## Migrating from Cori to Perlmutter



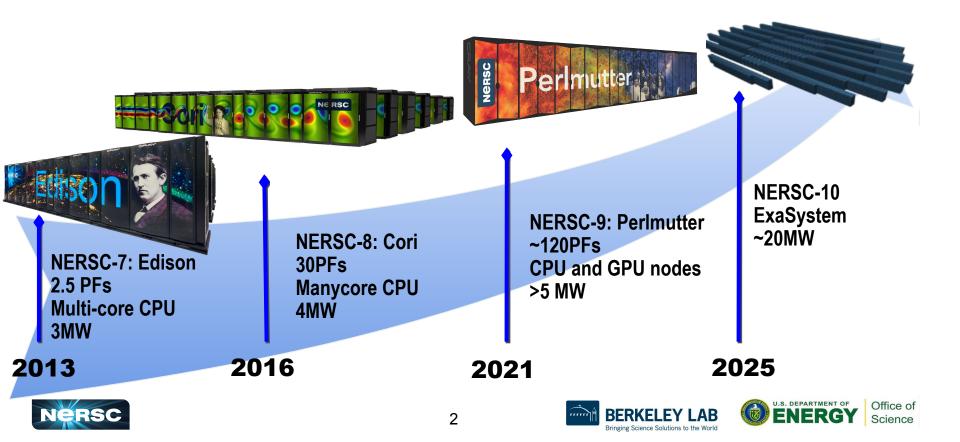
### Intro to Perlmutter and GPUs

### **Overview**

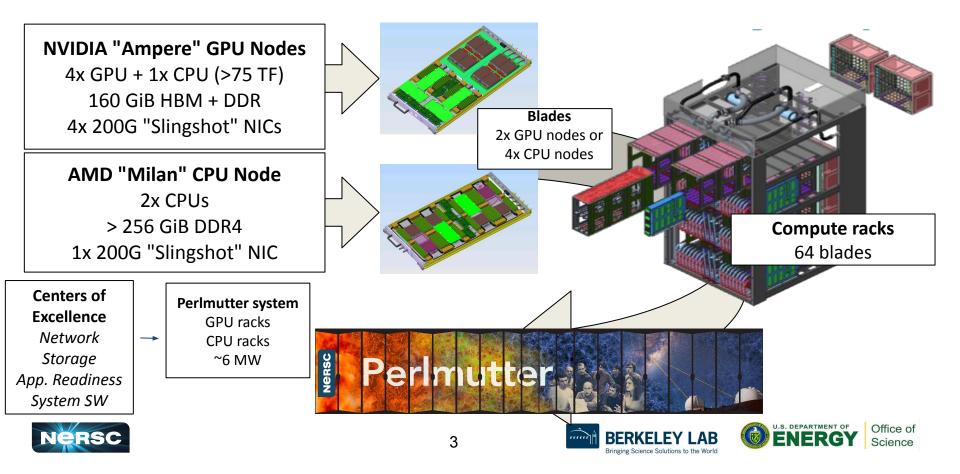
December 2022

Jack Deslippe Application Performance Lead

## **NERSC Systems Roadmap**



## Perlmutter system configuration



### The System





#### System Specifications

Partition	# of nodes	CPU	GPU	NIC
GPU	1536	1x AMD EPYC 7763	4x <u>NVIDIA A100</u> (40GB)	4x HPE Slingshot 11
CPU	3072	2x AMD EPYC 7763	-	1x HPE Slingshot 11
Login	40	1x AMD EPYC 7713	1x <u>NVIDIA A100</u> (40GB)	-
Large Memory	4	1x AMD EPYC 7713	1x <u>NVIDIA A100</u> (40GB)	1x <u>HPE Slingshot 11</u>

#### System Performance

Partition	Туре	Aggregate Peak FP64 (PFLOPS)	Aggregate Memory (TB)
GPU	CPU	3.9	384
GPU	GPU	59.9 tensor: 119.8	240
CPU	CPU	7.7	1536

#### More Details:

https://docs.nersc.gov/systems/perlmutter/architecture/





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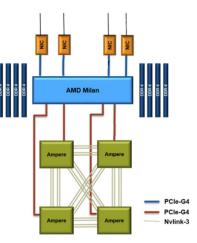
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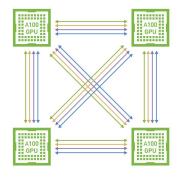
### The System

#### **GPU Nodes:**

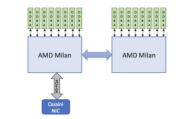
- Single AMD EPYC 7763 (Milan) CPU
- 64 cores per CPU
- Four NVIDIA A100 (Ampere) GPUs
- PCIe 4.0 GPU-CPU connection
- PCIe 4.0 NIC-CPU connection
- 4 HPE Slingshot 11 NICs
- 256 GB of DDR4 DRAM
- 40 GB of HBM per GPU with
- 1555.2 GB/s GPU memory bandwidth
- 204.8 GB/s CPU memory bandwidth
- 12 third generation NVLink links between each pair of gpus
- 25 GB/s/direction for each link

Data type	GPU TFLOPS
FP32	19.5
FP64	9.7
TF32 (tensor)	155.9
FP16 (tensor)	311.9
FP64 (tensor)	19.5





#### **CPU Nodes:**



- 2x AMD EPYC 7763 (Milan) CPUs
- 64 cores per CPU
- AVX2 instruction set
- 512 GB of DDR4 memory total
- 204.8 GB/s memory bandwidth per CPU
- 1x HPE Slingshot 11 NIC
- PCIe 4.0 NIC-CPU connection
- 39.2 GFlops per core
- 2.51 TFlops per socket
- 4 NUMA domains per socket (NPS=4)









### The System

#### All Flash Filesystem:

- 35 PB of disk space
- an aggregate bandwidth of >5 TB/sec
- 4 million IOPS (4 KiB random)
- It has 16 MDS (metadata servers)
- 274 I/O servers called OSSs
- 3,792 dual-ported NVMe SSDs.







### Enable a diverse community of scientific users and codes to run efficiently on advanced architectures like Cori, Perlmutter and beyond





## Comparison of Perlmutter and Cori

Attribute	Cori (2016)	Perlmutter (2021)
Peak Performance	~30 PF	~120 PF
Peak Power	< 4MW	~6 MW
System Memory	~ 1PB (DDR4 + HBM)	> 2PB (DDR4 + HBM)
Node Performance	> 3 TF	> 70 TF
Node Processors	Intel KNL + Intel Haswell	AMD EPYC (Milan) + Nvidia A100 GPUs
# of Nodes	9300 KNL + 1900 Haswell	1536 GPU Accelerated + 3072 CPU only
Intra-Node Interconnect	N/A	NVLink across GPUs; PCIe
Inter-Node Interconnect	Aries	Slingshot
Filesystem	28 PB, 0.75 TB/s	35PB All-Flash; > 4TB/s

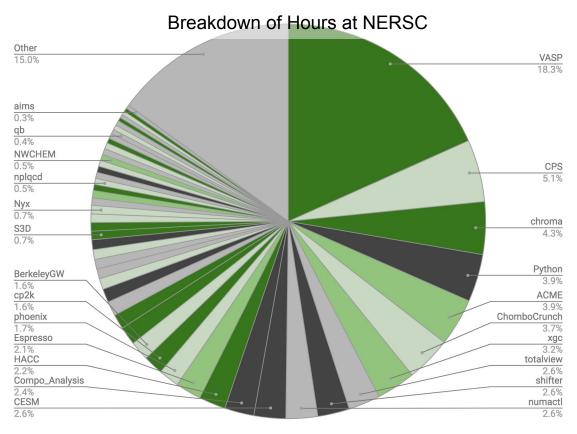






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### GPU Readiness Among NERSC Codes (Aug'17 - Jul'18)



GPU Status & Description	Fraction
Enabled: Most features are ported and performant	32%
<b>Kernels:</b> Ports of some kernels have been documented.	10%
<b>Proxy:</b> Kernels in related codes have been ported	19%
<b>Unlikely:</b> A GPU port would require major effort.	14%
Unknown: GPU readiness cannot be assessed at this time.	25%

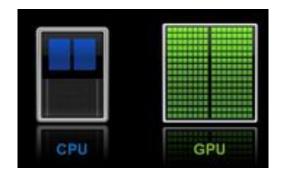
A number of applications in NERSC workload were GPU enabled already. We leveraged existing GPU codes from CAAR + Community

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## NESAP Motivation: CPUs vs GPUs

### CPU (Haswell)

- 64 cores
- 2 threads each
- 2x256-bit vectors
- double precision
  - ~2000 way parallelism (64\*4\*8)



### GPU (A100)

- 108 SM
- Up to 64 warps per SM (2 active at a time)
- 32 SIMT per warp
- double precision
  - 200,000+ way parallelism
     (108\*64\*32)



GPU - Throughput



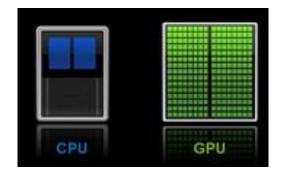




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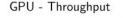
- 32 SIMT per warp
- double precision
  - 200,000+ way parallelism (108\*64\*32)

Oversubscribing GPUs (w/ Warps and Streams) helps hide latency, too!





CPU - Speed





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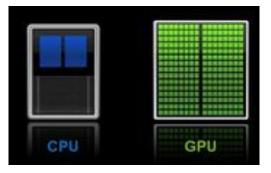




## GPUs vs. CPUs Memory Bandwidth

### CPU (Haswell)

- 128GB DDR
- ~120 GB/Sec Memory Bandwidth



### GPU (A100)

- 40GB HBM
- 1,500 GB/Sec Memory Bandwidth



PCIe ~ 32 GB/Sec

CPU - Speed

GPU - Throughput





Try to avoid moving data back and forth frequently







**Challenge** - There are Multiple GPU Optimization Avenues

- 1. You Need Orders of Magnitude More Parallelism
- 2. A100 GPU Memory is Very Fast. But, moving data to the GPU is Not.

Other Second Order Considerations:

- 3. There is some overhead in launching kernels. Fusing short kernels together and defining "CUDA Graphs" can help.
- 4. HBM is fast, but keeping data in registers, cache and "shared" memory is better! Find optimal balance between maximizing parallelism and minimizing register spills.

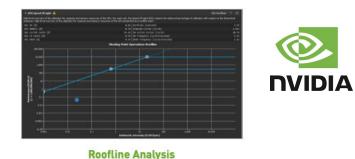




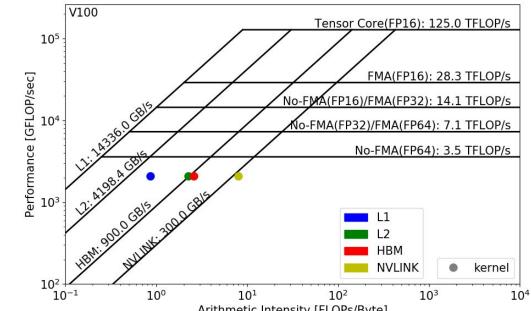


## **Determining Which Optimizations to Pursue**

Co Designing-Vendor Tools



NERSC worked closely with NVIDIA to design speed of light and roofline modeling in NVIDIA's NSIGHT profiler.



Arithmetic Intensity [FLOPs/Byte]







## **NESAP** Strategy

**NESAP** is NERSC's Application Readiness Program for preparing our workload for new systems.

**Strategy**: Partner with application development teams and vendors to port & optimize key applications of importance to the Office of Science. Share lessons learned with with NERSC community via documentation and training.

**Resource Available to Teams**: NERSC Staff technical liaisons, performance postdocs, access to vendor application engineers, hackathons, early access to hardware (GPU nodes on Cori and Perlmutter)

Simulation: 14 application teams Data: 9 applications Learning: 5 applications







## This was an all hands on deck activity!



Jack Deslippe (NESAP Lead)



Brandon Cook (Simulation Area Lead)



Johannes Blaschke (Data Area Lead)



Steve Farrell (Learning Area Lead)



Lisa Gerhardt (User Int lead)

Paul Lin (Early Science

Lead)



Stephen Leak (PE Lead)

Hannah

Ross

Rahul

Gayatri

Woo-Sun Yang



Chris

Dalev

Neil Mehta



16

Phillip

Thomas

Zhengji Zhao



Amanda

Dufek

Helen He Training



Kevin Gott



**Rollin Thomas** (Hackathons) (Jupyter)



Laurie Stephev (Python)











Bjoern Enders



Muaaz Awan

(Math Libs)

Wahid **Bill Arndt** Bhimii

### Hackathons Have Been Effective for Reaching Code Teams

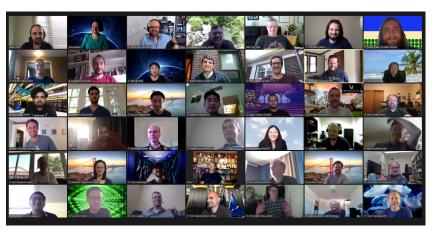
"Hackathons" have proven to be a highly effective tool for preparing applications for new architectures.

#### NERSC Supports Two Types of Hackathons:

- Private N9 Project COE Hackathons
   Quarterly with 2-3 NESAP teams + Cray and NVIDIA engineer
   support. Project controlled and focused on FOM
   optimizations. 12 conducted!
- 2. Public GPU Hackathons (<u>https://www.gpuhackathons.org</u>) NERSC provided more team mentors than any other institution to worldwide events.

Allows us to reach NERSC teams all around the country and world - **amplifies NESAP impact to the broad NERSC workload**.





NERSC adapted the hackathon format for the COVID work-from-home environment. Instead of on-site, multiple-day, full-day sessions, we moved to a series of shorter sessions spread out over 6-8 weeks. Some features of this format were popular and effective and we plan to incorporate them into future hackathons.





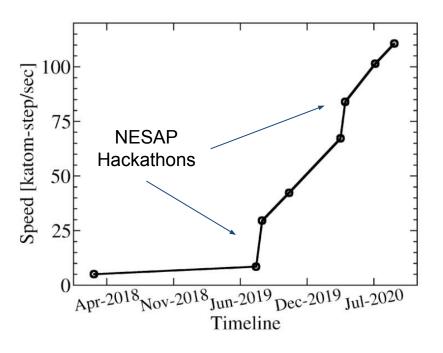


## NESAP Had a Big Impact on Applications (Example)

#### LAMMPS

- LAMMPS is a classical molecular dynamics code with a focus on materials modeling
- Production LAMMPS Kokkos version was highly optimized over a series of hackathons (joint effort of NERSC/NESAP, ECP, NVIDIA and HPE)
- Every kernel was rewritten and optimized individually
- SSI (system-wide throughput increase over Edison) in atom-steps/second

SSI:	35.3
Node vs Node Speedup:	171



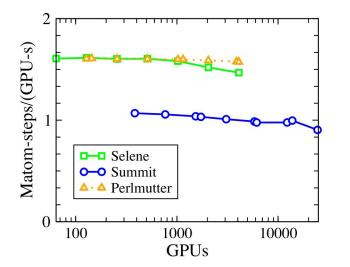


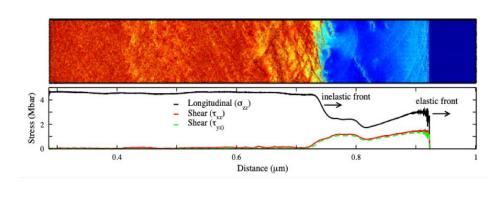




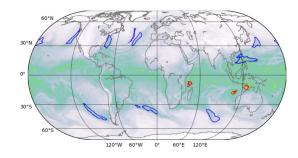
### Record Scale MD With LAMMPs Gordon Bell Finalists

- Collaborative effort: University of South Florida, Sandia, NERSC and NVIDIA
- Billion atom molecular dynamics simulation (20B atoms)
  - SNAP quantum-accurate machine learned interatomic potential
  - Kokkos CUDA backend for NVIDIA GPUs
- Simulation model shock compression of carbon at extreme pressures and temperatures.





## **NERSC Staff Gordon Bell Finalists/Winners**

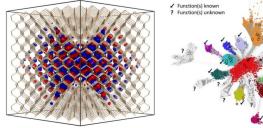


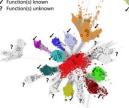
2018 (Winners): Climate/AI

2020 (Finalists): **Materials** 

Thorsten Kurth, Jack Deslippe, Mr. Prabhat

Charlene Yang, Mauro Del Ben, Jack Deslippe





2021 (Finalists): Molecular Dyn./Al

2022 (Finalists): **Bio-Informatics** 

2022 (Winner):

**Accelerator Physics** 

Muaaz Awan

Kevin Gott

Rahul Gayatri





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## **Observations**

- Many applications have been successful is preparing for Perlmutter
- We'd like to keep engaging with the broad NERSC community to enable it to use Perlmutter productively
  - We are continuing to encourage everyone to join community hackathons at GPUHackathons.org events all over the country in the next year
- Multiple GPU optimization angles exist. Profiling and roofline modeling are key to determining optimization paths.
- The scientific community is motivated to optimize their codes for GPUs.







## Perlmutter Supports Every GPU Programming Model

	Fortran/ C/C++	CUDA	OpenACC 2.x	OpenMP 5.x	CUDA Fortran	Kokkos / Raja	ΜΡΙ	HIP	DPC++ / SYCL
NVIDIA									
CCE									
GNU									
LLVM									

Vendor Supported Supported







### The System Has a Robust Programming Environment



DDT

GDB (CUDA-GDB)

Profilers
NSIGHT
CrayPat
Tensorboard







## Getting started with GPUs in Python

NumPy and SciPy do not utilize GPUs out of the box

- There are many Python GPU frameworks out there:
- "drop in" replacements for numpy, scipy, pandas, scikit-learn, etc 0
  - **CuPy**, **RAPIDS**, **cuNumeric** (coming soon?)
- "machine learning" libraries that also support general GPU computing
  - PyTorch, TensorFlow
- "I want to write my own GPU kernels"
  - Numba, PyOpenCL, PyCUDA
- Many of these GPU libraries have adopted the <u>CUDA Array</u> Interface which makes it easier to share array-like objects stored in GPU memory between the libraries
- There is also some effort in the community to standardize around a common Python array API



numpy:	<pre>mean(a, axis=None, dtype=None, out=None, keepdims=<no value="">)</no></pre>
dask.array:	<pre>mean(a, axis=None, dtype=None, out=None, keepdims=<no value="">)</no></pre>
cupy:	<pre>mean(a, axis=None, dtype=None, out=None, keepdims=False)</pre>
jax.numpy:	<pre>mean(a, axis=None, dtype=None, out=None, keepdims=False)</pre>
mxnet.np:	<pre>mean(a, axis=None, dtype=None, out=None, keepdims=False)</pre>
sparse:	<pre>s.mean(axis=None, keepdims=False, dtype=None, out=None)</pre>
torch:	<pre>mean(input, dim, keepdim=False, out=None)</pre>
tensorflow:	<pre>reduce_mean(input_tensor, axis=None, keepdims=None, name=None,</pre>

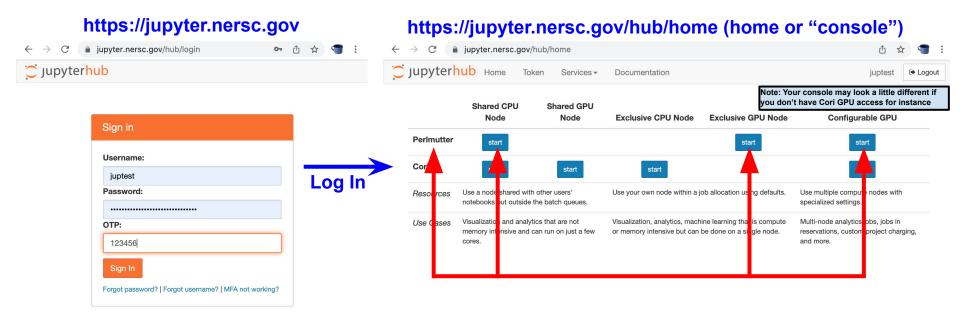






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### How do I run Jupyter notebooks on Perlmutter









### The Programming Environment Supports All Major GPU Prog. Models

- The NVHPC, GCC, CCE and LLVM (Clang) compilers provide additional support for applications. NERSC Staff are part of ECP Flang (in testing)
- **OpenMP 4.5/5.x** support has been enabled in NVHPC through NERSC NRE
- NERSC is a member of the **OpenACC** board. Supported in multiple compilers.
- **DPC++** supported on Perlmutter enabled via CodePlay NRE (LLVM)
- NERSC participating in ECP **HIP** project Enabling/Testing on Perlmutter
- Kokkos works well on the system. Multiple NERSC Staff members are part of the ECP Kokkos team.







## Broad impact and enablement

Perlmutter Supports all Major Programming models and languages



Pre-installed/Optimized Community Codes

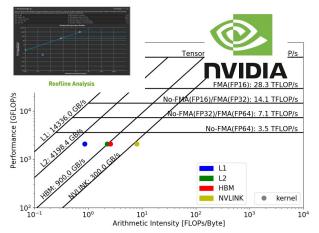


Community Resources

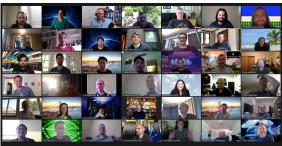
NERSC Documentation



#### Co Design-Vendor Tools



#### Community GPU hack-a-thons









NERSC Invested in Performance Portable Programming with OpenMP & DPC++ NRE (Off Project)

• **OpenMP 4.5/5.x** support has been enabled in NVHPC through NERSC NRE

Multi-Year NRE that Utilized NESAP and ECP applications for testing

Settled on a well-defined subset of the OpenMP standard for optimized GPU acceleration

Released in production NVHPC SDK

• **DPC++** supported on Perlmutter enabled via CodePlay NRE (LLVM)

Multi-Year NRE in collaboration with ALCF to enable optimized DPC++ execution on A100.

Based on Open-Source LLVM and available to use on Perlmutter





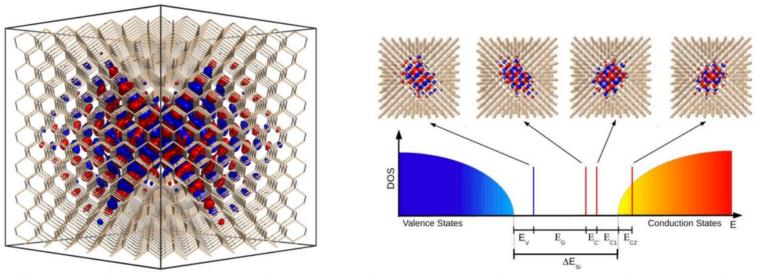


## Science Examples





## **Qubit Design With BerkeleyGW**



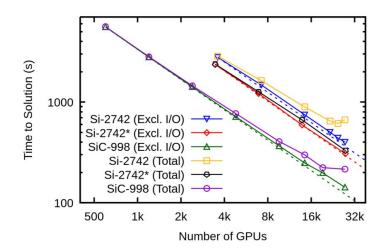
Example: Divacancy point defect in crystalline silicon, prototype of a solid-state Qubit

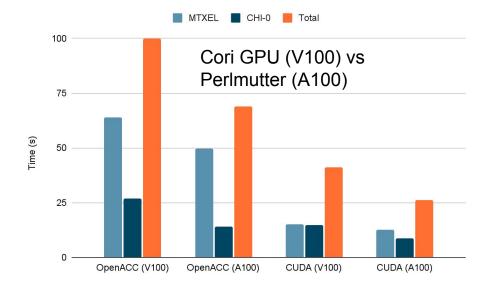
Accurate prediction requires:

- Accuracy beyond DFT: GW and GW+BSE
- Unprecedented simulation sizes: 1000's of atoms

## **Qubit Design**

The BerkeleyGW NESAP team was recognized as a Gordon Bell finalist in 2020.



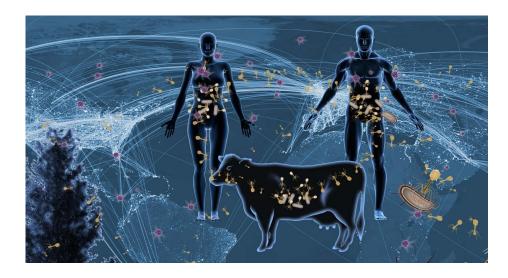


	MTXEL	CHI-0	Total
OpenACC (V100)	64	27	100
OpenACC (A100)	49.8	14.2	69
CUDA (V100)	15.2	14.7	41
CUDA (A100)	12.6	8.7	26.2

 Si-214 system (scaled: 4Ry CT; 3000 bands). 8 GPUs each.



### Exabiome (Meta-Genomics)



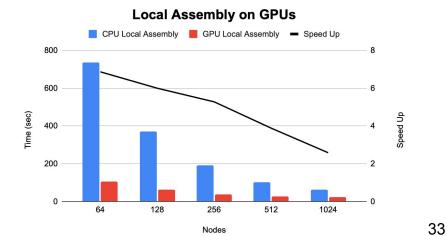


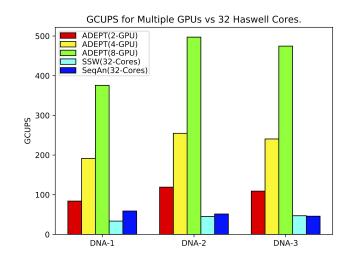
- Microbes: these are single cell organism, e.g. viruses, bacteria
- Microbiomes: communities of microbial species living in our environment.
- Metagenomics: genome sequencing of these communities.



### **Exabiome (Meta-Genomics)**

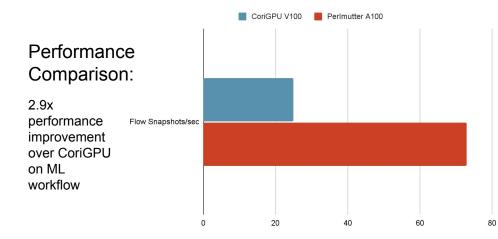
- A lot of progress has been made on GPU algorithms for meta-genomics.
- This NESAP team wrote the world's fastest GPU aligners using a lot of clever strategies, newly available GPU intrinsic instructions etc.
- With the help of warp level intrinsics, dynamic data structures were written for GPUs from scratch to re-write the Local Assembly stage.

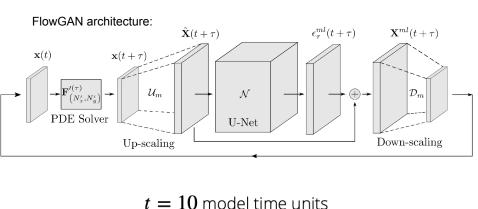


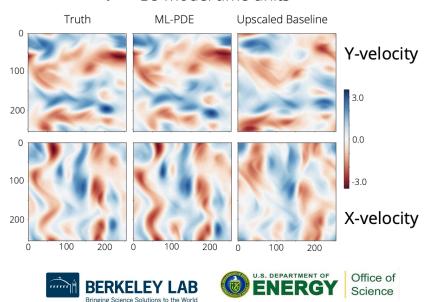


# Accelerating CFD with GANs on Perlmutter

The FlowGAN project introduces a technique based on a deep neural network architecture to augment traditional numerical simulations of fluid flows. The ML model is used to correct the numerical errors induced by a coarse-grid simulation of turbulent flows at high-Reynolds numbers.



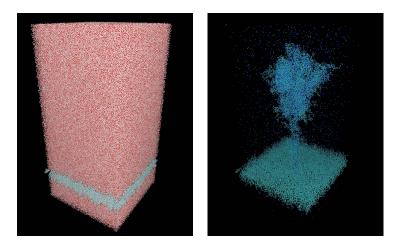




### Exaop Performance for the *Ab-Initio* Molecular Dynamics

Ground-breaking real-world exaop calculation in mixed FP16/32 run on Perlmutter

- The non-orthogonal local submatrix method applied to electronic-structure based molecular dynamics simulations exceeds 1.1 EFLOP/s in FP16/FP32 mixed floating-point arithmetic
- Used 4,400 NVIDIA A100 GPUs on Perlmutter
- The method achieves a sustained fraction of peak performance of about 80%.
- Example calculations are performed for SARS-CoV-2 spike proteins with up to 83 million atoms.



SARS-CoV-2 spike protein in aqueous solution: full cell (left) and without hydrogen and oxygen atoms (right).

Robert Schade, Tobias Kenter, Hossam Elgabarty, Michael Lass, Thomas D. Kühne, Christian Plessl, Paderborn University

arXiv:2205.12182v1 24 May 2022





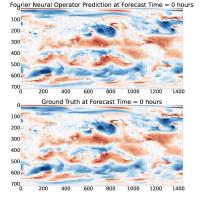
### Early Successes in Data/Learning

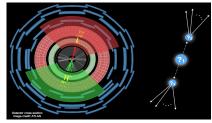
#### **DESC (Dark Energy Science Collaboration)**

- Using GPUs with Tensorflow, via Jupyter, for redshift model-fitting
- Distributed TF at scale on GPU w/ NCCL
- Tested up to 2048^3 N-body simulation, distributed on 256 GPUs
- Multiple TB of RAM

#### Data-driven Atmospheric Modeling

- ML Data-driven prediction of high-resolution atmospheric flow variables
- 2.9x improvement in throughput using Perlmutter A100 compared to Cori V100 GPUs





#### Anomaly Detection, Unfolding & Fast Simulation in Particle Physics

- DL techniques used in searches for fundamental particles at the LHC
- Expanding to more complex models/approaches and higher-fidelity generative networks

#### **Open Catalyst Project**

g Science Solutions to the World

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- Deep learning to accelerate catalyst discovery for reactions that are critical for energy storage and climate change mitigation
- Scaling current models from O(10-100) GPUs to O(1000) GPUs



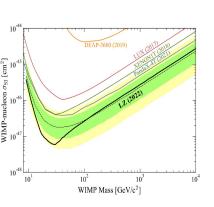
### Early Successes in Superfacility

#### LCLS

- Reconstruct molecular structure form X-Ray scattering data
- Used Perlmutter for live data processing (ie., determining molecular structures during data collection), enabling real-time steering of the experiment

#### Lux-Zepplin (LZ)

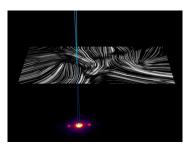
- Dark matter detection experiment used GPUs for<sup>1</sup> ray tracing in detector simulation
- Used Perlmutter to extract Imits on dark matter-nucleon interaction
   for first science results



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#### NCEM

- Multi-TB scale electron microscopy image simulation to train NN for materials research
- VASP to calculate XAS spectra to train a ML model for automated assignment of bond valence
- Real-time processing and reduction of 4D-STEM data with distiller.lbl.gov



#### Dark Energy Spectroscopic Instrument

- DESI Spectral Extraction is an image processing code implemented in Python.
- 2.5x improvement in per-node throughput using Perlmutter A100 compared to Cori V100 GPU (x25 compared to Edison).









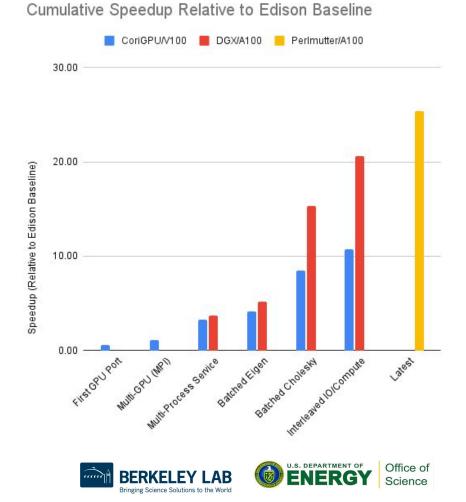
## Questions?



## DESI

### Dark Energy Spectroscopic Instrument

- DESI Spectral Extraction is an image processing code implemented in Python.
- Completed major refactor of optimized CPU code and initial GPU port in early 2020.
- Major optimization milestones include: saturating GPU utilization using MPI and CUDA Multi-Process Service, refactoring code to leverage batched linear algebra operations on GPU, and interleaving IO with computation.
- **25x** improvement in per-node throughput using Perlmutter compared to Edison baseline.

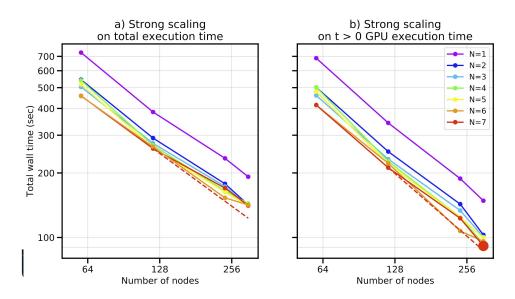




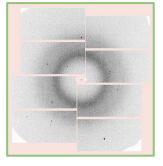
### ExaFEL

XFEL requires **real-time data analysis** to make decisions **during ongoing experiments**. Data collection rates outpacing computational resources at the experimental sites, **requiring a Superfacility approach**.

In two years, NESAP has developed a highly scalable CUDA/GPU application. CCTBX/nanoBragg w/ runtime improved from 12.3 hours on Edison, to 2 minutes



**CCTBX/nanoBragg** strong scaling on Summit. Colored lines show number of concurrent streams per GPU



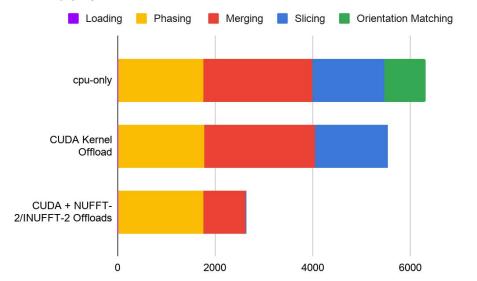
Bringing Science Solutions to the World



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### ExaFEL

NESAP has been essential in **developing a scalable version of the MTIP algorithm** (figure, right). By offloading kernels to CUDA, **MTIP/Spinifel runtime was decreased by 2.4x over CPU-only code**.



#### Time (s) spent in different modules

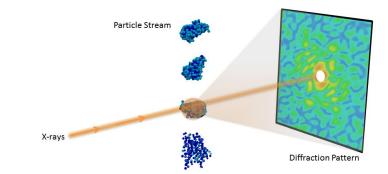
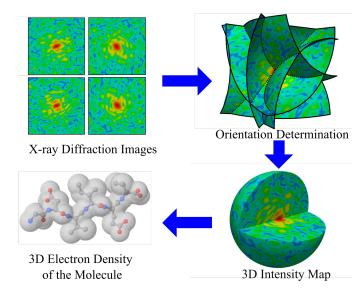


Illustration of **SPI technique**: the X-ray beam interacts with only a few molecules a time



8000

## Large Scale Combustion Modeling w/ Pele

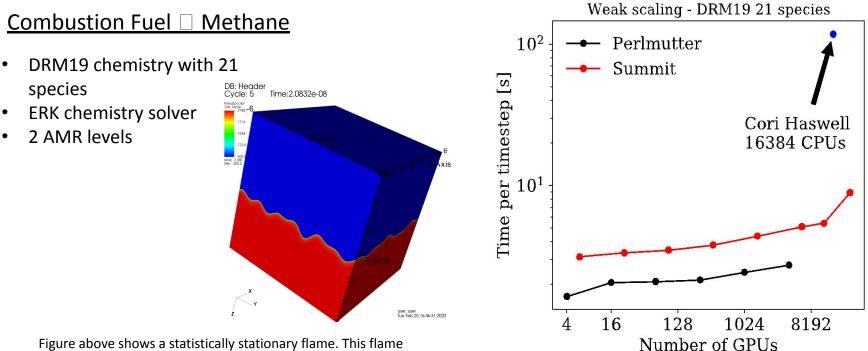


Figure above shows a statistically stationary flame. This flame configuration has been extensively used in DNS calculations and in this case it is used for scaling tests.

The configuration can be easily reproduced with different chemical

NERSC





## NERSC, ALCF and Codeplay partnership on SYCL

- Target SYCL 2020 (latest specification) support on Ampere A100 GPUs
- Open LLVM based compiler
- Provides Portability for Apps Developed for Aurora
- Extensions for A100
  - Asynchronous Copy
  - Asynchronous Barrier
  - Tensor core types/ APIs



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#### NERSC, ALCF, Codeplay Partner on SYCL for Next-generation Supercomputers

#### FEBRUARY 3, 2021 Contact: cscomms@lbl.gov

The National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (Berkeley Lab), in collaboration with the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory, has signed a contract with Codeplay Software to enhance the LLVM SYCL™ GPU compiler capabilities for NVIDIA® A100 GPUs.

This collaboration will help NERSC and ALCF users, along with the high-performance computing community in general, produce high-performance applications that are portable across compute architectures from multiple vendors.

Codeplay is a software company based in the U.K. that has a long history of developing compilers and tools for different hardware architectures. The company has been the lead implementor of SYCL compilers and a main contributor to the existing open source support for NVIDIA V100 GPUs through the DPC++ project. NVIDIA A100 GPUs are available in the ThetaGPU extension of ALCF's Theta and will power NERSC's next-generation supercomputer, Perlmutter.







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