Fermilab Software and Computing R&D

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A Coordinated Ecosystem for HL-LHC Computing R&D
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Some disclaimers

• I am speaking on behalf of a large R&D program at Fermilab
  - Spans many areas of software and computing
  - Impossible to do it justice in a 20 minute talk
  - Work presented is done by others; any mistakes in presentation are mine

• Significant overlap with US CMS Ops R&D program in S&C
  - Fermilab is the host lab for US CMS
  - Tried to minimize overlap with Lindsey’s talk this morning

• Presentation format
  - Showing most projects answers for suggested questions by the workshop organizers
Previously, on FNAL S&C R&D… [2019]

Software R&D Strategy

- Evolve the Fermilab facility for future experiment needs using modern computing hardware
  - CMS
  - DUNE
  - Mu2e
  - Other Intensity Frontier experiments
  - Cosmic Frontier
- Support the use of external computing, including both HTC resources and HPC resources, especially Exascale
- Assist the experiments in taking advantage of advances in computing hardware and software

- Topics
  - Artificial Intelligence
  - Evolving Computing Architectures
  - Compute (aka HEPCloud)
  - Storage
  - Networking
  - Analysis Facility Concepts
  - Quantum Computing
    - in support of Lab program
    - not covered here
Fermilab Scientific Software and Computing

• Evolve Fermilab facility for future experiment needs
  - Primarily driven by DUNE and HL-LHC CMS
  - Leverage advances in hardware (particularly heterogeneity)

• Evolve software and tools used by experiments to produce science
  - Leadership in this area: create solutions rather than fix problems
  - Embrace AI in all applicable aspects

• Organizational change: Scientific Computing Division Computational Science and Artificial Intelligence Directorate (CSAID)
  - Three divisions within directorate with core competencies
    • Scientific Computing Systems and Services; Data Science, Simulation, and Learning; Real Time Processing Systems
    • AI office coordinating lab-wide AI activities within CSAID
Artificial Intelligence Strategy

- Develop **AI capabilities to accelerate HEP science** & contribute to overall DOE AI strategy and greater science/industry AI ecosystem
- Build **diverse, inclusive community; assemble multi-disciplinary collaborations** around cross-cutting HEP AI challenges

**Strategic pillars**

- **Operations and control systems**
- **Algorithms for HEP science**
- **Real-time AI systems at edge**
- **Computing hardware and infrastructure**

- **Physics-inspired data & models**
  Tailor AI to data representations that integrate physics knowledge for simulation and reconstruction
- **Robust & generalizable learning**
  Build robust models that can interpolate/extrapolate; quantify uncertainties and understand anomalies; towards explainable algorithms
- **“Fast” & efficient algorithms**
  ML in resource-constrained environments mapped to heterogeneous hardware
Accelerating ML data processing

- For HL-LHC, computing will be bottleneck - goal to enable more powerful algorithms beyond projections
- Coprocessors (GPUs, FPGAs, ASICs, …) naturally accelerate ML workloads by orders of magnitude
- No way to guarantee access to HW at all grid sites
- Leverage industry hardware and tools - provide coprocessors as-a-service

SONIC:

**Services for Optimized Network Inference on Coprocessors**

- Scalable, flexible, adaptive, and non-disruptive deployment of coprocessors for HL-LHC
- Explore with on-prem, clouds, HPC and also for analysis facilities for all types of emerging hardware
- Testing now on CMS production workflows for Run 3
- Developed for ProtoDUNE and LIGO as well

Scaling off-site usage to 24 GPUs!
Networking R&D

- FNAL, along with Vanderbilt and Nebraska joining SENSE/Rucio prototype effort with Caltech, UCSD, and ESNet
  - Goal: Use SENSE to open SDN channels for prioritized transfers, provide bandwidth accountability, and bandwidth sharing/prioritization
  - Final goal: manage the WAN connectivity of FNAL for simultaneous use by experiments
- Fits into HL-LHC S&C ecosystem as a crucial element of storage strategy
  - Key for a viable caching infrastructure
- Collaborating with NOTED from CERN and ESNet caches in the network
  - Will be part of next WLCG data challenge in 2024
- USCMS ops funds 1 FTE at FNAL and 1 FTE at Caltech and some effort at Nebraska
  - Offer for hire at FNAL accepted; will start in the Spring
- Missing connections: would be good to build closer ties with LCFs
Storage R&D

- Evolve Fermilab storage R&D infrastructure for needs of the Exabyte era
  - Not experiment specific but heavily based on needs of HL-LHC CMS and DUNE
  - Consider all aspects of existing infrastructure
- Essential component of HL-LHC computing infrastructure for CMS
  - FNAL will continue to be the largest Tier-1 site for CMS during HL-LHC
- Connections with US CMS Ops: Funds ~50% of effort
  - Includes postdoc R&D funding for Object Store exploration
- Missing connections
  - More coordination with WLCG
  - Working with LCFs to understand optimal storage for data delivery to HPCs
Computing Resource Evolution STrategy (CREST)

• Document/plan strategy to evolve FNAL facility for 2029/2030 needs
  - Networking and Storage R&D represent pillars of this effort
  - Facility needs primarily driven by HL-LHC CMS and DUNE
  - Includes strategy for machine rooms, hardware type and cost evolution, services including monitoring and databases, central resources and user-facing resources (analysis facilities, etc.) and much more

• Essential component of HL-LHC computing infrastructure for CMS
  - FNAL will continue to be the largest Tier-1 site for CMS during HL-LHC

• USCMS Ops program funds many areas of R&D for facility evolution
  - Includes Storage R&D, Networking R&D, and HEPCloud
HEP-CCE: Portable Parallelization Strategies (PPS)

• Investigate range of software portability solutions using HEP testbeds
  - HEP-CCE PPS involves Fermilab, ANL, BNL, and LBNL
  - FNAL contribution is ~1.5 FTE
  - Participation includes ATLAS, CMS, and DUNE
• Vital for use of heterogenous architectures/accelerators for HL-LHC compute
• Software projects as use cases in collaboration
  - CMS Heterogeneous Pixel Reconstruction (patatrack) at CERN
  - p2r/p2z which includes effort from mkFit
  - Wire-cell toolkit
  - ATLAS FastCaloSim and ACTS
• Includes collaboration with US CMS Ops supported CMS Core Software experts
HEP-CCE Fine-Grained I/O and Storage (IOS)

• Develop strategies for effective use of storage at HPC sites for HEP experiments
  - Involves effort from FNAL and ANL
  - FNAL contribution is ~1.5 FTE
• Will significantly impact ability to use HPC resources for HL-LHC computing
• Collaborating with
  - ROOT I/O team (one expert)
• Connections to US-LHC operations program
  - Includes effort from CMS framework developers and USCMS Software L2
Detector Simulation using GPUs: Celeritas and Acceleritas

• Developing a full-fidelity detector simulation on GPU
  - Current focus: offloading EM tracks from Geant4 to GPUs
  - Leveraging architectures available at LCFs
  - Current FNAL effort is 1.9FTE
  - Collaborating with ORNL and ANL; partial FNAL funding from SciDAC

• Essential for speeding up simulation workflows for HL-LHC

• Collaborating projects
  - Geant4, VecGeom, Adept simulation GPU R&D (CERN), ADIOS (Exascale computing project), SWIFT-HEP

• Collaborating with US-CMS ops framework and simulation experts

• Missing connections
  - Integration with experiment framework; lack of support currently
Framework R&D LDRD

• Developing framework software that supports user-defined processing levels
  - Experiment agnostic but motivated by DUNE requirements
  - Total effort is ~0.5FTE, funded by LDRD

• Potentially applicable to HL-LHC S&C
  - Rethinks how framework jobs are assembled and executed

• Collaborating with
  - DUNE, ensuring alignment with requirements
  - WireCell: BNL-funded project supporting neutrino physics simulation and reconstruction
  - Will be presented within context of HSF frameworks working group

• Connection to US LHC operations program
  - USCMS ops leaders are aware of effort and have provided feedback
GPU Algorithm R&D

- Develop high-performance GPU-based algorithms for multidimensional numerical integration
  - Supported by FNAL LDRD
  - In collaboration with computer scientists at Old Dominion
- Producing freely available algorithms: can be used by HL-LHC experiments
- Collaborating with
  - DES actively using algorithms in Year 3 galaxy cluster analysis
  - LSST DESC members have expressed interest
- Missing connections
  - More interested users
**mkFit**

- Parallel track reconstruction for HEP experiments
  - Already used in track building in CMS Run3 w/ 3.5x speedup
  - Being expanded for generic detectors

- Targeting usage as part of HL-LHC reconstruction
  - Being expanded for HL-LHC detector geometry

- Collaborating with UCSD, Cornell, Princeton
  - Support from IRIS-HEP
  - Support from SciDAC4 ran out
  - USCMS Ops is directly supporting effort

- Collaborating with other projects
  - HEP-CCE PPS; using mkFit as benchmark code. Can integrate back into mkFit for GPU execution
Exa.TrkX

• Graph NN (GNN) for tracking and reconstruction in HEP
  - Coordinated by LBNL with primary focus on HL-LHC ATLAS
  - FNAL focus on GNNs for LArTPC detectors (e.g. DUNE)
  - Collaborating with Cincinnati and Northwestern (CS/ASCR)

• Collaborating with other projects working on GNNs
  - e.g. HGCal reconstruction on HL-LHC CMS
  - Experts on other aspects of reconstruction (e.g., HPC workflows and reference dataset definition)
Analysis software tools: coffea

• Single point of entry and incubator for developing effective concepts in columnar analysis
  - Basic array manipulation->high-level physics analysis data transformations
  - Scale out across a wide variety of cluster types and execution engines (i.e. dask)
  - Large user community on CMS, O(100) with multiple published analyses
  - Platform from which to build HL-LHC analysis capable software frameworks

• Collaborating with:
  - Currently: awkward-array, uproot, boost-histogram, fastjet, coffea-casa, EAF
  - Planning: the incarnations of these projects post IRIS-HEP, pytorch, tensorflow, nvidia

• Missing connections
  - Deeper connection and develop road to adoption within ATLAS (started in some capacities, simplified systematics efforts)
  - ML researchers on nested, jagged, structured data

• Ecosystem wishes
  - More widely adopted standards for thin, simple analysis data tiers
  - Adoption of standards for existing compute clusters to run execution engines like dask / parsl
## Conclusion

- A wide range of software and computing R&D activities are being undertaken at Fermilab
  - All focus on achieving solutions that enable HEP

- Computing facilities need to evolve before the end of the 2020s
  - Focus on Storage and Networking as core development areas
  - Take advantage of increasing heterogeneity in compute resources

- Software
  - Advance software tools to use range of architectures; reduce time-to-insight
  - Take advantage of AI/ML