MEIFENG LIN
BROOKHAVEN NATIONAL LABORATORY

# COMPUTATIONAL SCIENCE INITIATIVE

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NATIONAL LABORATORY

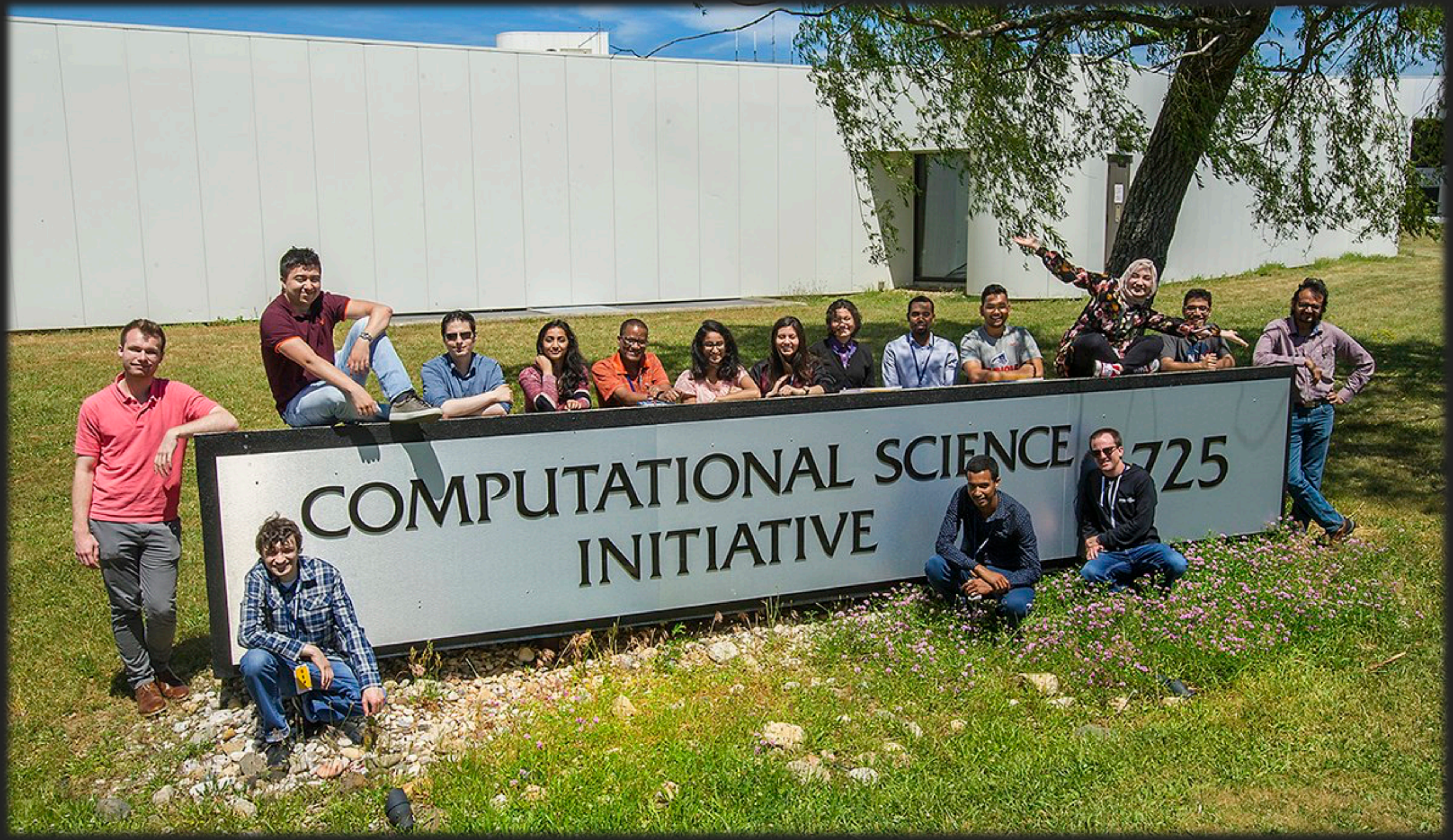
# OUTLINE

- BNL/CSI Overview
- HPC Project Highlights
- Some Comments/Thoughts on Exascale Computing
- Some Side Notes

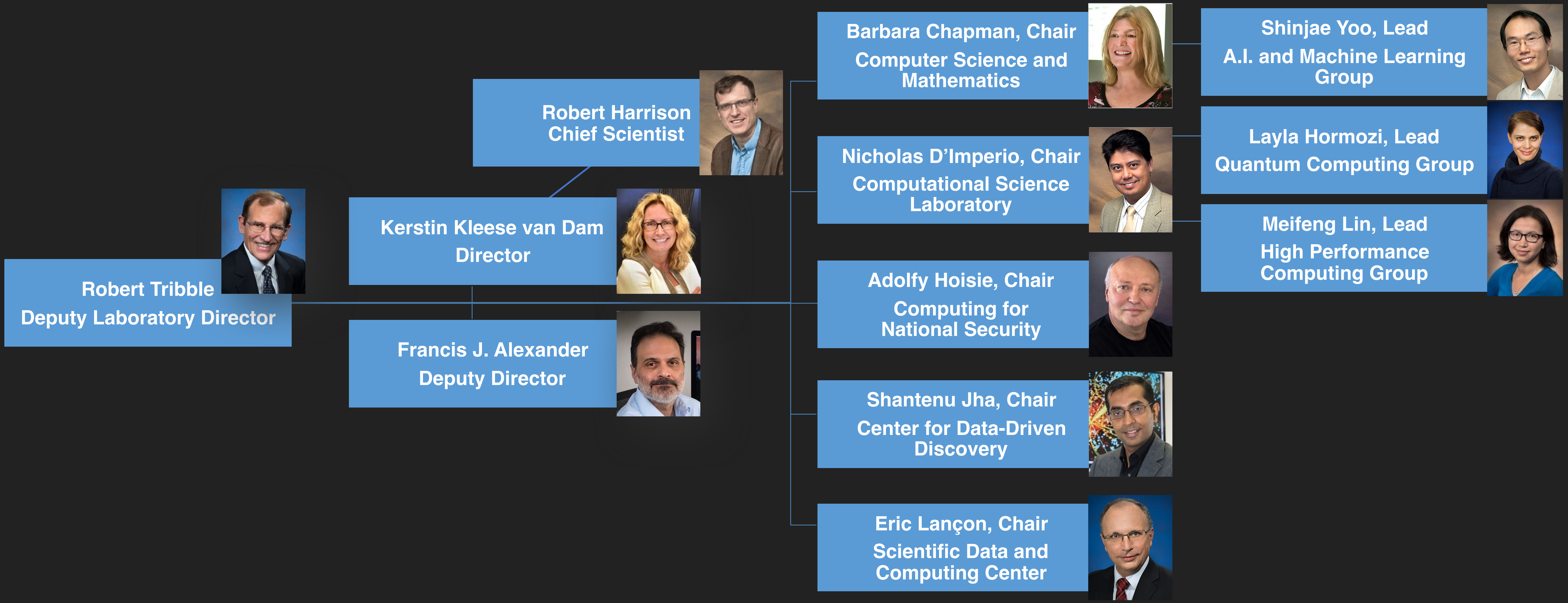
# COMPUTATIONAL SCIENCE INITIATIVE



- Established in 2015
- An umbrella to bring together computing and data expertise across BNL
- Aims to foster interdisciplinary collaborations in domain sciences, computer science, applied math and data analytics.
- **Focus areas:**
    - High performance and novel computing, including quantum computing
    - Data analytics at scale, incl. scalable machine learning, visual analytics, workflow, provenance, etc.
    - State-of-the-art computing and storage facility
- 5 departments, ~50 staff members and growing!



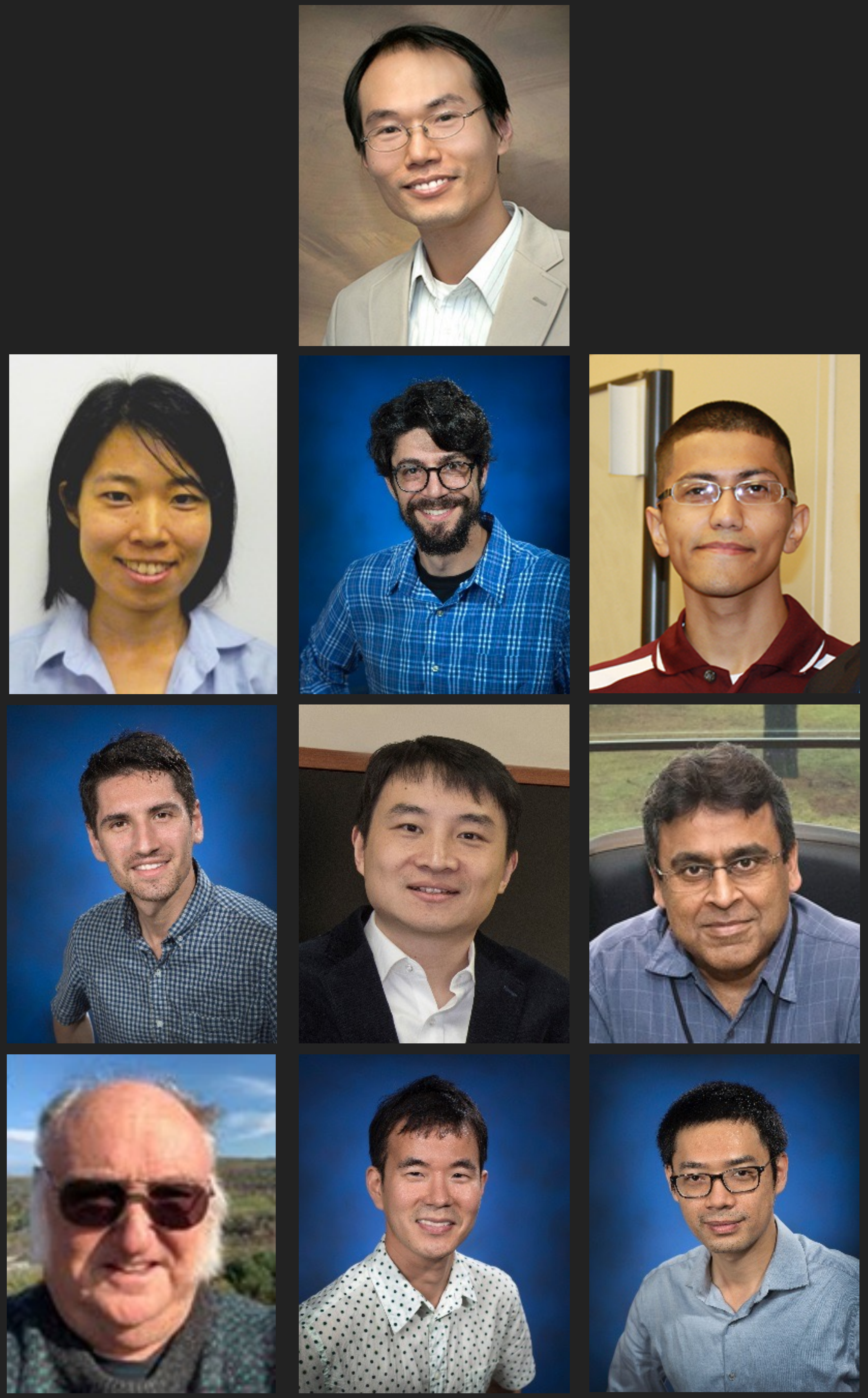

# CSI ORGANIZATIONAL STRUCTURE



# MACHINE LEARNING AND A.I. GROUP



- Group Lead: Shinjae Yoo
- Specific Focus:
  - Real-Time Analysis of Experimental Data (NSLS II, CFN, Cryo-EM, Solar Power)
  - Causal Analysis (Biology, Power Grid)
  - Natural Language Processing for Science
  - Robustness, Explainability, Reproducibility
  - Quantum Machine Learning



# NEW QUANTUM COMPUTING GROUP

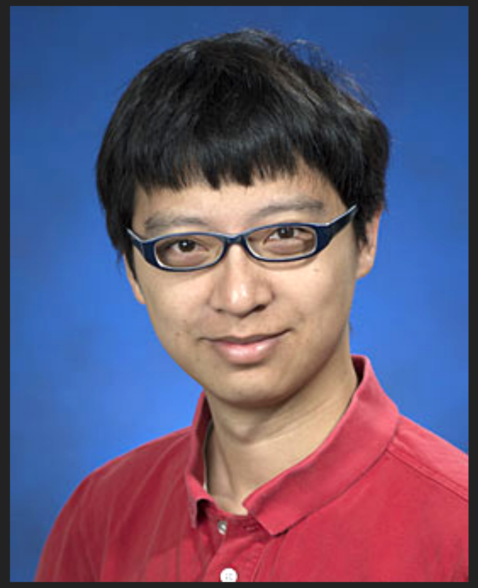


- Group Lead: Layla Hormozi
- Specific Focus:
  - Quantum Networking
  - Connecting Quantum Networking and Quantum Computing
  - Optimized Quantum Algorithm Development for Nuclear, High Energy, and Condensed Matter Physics
  - Quantum Error Characterization and Correction





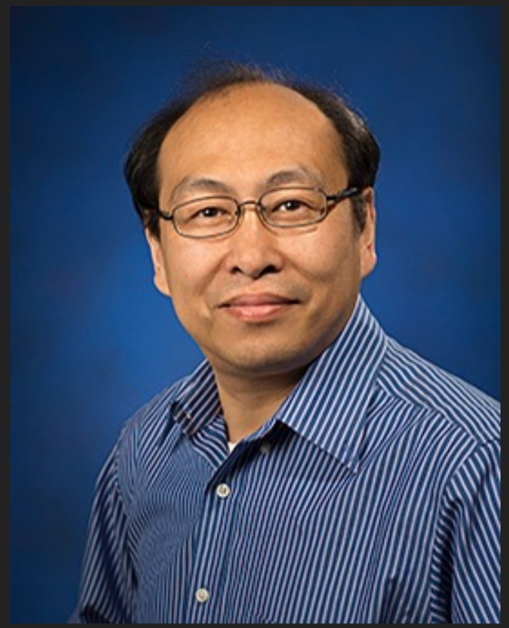


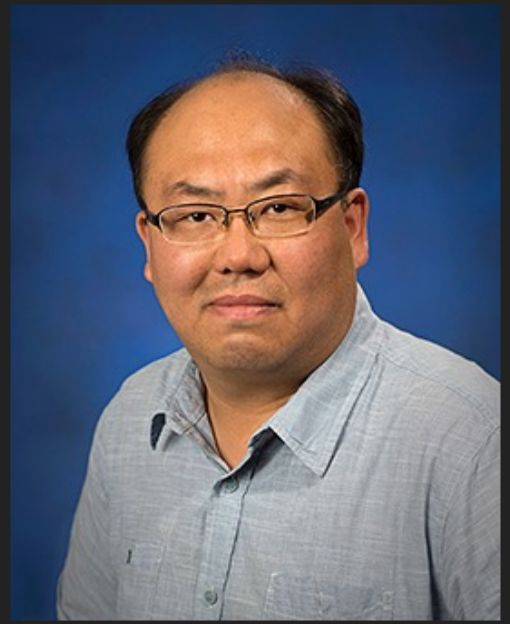


# HIGH PERFORMANCE COMPUTING GROUP



- Group Lead: Meifeng Lin
- The High Performance Computing Group at CSI help the scientists get their codes to run on modern computing architectures
- Research domains range from materials science, quantum chemistry, high energy and nuclear physics, climate science, etc.
- Making use of state-of-the-art software tools and hardware architectures:
    - Performance profiling, analysis and modeling
    - MPI, OpenMP, OpenACC, …
    - CUDA, HIP, SyCL, …
    - Performance portable frameworks





# HPC PROJECT HIGHLIGHTS

# HPC for NSLS II: X-ray Ptychographical Image Reconstruction via Distributed & GPU Computing


**Leo Fang** CSI | Zhihua Dong CSI | Xiaojing Huang NSLS-II | Hanfei Yan NSLS-II | Sungsoo Ha CSI | Wei Xu CSI | Yong Chu NSLS-II | Stuart Campbell NSLS-II | Meifeng Lin CSI


References:


1. Dong *et al.*, NYSDS 2018 (arXiv:1808.10375)
2. Fang *et al.*, "*Accelerated Computing for X-ray Ptychography at NSLS-II*", book chapter in "*Handbook on Big Data and Machine Learning in the Physical Sciences*"
3. Fang *et al.*, in preparation


Work supported by BNL LDRD #17-029, and in part by DOE BES

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# REAL-TIME ANALYSIS AND STEERING OF EXPERIMENTS

- Facility users at CFN and NSLS II typically have limited time allocated.
- Getting the right setup of the experiments often takes trial-and-error.
- Brighter light sources mean faster data rates and larger data volumes.
  - Analyzing data could take a long time
  - Affects the number of experiments users can do
- Need to improve *in-situ* data analysis tools
  - Speed - HPC
  - Usability - intuitive GUI
  - Maintainability - high-level programming abstractions

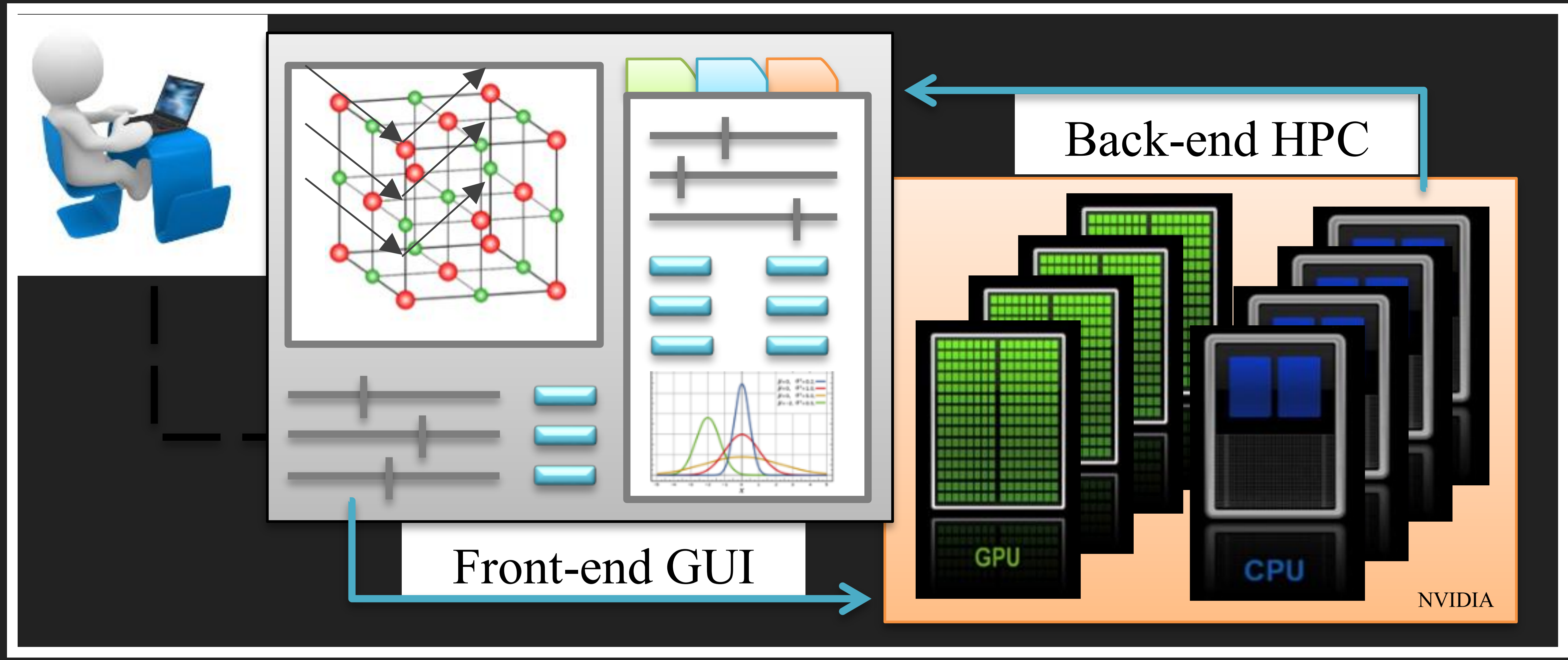
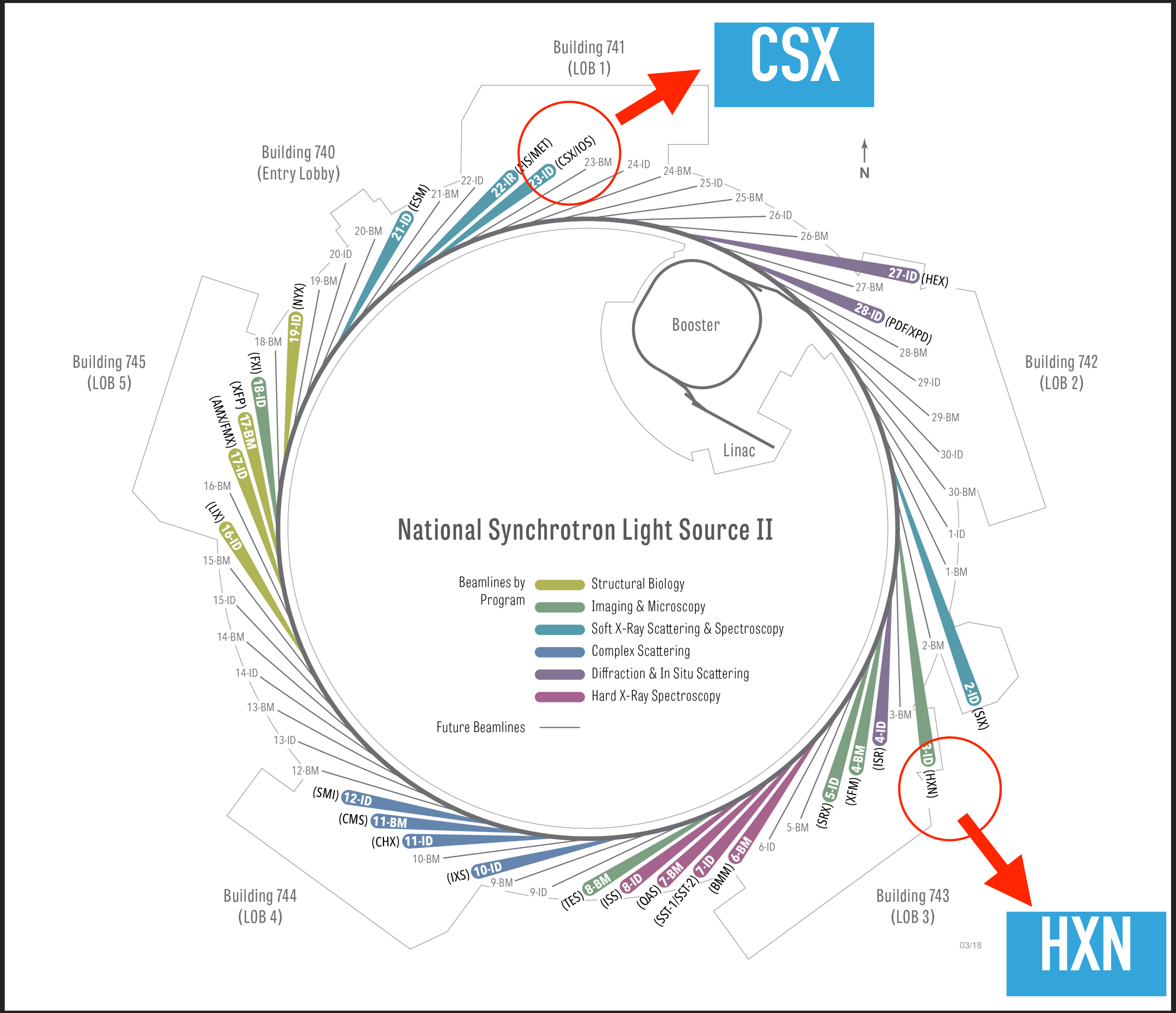



Image Credit: Wei Xu

# NSLS II



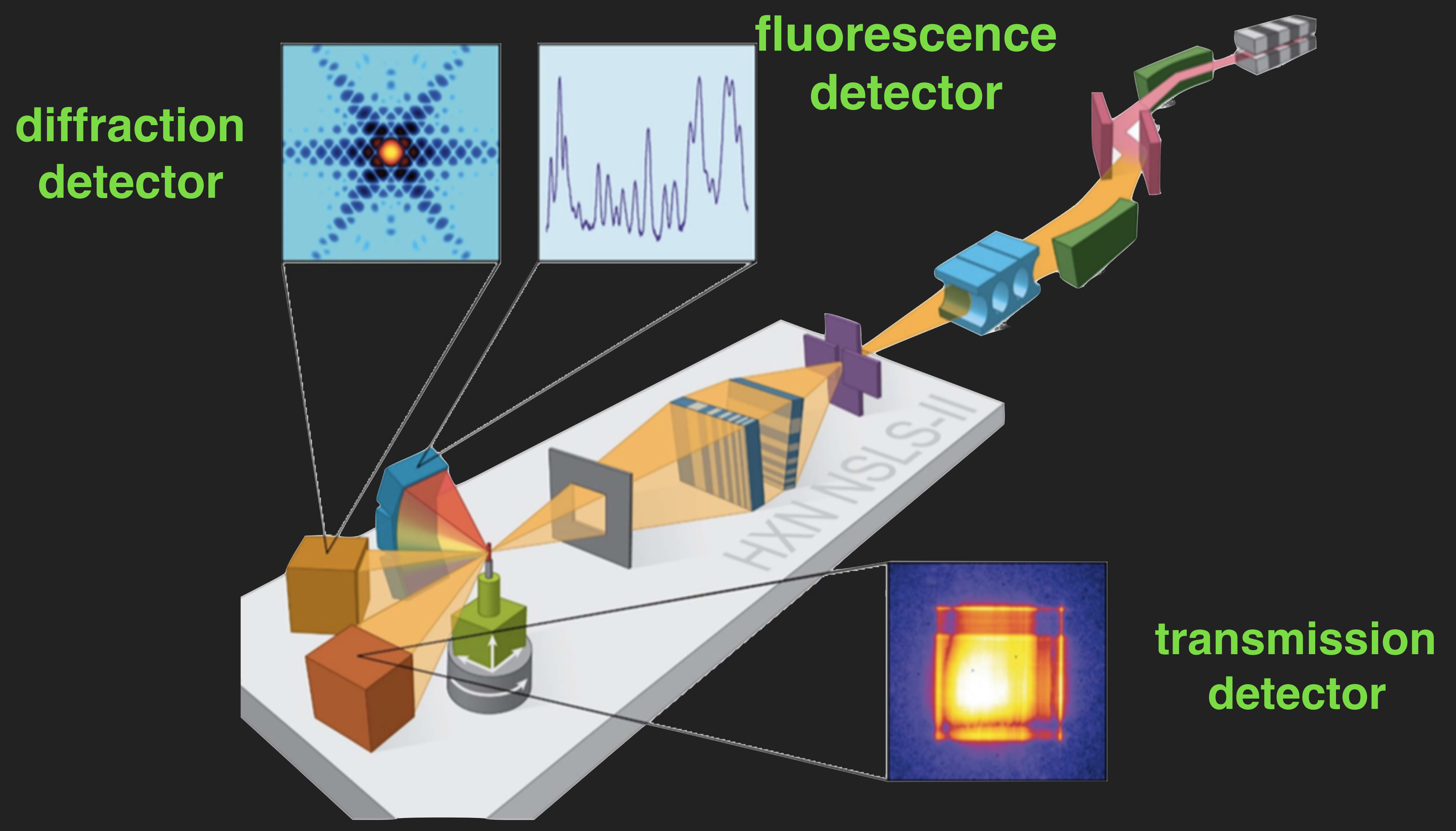
- NSLS II - National Synchrotron Light Source II (there was an NSLS at BNL - now CSI)
- State-of-the-art, medium-energy (3-billion-electron-volt, or GeV) electron storage ring that produces x-rays up to 10,000 times brighter than the NSLS
- First light: 2014
- 28 beam lines in operation; 1 under development
- HXN - Hard X-ray Nanoprobe
- CSX - Coherent Soft X-ray Scattering



# DATA AND COMPUTATION CHALLENGES



- Ptychography reconstruction at HXN
  - Typically O(10,000) - O(100,000) scan images
  - ~200x200 pixels (in floating points) per image
  - Data size of <u>input</u> images:  O(1GB) to O(10 GB)
- Memory requirements for the DM algorithm (including temporary buffers):
  - Single-mode: >4x of input size
  - Multi-mode: >10x of input size
  - **Need multiple GPUs for sufficient memory**
- Difference map iterative algorithm: O(100) iterations
- **Serial Python code:** typically takes hours, and sometimes days (e.g., multislice reconstruction), to complete one ptychography reconstruction.




Yan et al., Nano Futures 2, 011001 (2018)

# NSLS-II PTYCHOGRAPHY SOFTWARE – CURRENT STATUS



- Fully Python-based (numpy + scipy + …) software stack
- ➡ for easy integration with NSLS-II control, data acquisition & analysis environment (databroker, bluesky, ophyd, etc)
- CPU version: **mpi4py** + numpy
- GPU version: **mpi4py + cupy + numba**
- Computationally intensive functions rewritten in CUDA C and/or Numba
- Graphical user interface (GUI) provided
- Already deployed in production at HXN & CSX beamlines

# USING CUPY WITH NUMBA



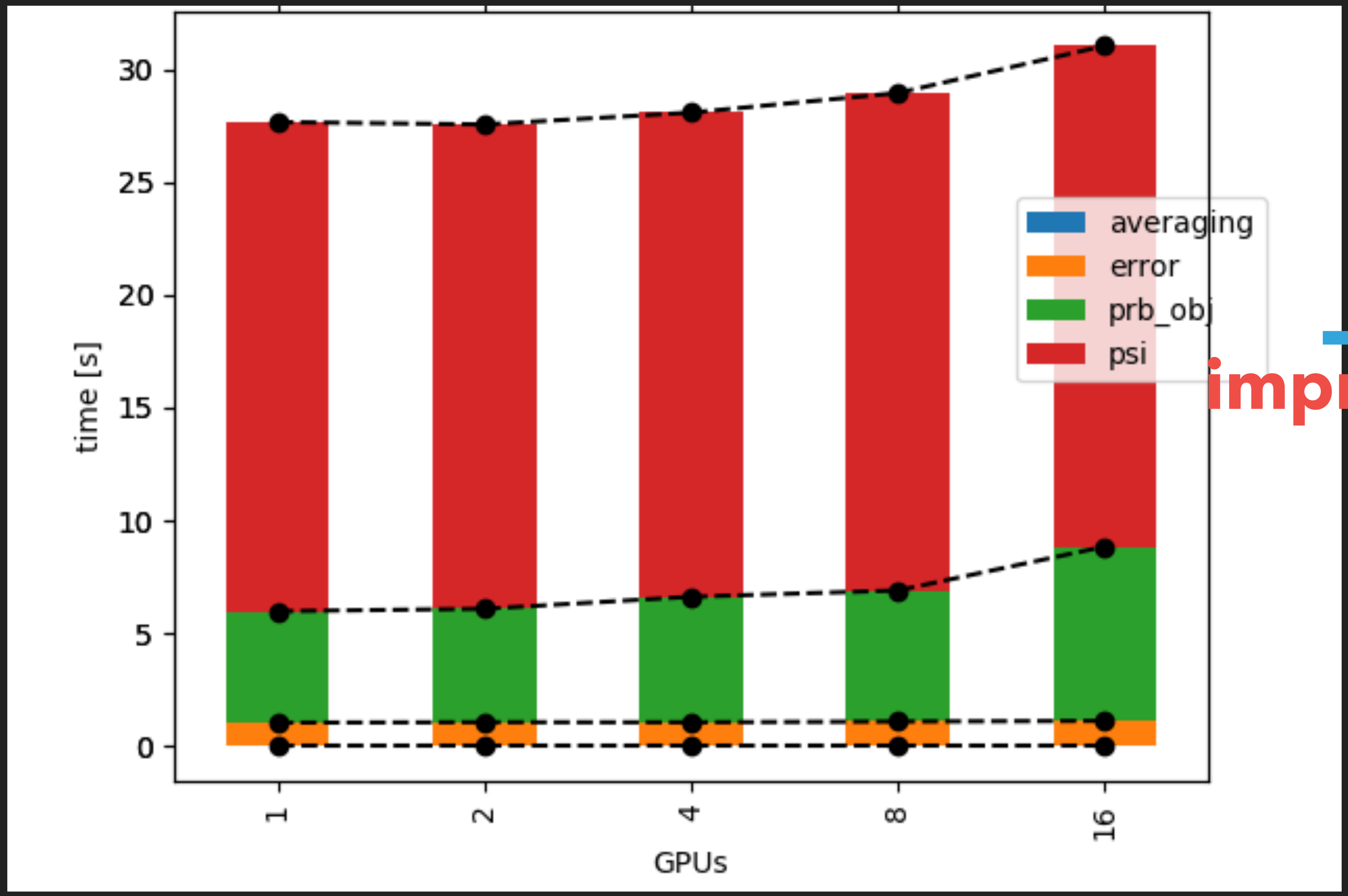
- Use CuPy to create and manage GPU arrays
- Use numba to JIT compile CUDA kernels - no need to write raw CUDA C kernels

```
@cuda.jit()
def accumulate_obj(prb_norm_d, obj_upd_d, prb_sqr_d, prb_conj_d, product_d,
point_info_l, start, batch):
    x, y, z = cuda.grid(3)
    x_max = int32(product_d.shape[-2])
    y_max = int32(product_d.shape[-1])
    if x < x_max and y < y_max and z < batch:
        x_start = point_info_l[start+z, 0]
        y_start = point_info_l[start+z, 2]
        temp = prb_conj_d[x, y] * product_d[start+z, 0, 0, x, y]
        cuda.atomic.add(prb_norm_d, (x_start+x, y_start+y), prb_sqr_d[x, y])
        cuda.atomic.add(obj_upd_d.real, (x_start+x, y_start+y), temp.real)
        cuda.atomic.add(obj_upd_d.imag, (x_start+x, y_start+y), temp.imag)
```

# RESULTS: WEAK SCALING*

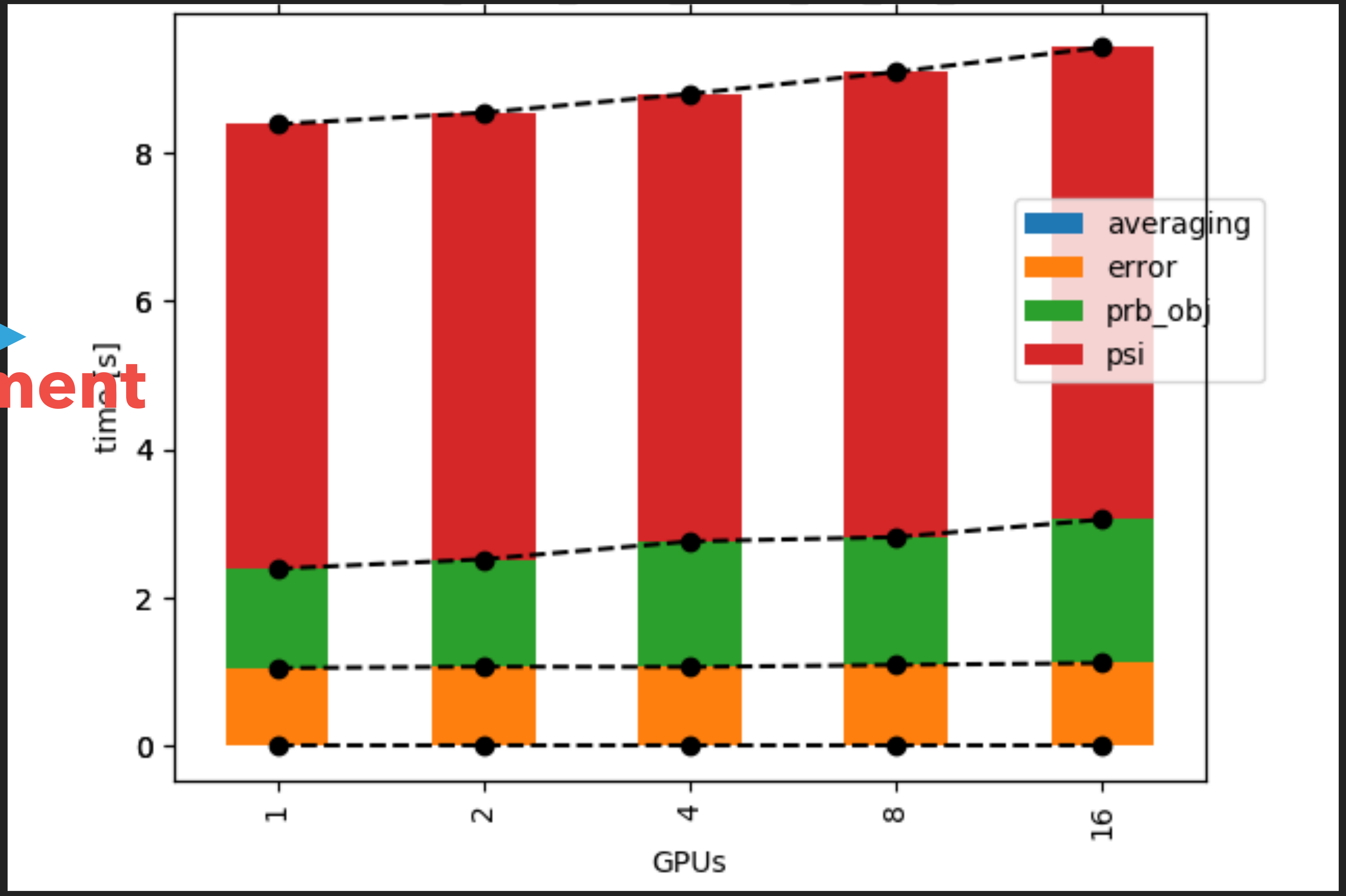


pure CuPy implementation




3X improvement

CuPy arrays + Numba kernels




Pure CuPy is suitable for quick prototyping
performance is reasonable but still much slower than CUDA/numba

* tested on single DGX-2 with single precision + **no mode** + CuPy v6.1.0 + Open MPI 4.0.1 + NCCL v2.4.2-1
* Test data size: 5000 images per GPU (each image 200x200 pixels)

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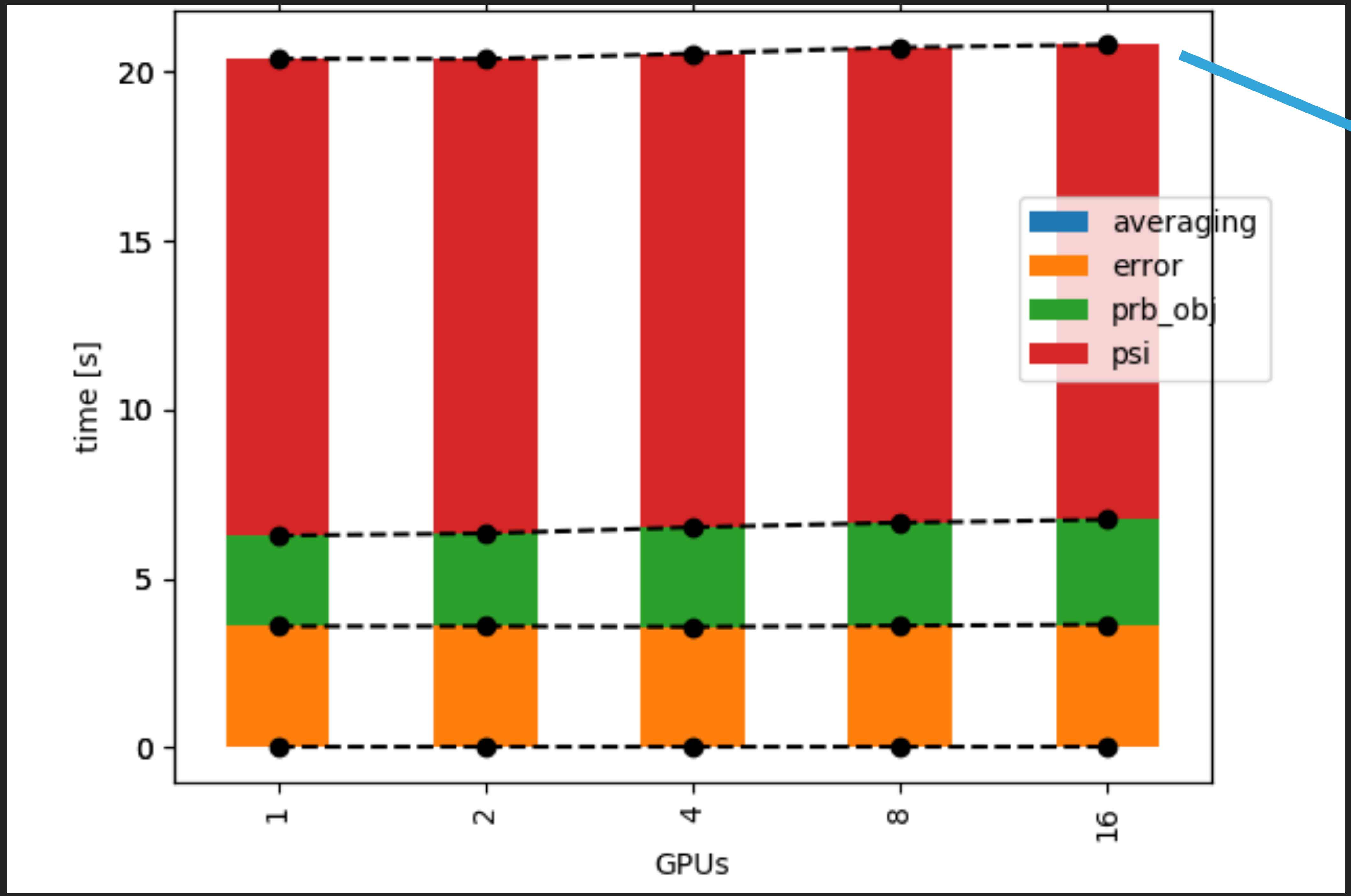
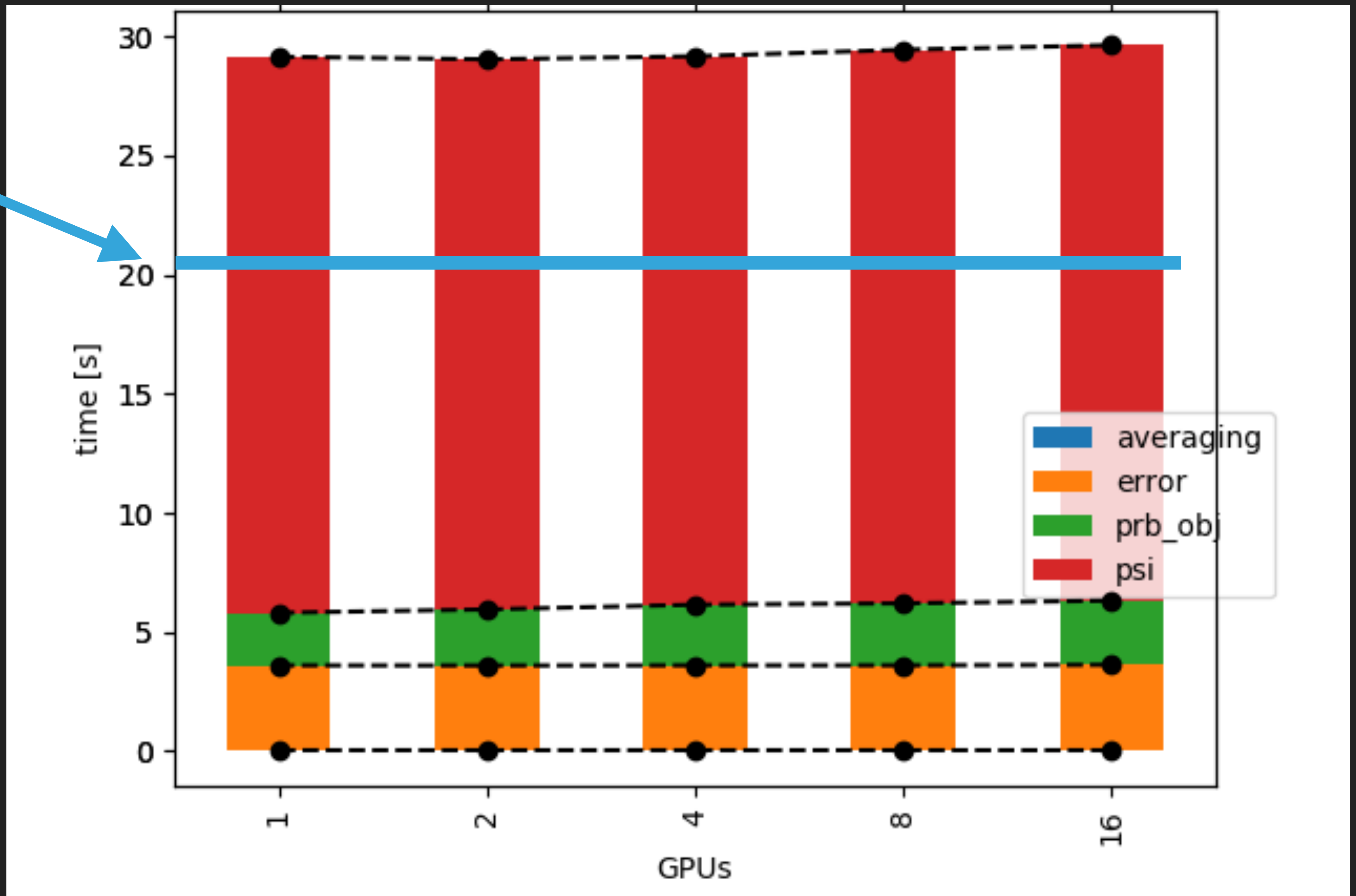
# RESULTS: WEAK SCALING



## CuPy arrays + CUDA kernels




## CuPy arrays + Numba kernels




CuPy + Numba is enough for further performance boost
(~50% slower than CUDA C)

* tested on single DGX-2 with single precision + **5 modes** + CuPy v6.1.0 + Open MPI 4.0.1 + NCCL v2.4.2-1
* Test data size: 5000 images per GPU (each image 200x200 pixels)

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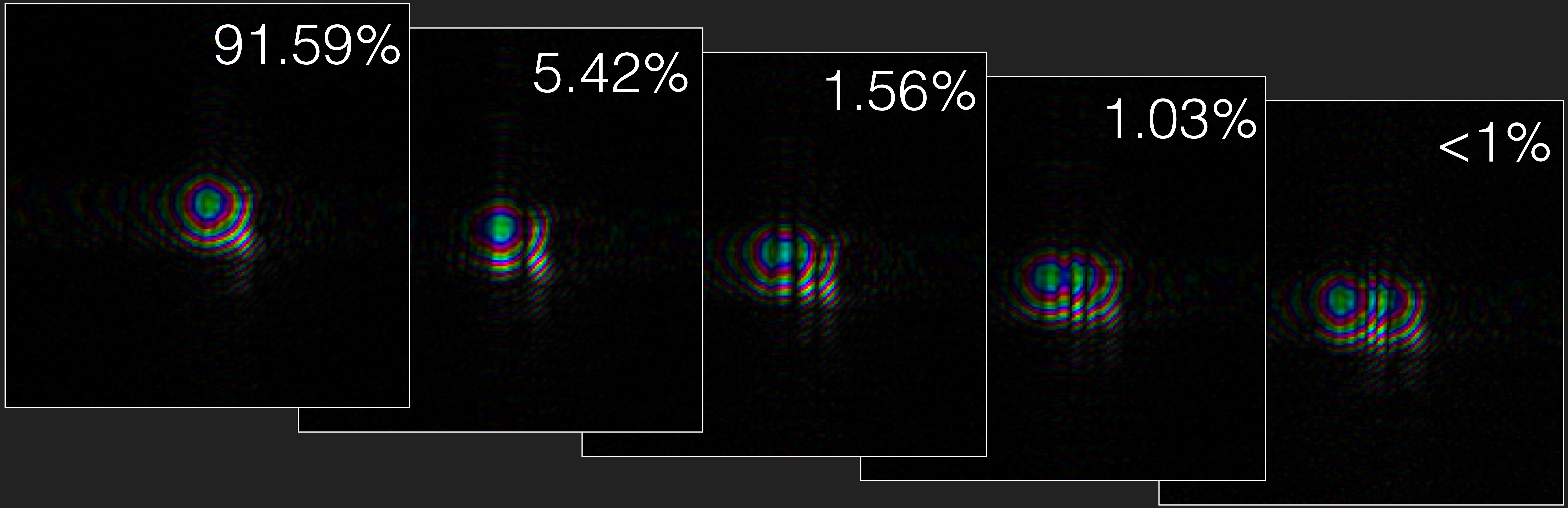
# RESULTS: GALLERY

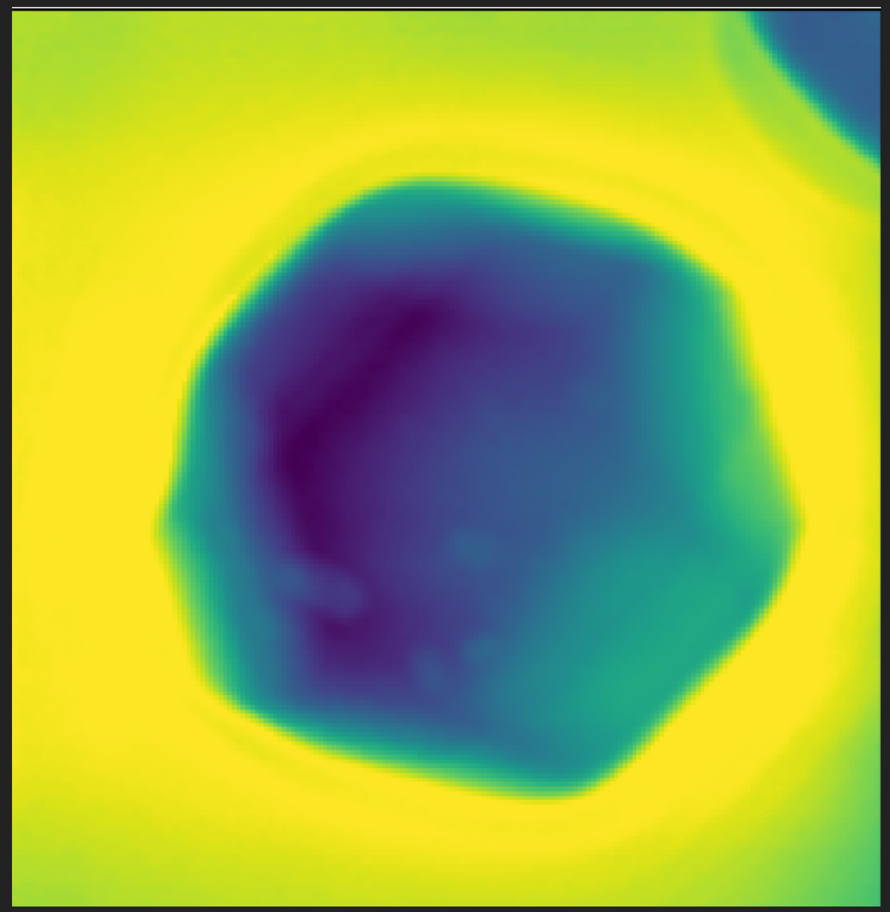


showcase: gold nano-crystal with multi-mode

Test machine: xf03id-srv5@HXN, Intel Xeon CPU E5-2630 v4 @2.20GHz, 256GB RAM, 4 NVIDIA Tesla V100 GPUs. 50 iterations used.



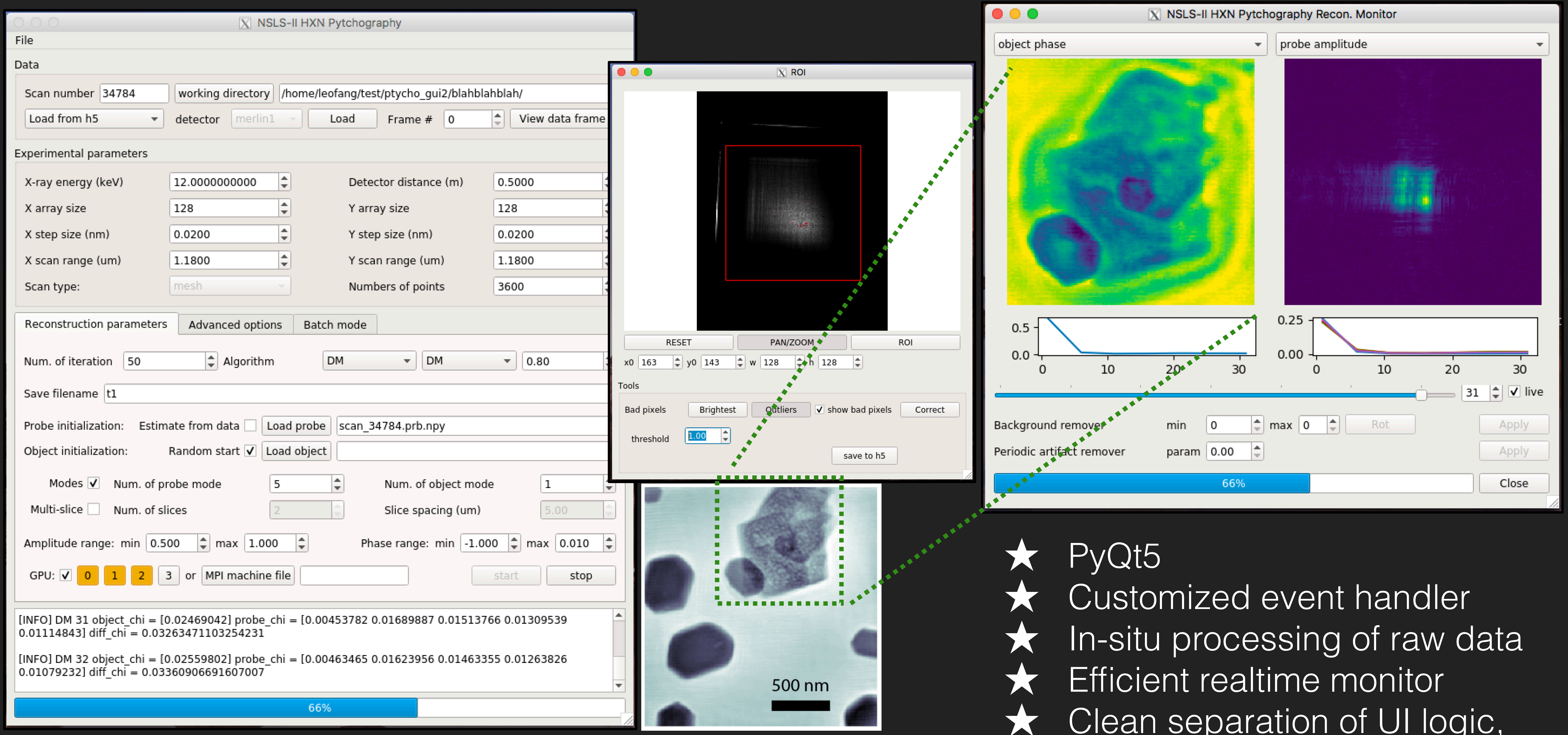

obj. phase



Serial CPU code: 8.8 hr —**>1000x speedup!**→ 4 V100 GPUs: 25.69s

# GRAPHICAL USER INTERFACE






- ★ PyQt5
- ★ Customized event handler
- ★ In-situ processing of raw data
- ★ Efficient realtime monitor
- ★ Clean separation of UI logic, implementation & computation

# HPC for LHC: Accelerating ATLAS Fast Calorimeter Simulations on GPUs





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**BNL**

Tadej Novak
Jozef Stefan Institute

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# HL-LHC: SOFTWARE AND COMPUTE CHALLENGES



- Upgrade planned for **High-Luminosity (HL) LHC** in 2026
  - ~10x luminosity of the original LHC design value
  - ~5x increase in event size
  - ~10x increase in event rate

→ **50x data**

- Currently none of ATLAS production software uses compute accelerators.
- "Business as usual" may not be able to meet the compute demands of HL-LHC.
- Need to be able to utilize HPC systems as well as traditional HTC/cloud
- Current and future HPC systems increasingly feature (different kinds of) compute accelerators
- **Portability across different architectures is essential!**

TOP500 The List.

PRESENTED BY

| | SYSTEM | SPECS | SITE |
|---|---|---|---|
| 1 | Summit | IBM POWER9 (22C, 3.07GHz), NVIDIA Volta GV100 (80C), Dual-Rail Mellanox EDR Infiniband | DOE/SC/ORNL |
| 2 | Sierra | IBM POWER9 (22C, 3.1GHz), NVIDIA Tesla V100 (80C), Dual-Rail Mellanox EDR Infiniband | DOE/NNSA/LLNL |
| 3 | Sunway TaihuLight | Shenwei SW26010 (260C, 1.45 GHz) Custom Interconnect | NSCC in Wuxi |
| 4 | Tianhe-2A (Milkyway-2A) | Intel Ivy Bridge (12C, 2.2 GHz) & TH Express-2, Matrix-2000 | NSCC Guangzhou |
| 5 | Frontera | Dell C6420, Xeon Platinum 8280 28C 2.7GHz, Mellanox InfiniBand HDR | TACC/U of Texas |

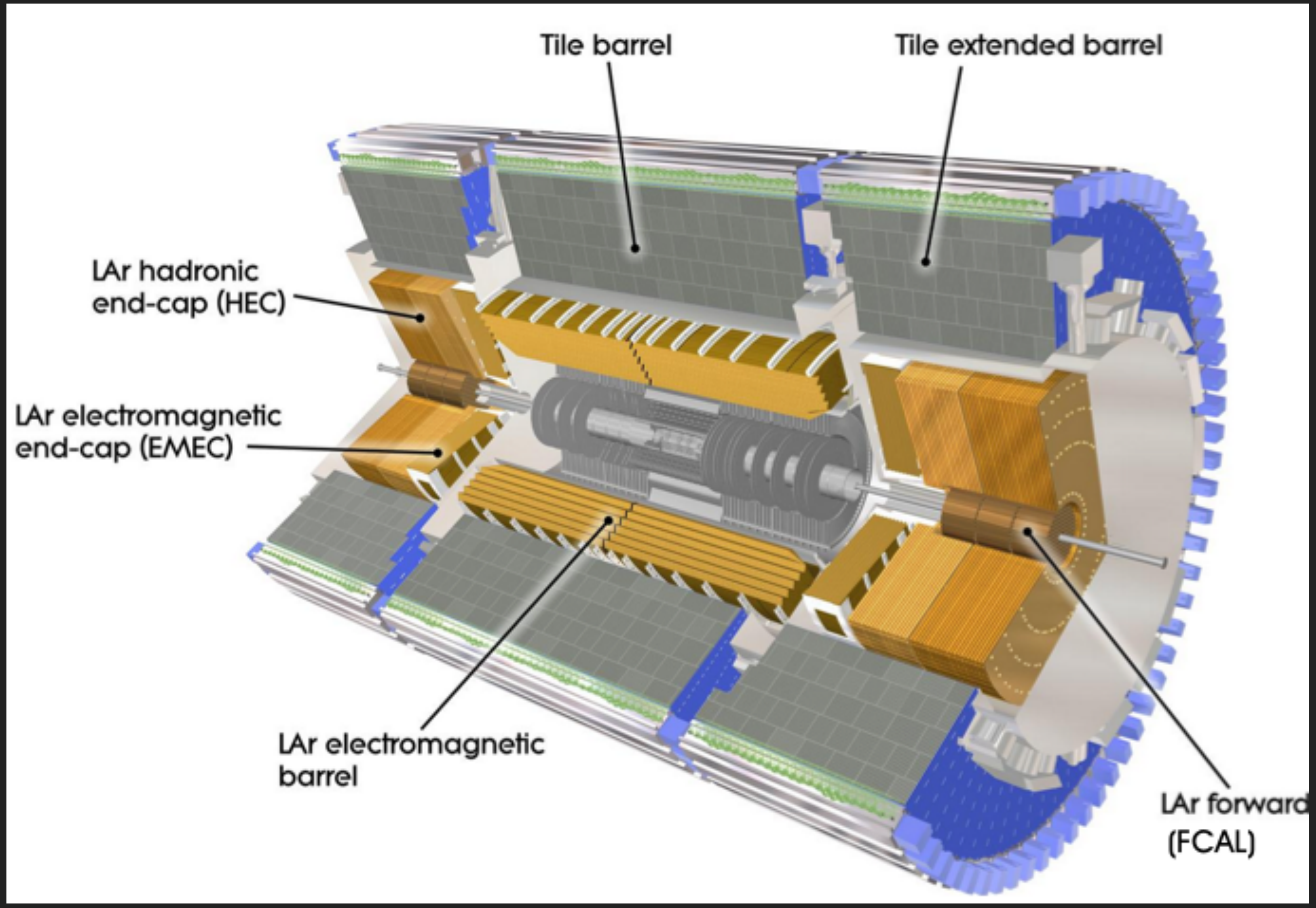
www.top500.org


Upcoming US exascale systems: Auroa (ALCF) and Frontier (OLCF)

# ATLAS FAST CALORIMETER SIMULATION



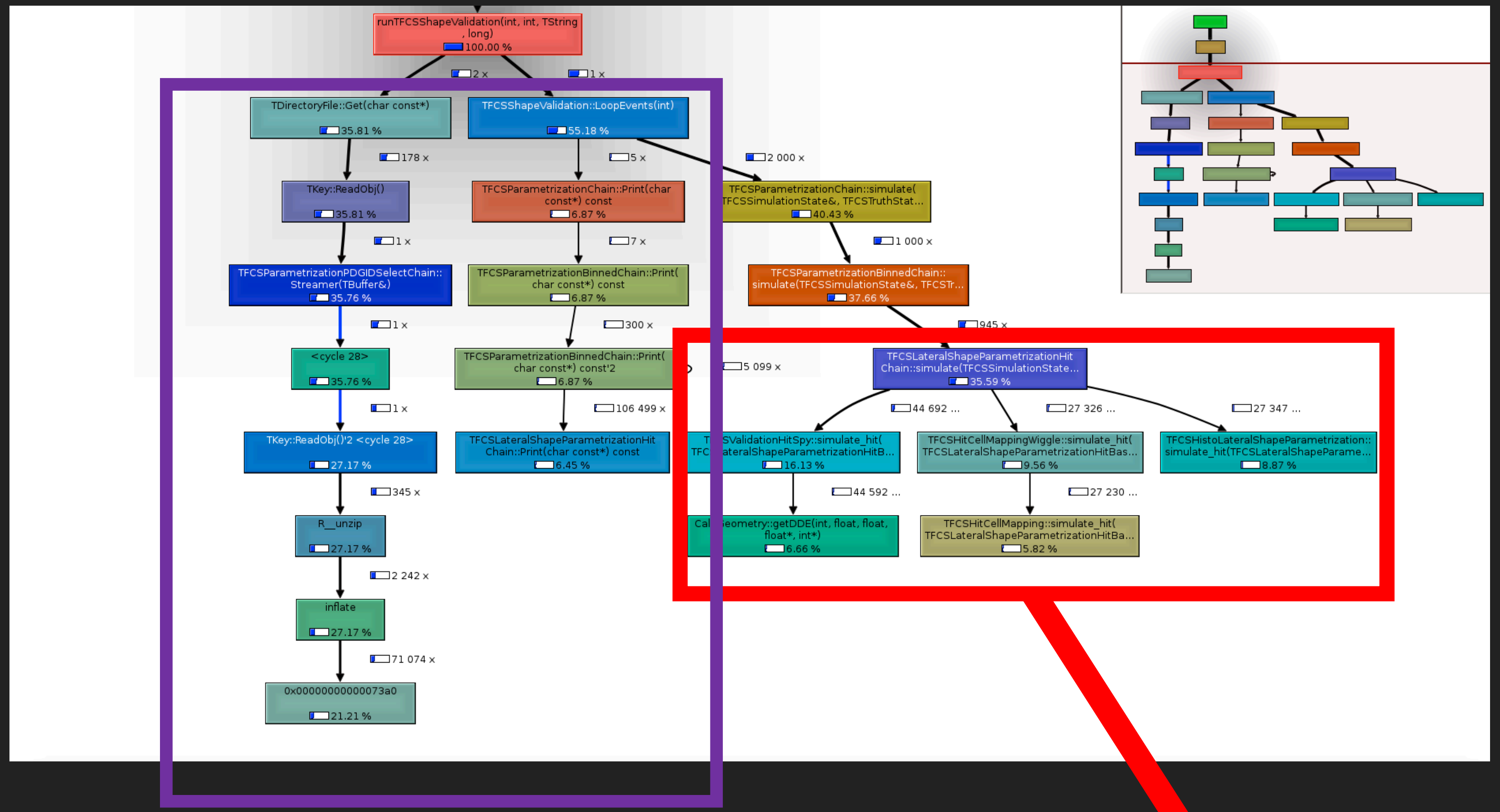
- Calorimeter simulation measures the energy depositions of O(1000) particles after each collision.
- Full detailed simulation uses Geant4, which is very slow
- Fast calorimeter simulation uses parametrization of the calorimeter: less accurate but much faster than Geant4 [T. Yamanaka (ATLAS) 2011]
- FastCaloSim (FCS): a relatively self-contained code for fast ATLAS calorimeter simulation
  - Good candidate for proof-of-concept GPU/ portability studies




Credit: ATLAS

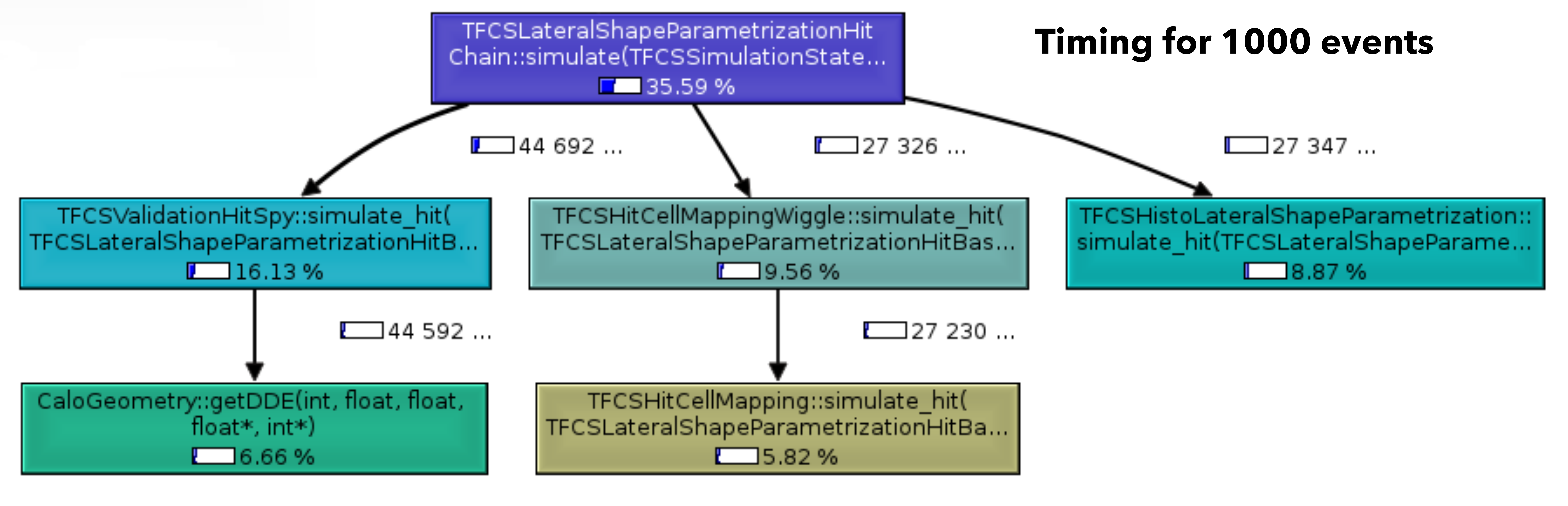
# PERFORMANCE PROFILING





I/O routines

- ➢ **TFCSLateralShapeParametrizationHitChain::simulate()** is the **most significant** routine except I/O (~30%).
- ➢ **TFCSLateralShapeParametrizationHitChain::simulate()** The running time **scales with the number of events.**
- ➢ **TFCSLateralShapeParametrizationHitChain::simulate()** is our target to parallelize/port to GPUs.




**Timing for 1000 events**

# GPU PORTING



- Initial strategy: CUDA
  - to identify feasibility and challenges with GPU porting
- Data structure modification from CPU to GPU:
  - Implemented new GPU CaloGeomory structure and supporting Classes
  - Simpler, no ROOT Dependence
  - CaloGeometry data can be loaded once and be reused: ~25MB
- Multi-stage CUDA kernels to generate histograms
  - Blockwise atomic update with shared memory
  - Followed by reduction across all blocks
- To get # of hits in the calo cells
  - only ~200 cells get hit out of 20,000 cells - trial run to narrow down the hit cells
  - Reduces memory requirement, and load imbalance

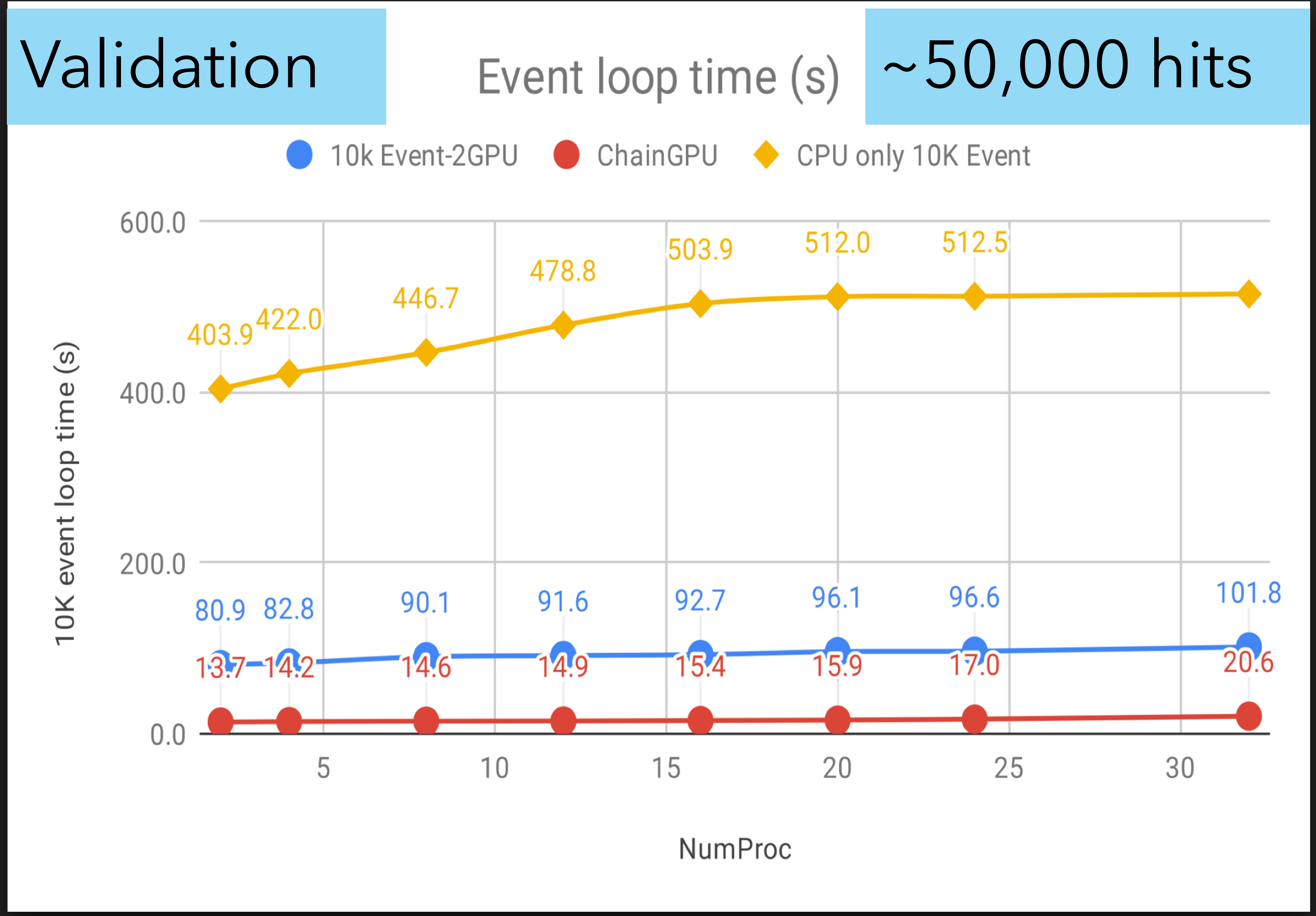
# CPU VS GPU PERFORMANCE COMPARISON



- Validation against GEANT4 most time consuming (~50K hits)
- CPU: "embarrassingly parallel" - different processes simulate different events
- GPU: Use CUDA-MPS to share 2 P100 GPUs on BNL Institutional Cluster*
- ~5X gain with 50K hits compared to CPU only runs (32 parallel processes).
- Actual production runs have fewer hits - less compute
  - Less performance gain: 2-3X vs. CPU

* CPU: Intel Xeon "Broadwell" 32 cores per node
* GPU: 2 NVIDIA P100 per node

Validation ~50,000 hits



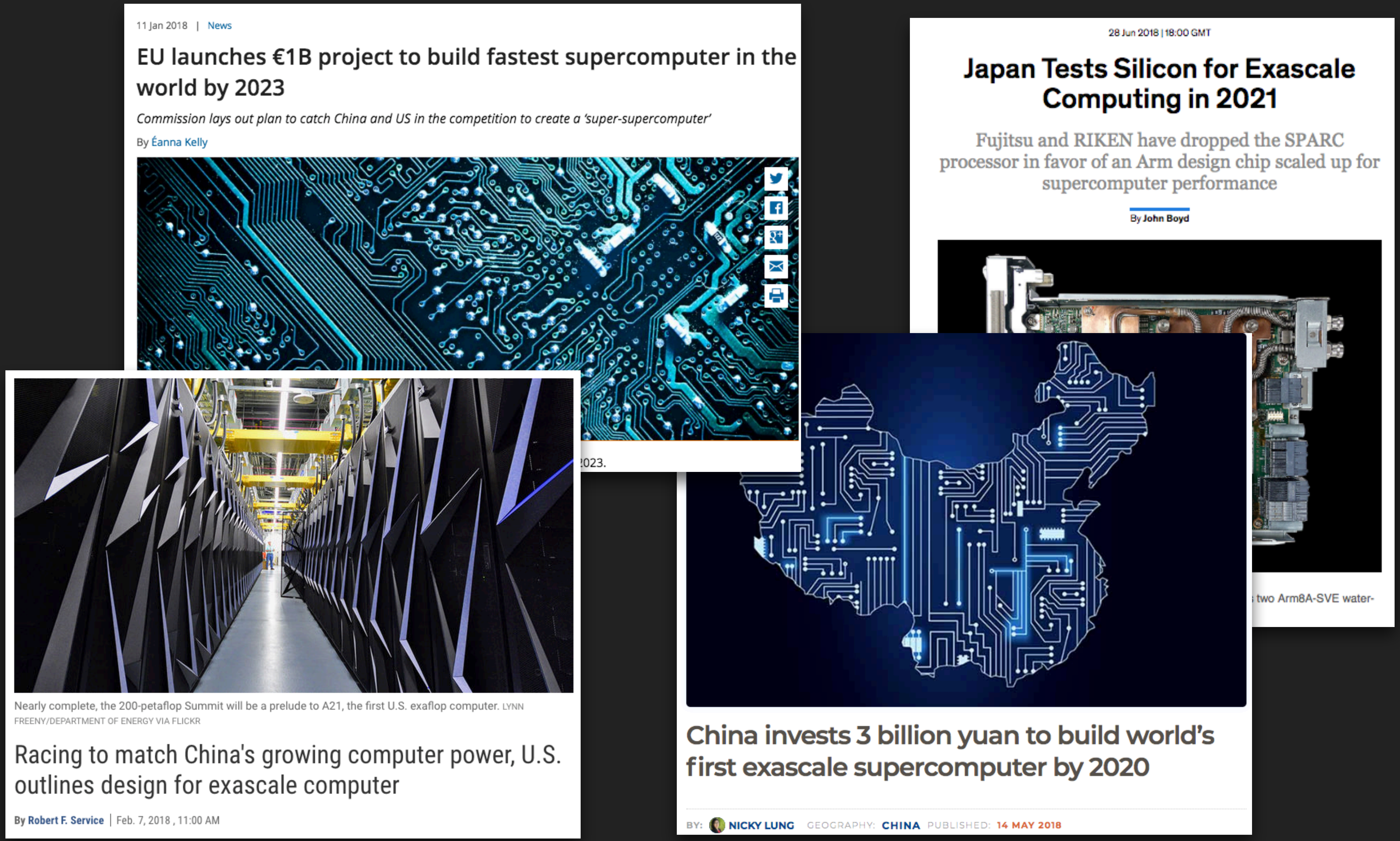

Simulations ~5,000 hits

| #MPI Processes | Particle | Energy | Min Eta | CPU (s) /10K event / process | GPU (s) / 10K event / process |
|---|---|---|---|---|---|
| 1 | Electron | 65536 | 2.2 | **18.8** | **6.0** |
| 32 | Electron | 65536 | 2.2 | **24.0** | **7.1** |

# EXASCALE COMPUTING

# THE RACE TO EXASCALE

- China, EU, Japan and US are all developing exascale supercomputers.



# DIVERSE EXASCALE ARCHITECTURES IN US ALONE



## Relevant US DOE Pre-Exascale and Exascale Systems for ECP

**Pre-Exascale Systems**

**Future Exascale Systems**

| 2012 | 2016 | 2018 | 2020 | 2021–2023 |
|---|---|---|---|---|
| TITAN – ORNL Cray/AMD/NVIDIA | CORI – LBNL Cray/Intel | SUMMIT – ORNL IBM/NVIDIA | PERLMUTTER – LBNL Cray/AMD/NVIDIA | FRONTIER – ORNL Cray/AMD |
| MIRA – ANL IBM BG/Q | THETA – ANL Intel/Cray | | | Aurora – ANL Intel/Cray |
| SEQUOIA – LLNL IBM BG/Q | TRINITY – LANL/SNL Cray/Intel | SIERRA – LLNL IBM/NVIDIA | | CROSSROADS – LANL/SNL TBD; EL CAPITAN – LLNL Cray |

ECP EXASCALE COMPUTING PROJECT

Doug Kothe @ 2019 NSF Blueprint workshop

# TWO MAJOR PARALLEL PROCESSING PARADIGMS (SINGLE-NODE)



- **SIMD - Single Instruction Multiple Data**
  - Intel Xeon Phi (AVX512): Cori/NERSC, Theta/ALCF
  - Intel Xeon "Skylake" (AVX512): Frontera/TACC
  - New! ARM SVE (Scalable Vector Extensions), supporting 128-bit to 2048-bit vector units: Post-K/Japan, new system at SBU
- **SIMT - Single Instruction Multiple Threads**
  - GPGPUs - NVIDIA, AMD, Intel New!
- Can we have the same data format/layout/programming model for both?

# PORTABILITY CONSIDERATIONS



**Given the diversity of current and upcoming HPC architectures, we may need to design our software with following considerations:**

- Performance Portability
  - How much tradeoff do you want to make between performance and portability?
  - Is it possible to design your software to be portable and at the same time reasonably performant?
- Programming Models
  - What programming models do you want to use c.f. performance portability?
  - OpenMP, OpenACC, OpenCL, CUDA, HIP, SyCL, OneAPI, Kokkos, etc.
- Programming Languages
  - Parallelism has increasing become part of the language itself, e.g. pSTL in C++.
- Data Layout
  - Is there a “one-size-fits-all” data layout for the diverse architectures?

# CSI ECP PROJECTS



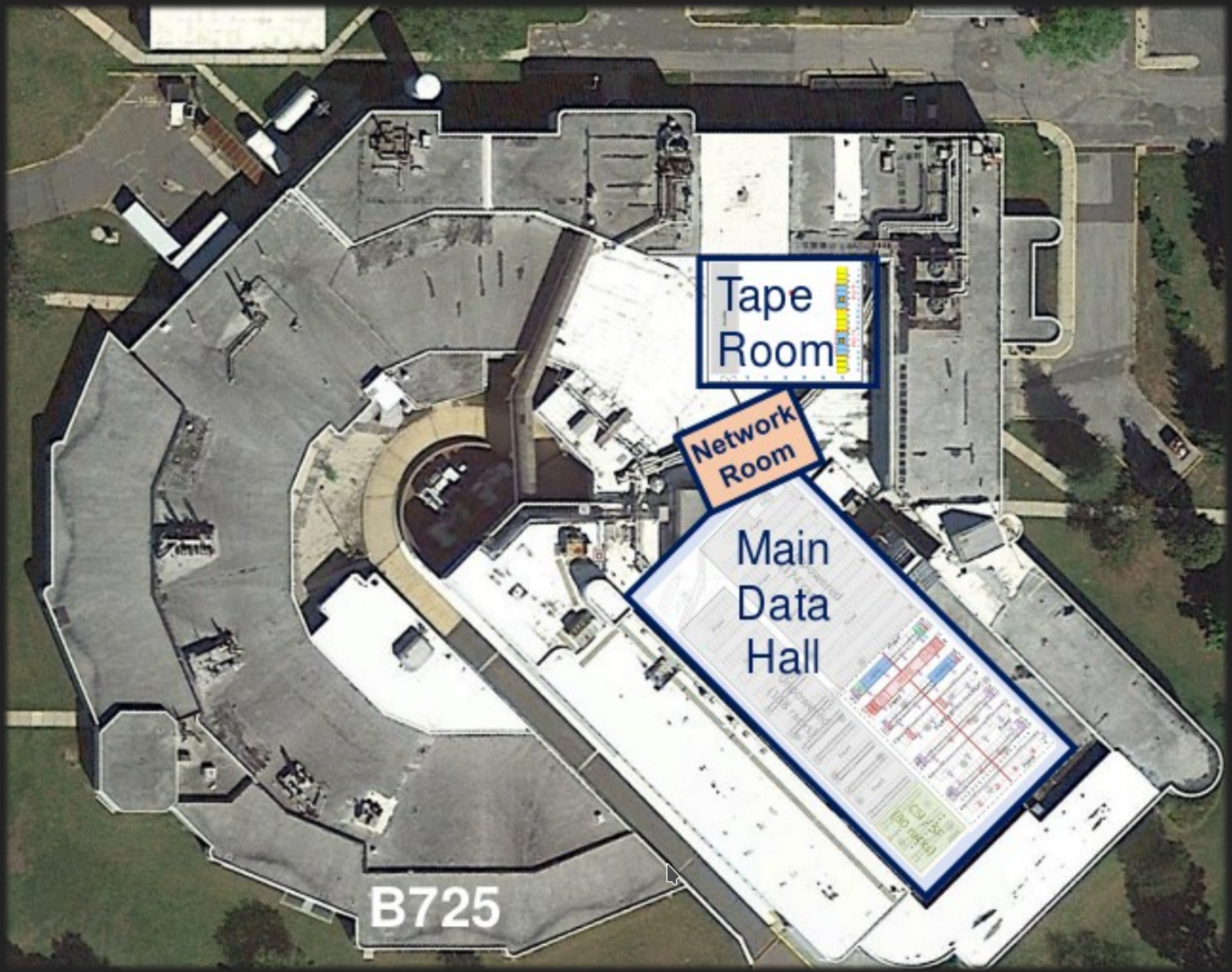
- Application Development
  - Lattice QCD - algorithms, performance portability, workflows
  - NWChemEX - newly-designed C++-based library (from Fortran-based NWChem)
- Software Technologies
  - SOLLVE (Scaling OpenMP LLVM Compiler towards Exascale) - OpenMP standard, LLVM compiler infrastructure
- Codesign Centers
  - CODAR - Center of Data Analysis and Reduction
  - ExaLearn - Machine Learning software for Exascale applications

# SIDE NOTES

# NEW DATA CENTER CONSTRUCTION UNDER WAY



- Repurposed NSLS Light Source building
- "Tier III" Class data center*
  - Redundant infrastructure
  - Concurrently maintainable
  - Completely self sufficient in emergencies
- New data center occupancy timeline
  - ATLAS areas ready before CY2021 - to coincide with LHC Run 3 start
  - Other areas become ready for occupancy throughout CY2021






* using the "Tier" classification defined by the Uptime Institute

Slide Credit: Shigeki Masawa, Imran Latif, Alexandr Zaytsev

# TRAINING EVENTS



- CSI regularly holds hands-on training events
- Hands-on training events (hackathons) give scientists access to expert guidance on modern HPC architectures and programming tools.
- Great way to jumpstart incorporating a new programming tool/model in your code
- Planned this year:
  - GPU Hackathon, August 17-21, 2020
  - OpenMP Hackathon, dates TBD
  - ML/AI Tutorials, dates TBD