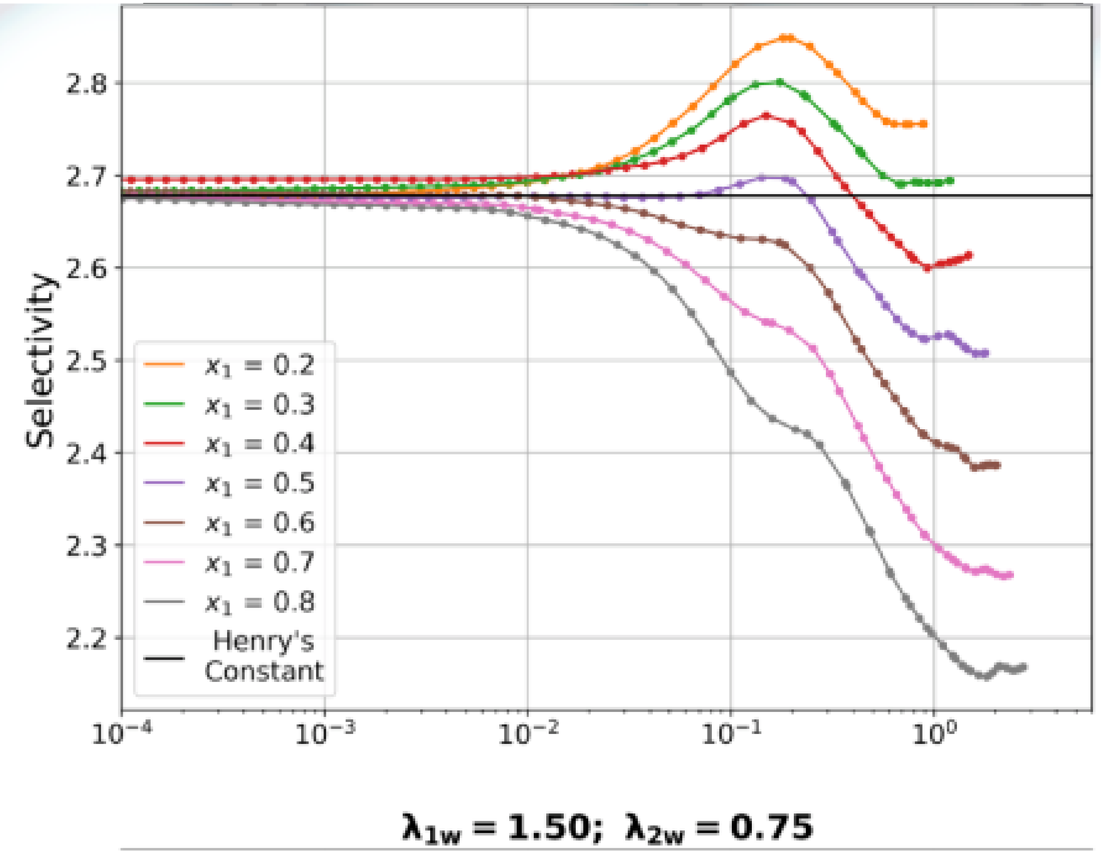
NIST

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.



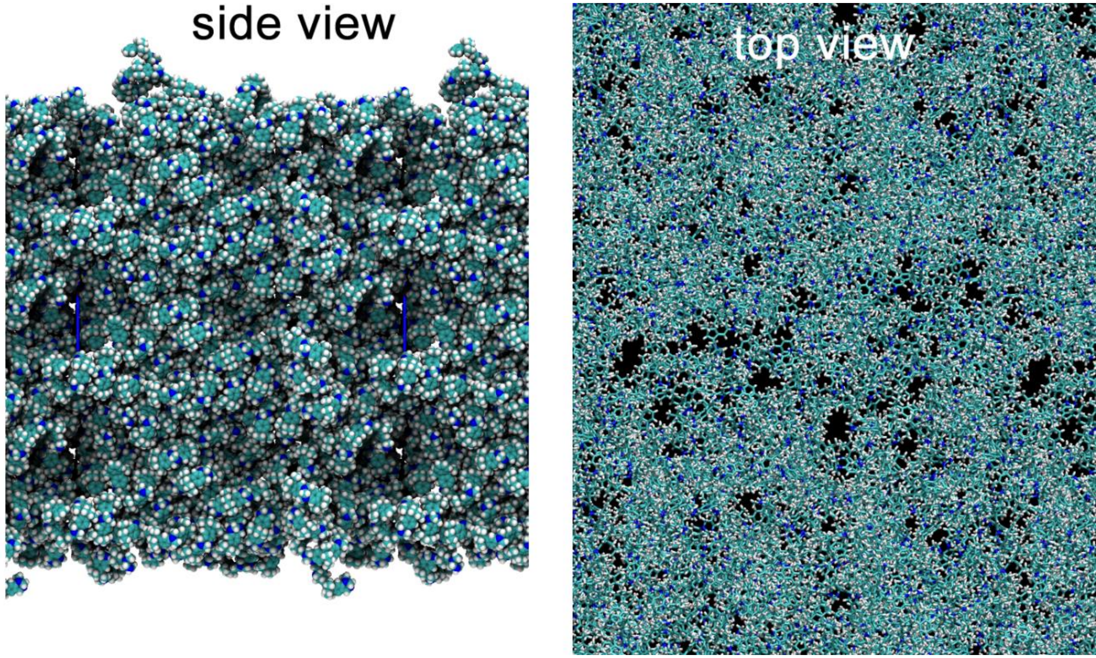
Impact → HPC simulations yield durable dataset for informatic MSA design.

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

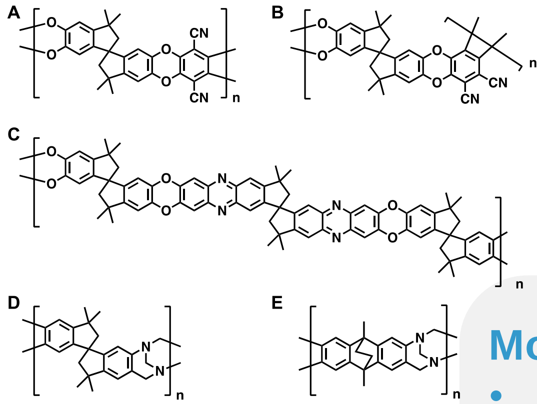
Li-S offers 5x energy density but membrane lifetime must be optimized

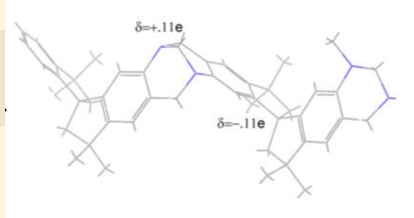


Computed molecular models of Sepion's polysulfide-blocking polymer membranes cast from polymers of intrinsic microporosity (PIMs).

HPC methods

polymer library





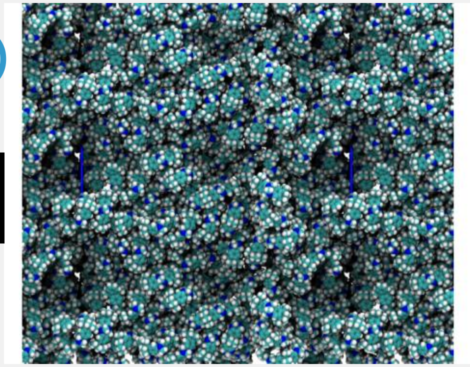
MF³ force-field development

- 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

Tod Pascal & David Prendergast

HPC science codes repurposed for product design

Pore size and chemistries simulated for 50K atoms

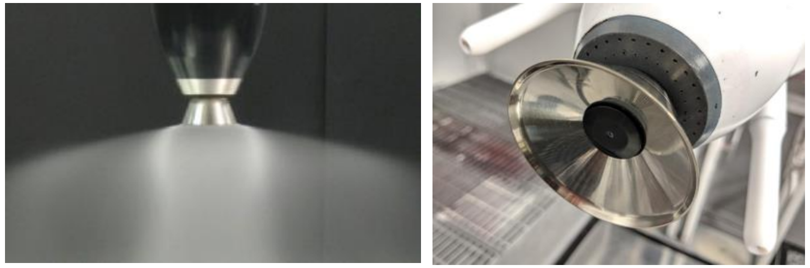
Membrane designs shaped by modeled chemistries

"Our success suggests a revolution in ion-transporting membranes is within reach." *NanoLett. 15, 9, 5724-5729*

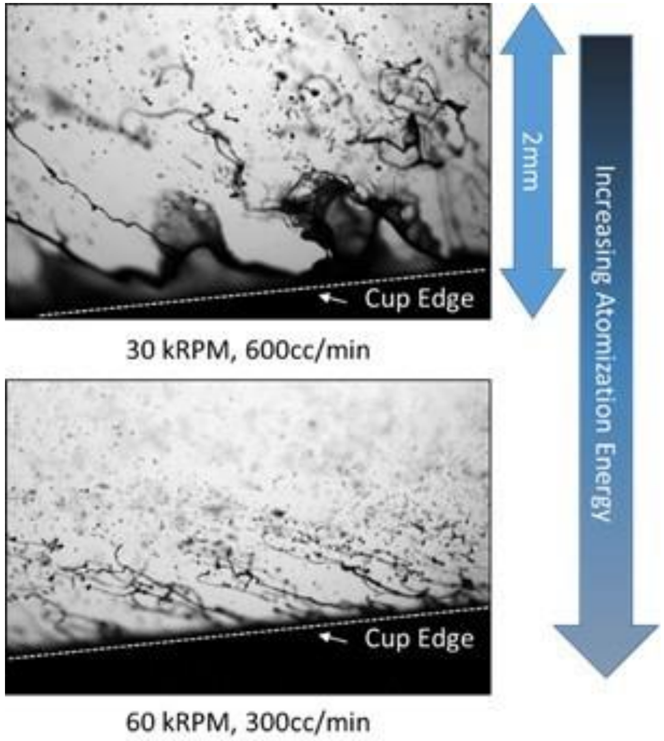
Industrial Spray Painting

In manufacturing settings, paints are frequently applied by an electrostatic rotary bell atomizer.

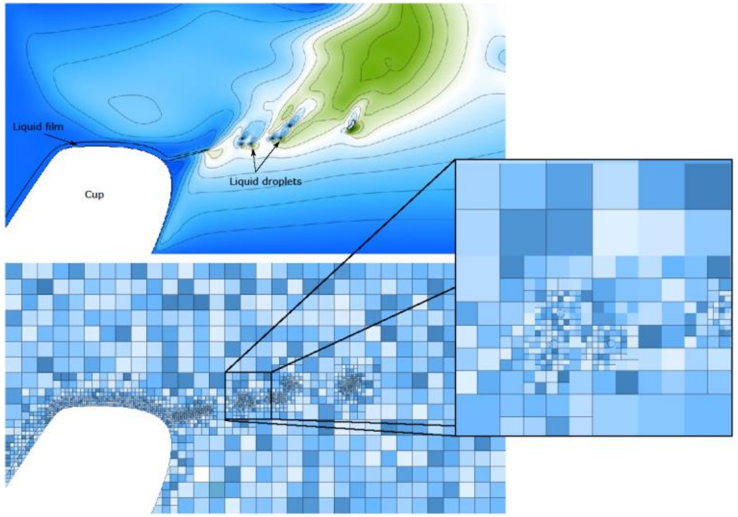
- Painting consumes 70% of the total energy used in automobile assembly
- **10,000s of gigawatt-hours each year** in the U.S. automotive industry alone



High-throughput spray painting using a rotary bell atomizer.

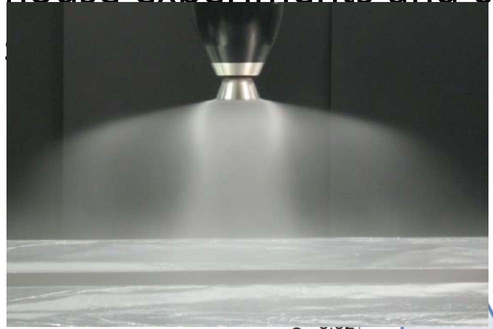


3d peta-scale model of surface tension forces, sheeting behavior dependence on film thickness, formation of tendrils and their breakup into droplets. 10K CPUs used.

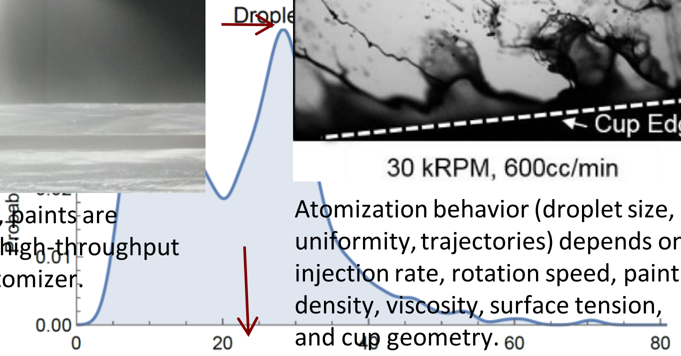


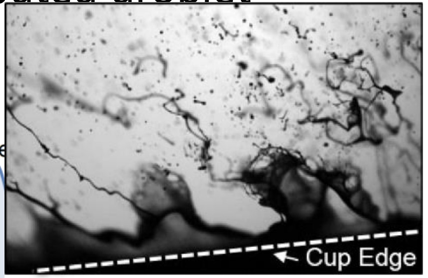
Method: Multiphase fluid using Discontinuous Galerkin

Quantitative agreement between PPG in-house experiments and computed droplet s



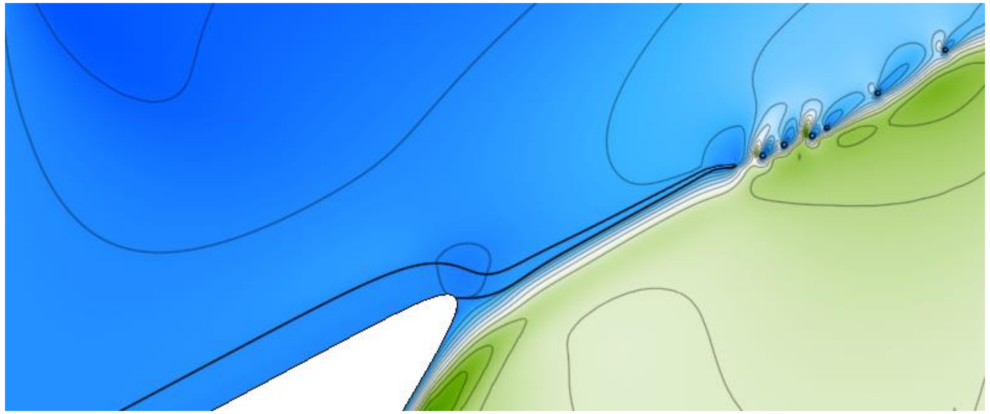
In manufacturing settings, paints are frequently applied with a high-throughput electrostatic rotary bell atomizer.





30 kRPM, 600cc/min

Atomization 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 a cup, breaking up into droplets.

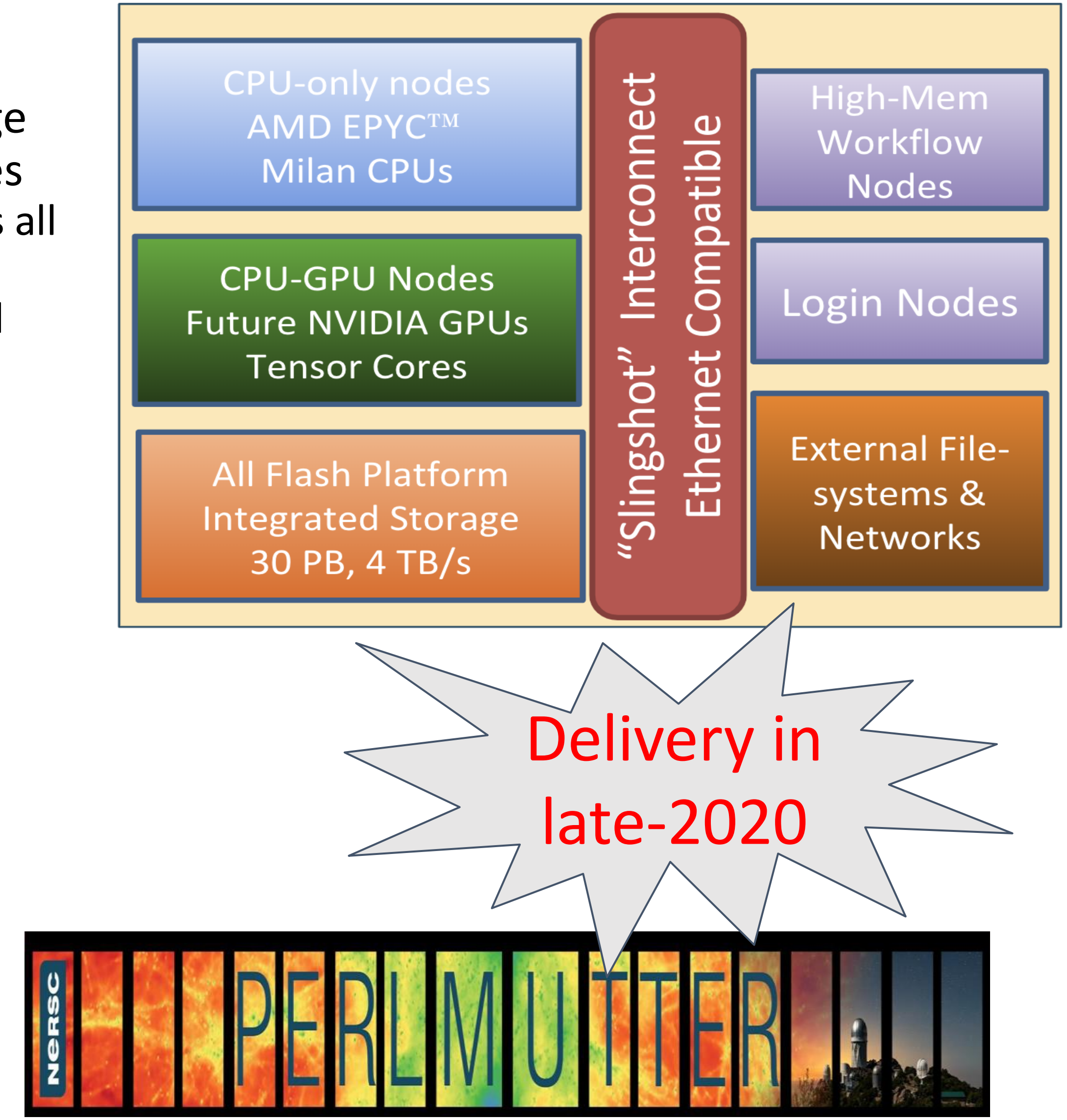
Adaptive mesh refinement – elements are refined near thin films or high-curvature interfacial features

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



Thanks!

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