Advanced technology: theory efforts & synergies

Fermilab

Lattice-QCD computing

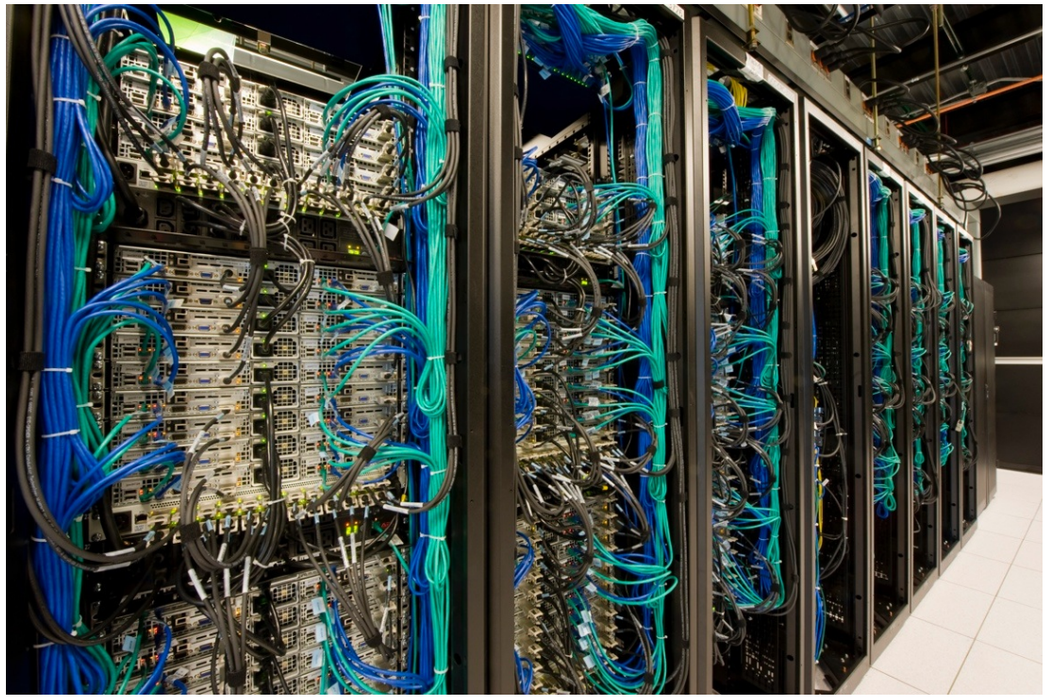
- Fermilab deploys and operates large computing clusters for the use of the U.S. lattice gauge theory community. These are organized by USQCD, of which almost all U.S. lattice theorists are members. Fermilab theorist Paul Mackenzie is spokesperson of USQCD.
  - Deployment and management of the clusters is carried out by the LQCD Project with Fermilab's Bill Boroski as project manager. In 2014, Fermilab deployed the pi0 cluster which consists of 128 K40 GPUs and a 3,900-core conventional cluster.
- DOE funds software for the particle and nuclear physics lattice communities through the SciDAC program. Paul Mackenzie is the PI of the particle physics SciDAC grant.

Synergies with lab hardware expertise: *Benefits to LQCD*

- Fermilab lattice computing effort benefits from and contributes to general lab expertise in computing hardware.

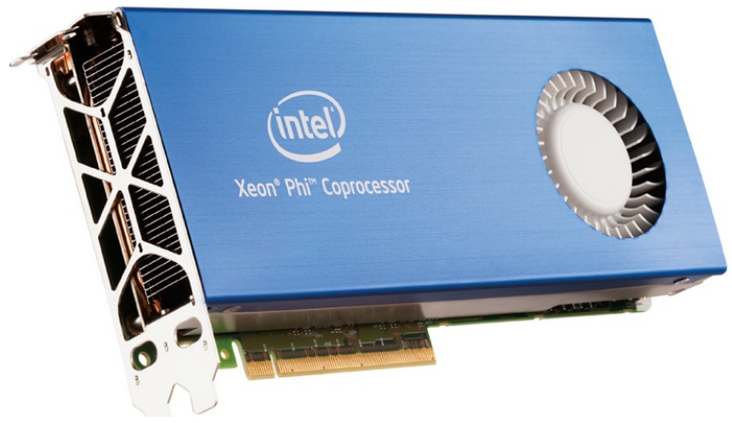
  -LQCD hardware performance depends on low-latency communications between processors, like those used for data acquisition. Benefited from lab expertise in DAQ applications (SDSS, CDF and D0 L3 triggers).

  -LQCD experience influenced design of proposed BTeV trigger.



Synergies with lab hardware expertise: *LQCD Contributions*

- LQCD early adopter of advanced networking (Myrinet, Infiniband).
  - artdaq toolkit development and design drawn from LQCD experience with MPI and infiniband
  - Current DAQ framework planned to be used by several Fermilab projects: Mu2e, NOvA, g-2, LArSoft, ArgoNeuT, μBooNE, and LBNE
  - LQCD influenced first artdaq cluster design and aided with deployment
- LQCD early adopter of advanced hardware.
  - Deployed first GPU cluster at FNAL in 2009.
  - Deployed small advanced computing hardware cluster ~2012 with GPUs and Xeon Phi (MIC) accelerators.
    - Used for accelerator modeling. Broad cross section of other Fermilab projects have also used this hardware and participated in training last September on Xeon Phi: LQCD, GEANT4, CMS offline, accelerator modeling, multicore frameworks, DES (2-pt correlation functions on GPUs), hardware/software for HEP triggers.

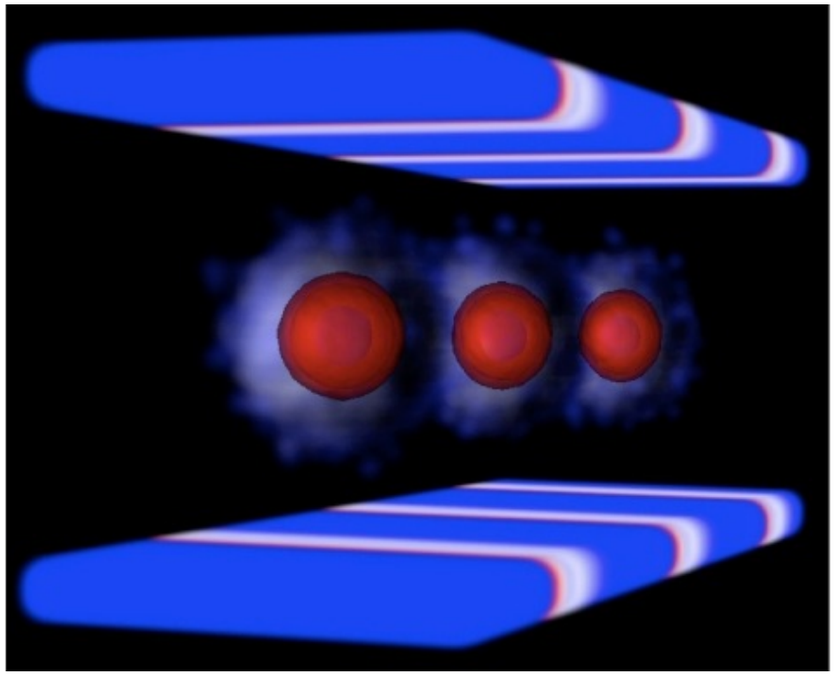


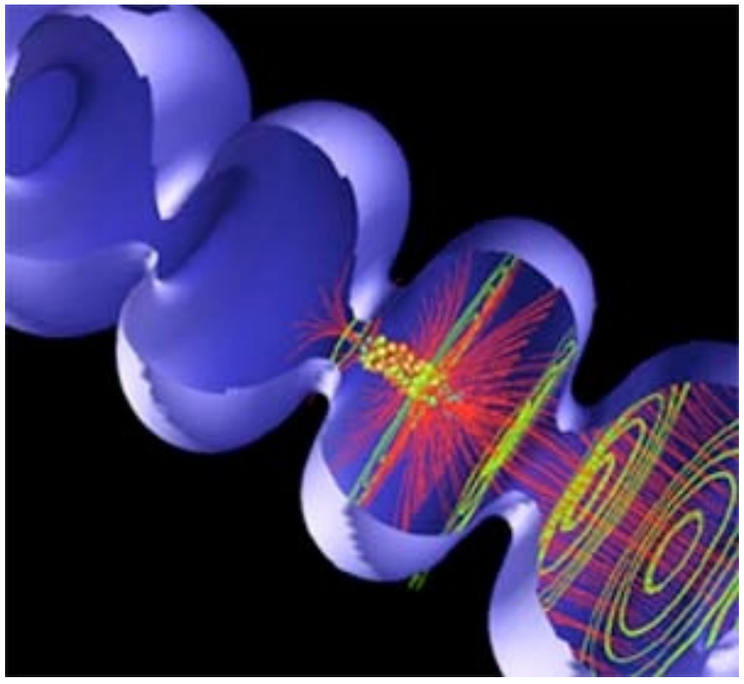
- LQCD early adopter of advanced filesystems.
  - Helped USCMS with testing and usage of Lustre filesystem..

Synergies with accelerator simulation: *Overlapping needs*

- Lattice QCD and Accelerator Simulation have cross-cutting needs in developing code for emerging state-of-the-art architectures, particularly in machines hosted at ALCF, NERSC and OLCF.

- LQCD and AS have an established pattern of inter-group cooperation, which also includes Geant4 and Computational Cosmology.
  - Share MIC/GPU software development cluster.
  - Share framework efforts, performance measurement, and analysis tools.
  - Joint NEAT-topics seminar series to share experience and knowledge.





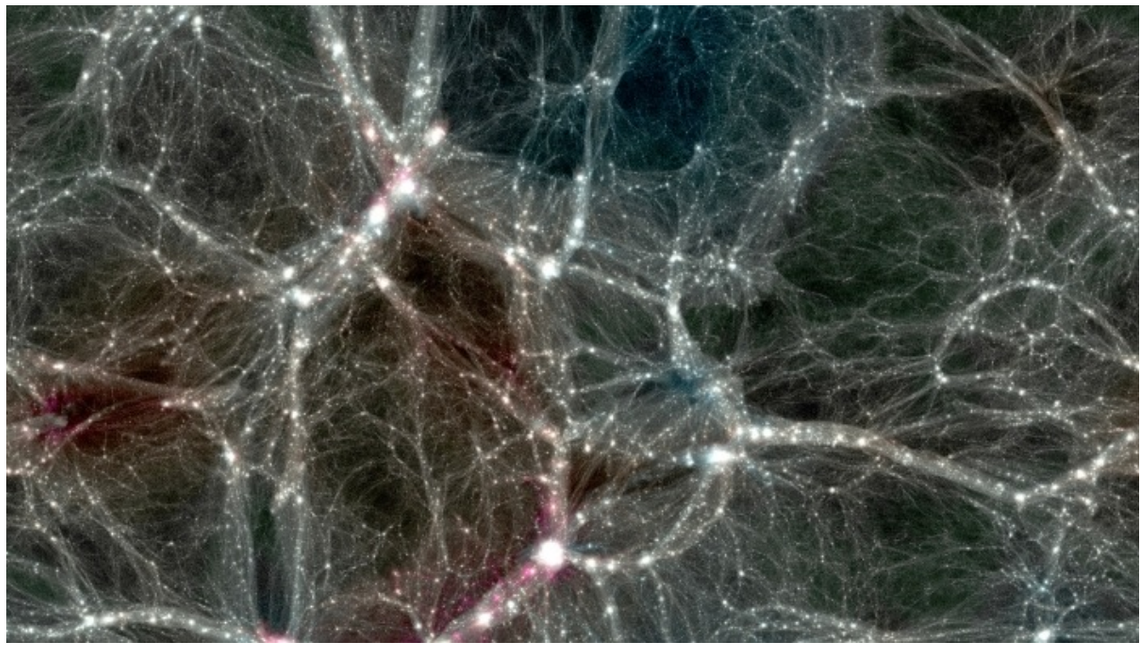
Synergies with accelerator simulation: *Joint plans*

- Plans for upcoming joint SciDAC work:
  - Share experience concerning low-level programming for Intel MIC and related architectures. Important aspects include vectorization, compiler-guided optimizations, data layout and communication optimization.
  - Share experience concerning GPU optimizations for large-scale NVIDIA GPU-based HPC systems. Focus on data layout, communication patterns, and optimizations for scaling.
  - Share experience for the POWER architecture. Important aspects for POWER include data layout and vectorization. Consider hybrid POWER-NVIDIA machines (e.g., Summit at OLCF) when they become available.
- New developments will be shared through the High Energy Physics Forum for Computational Excellence.

SciDAC
Scientific Discovery through Advanced Computing

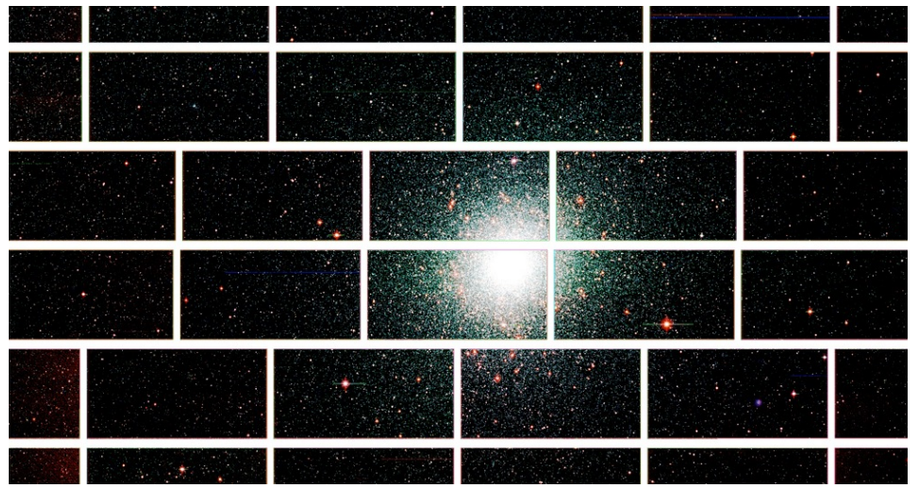
Cosmological computing: *Simulations*

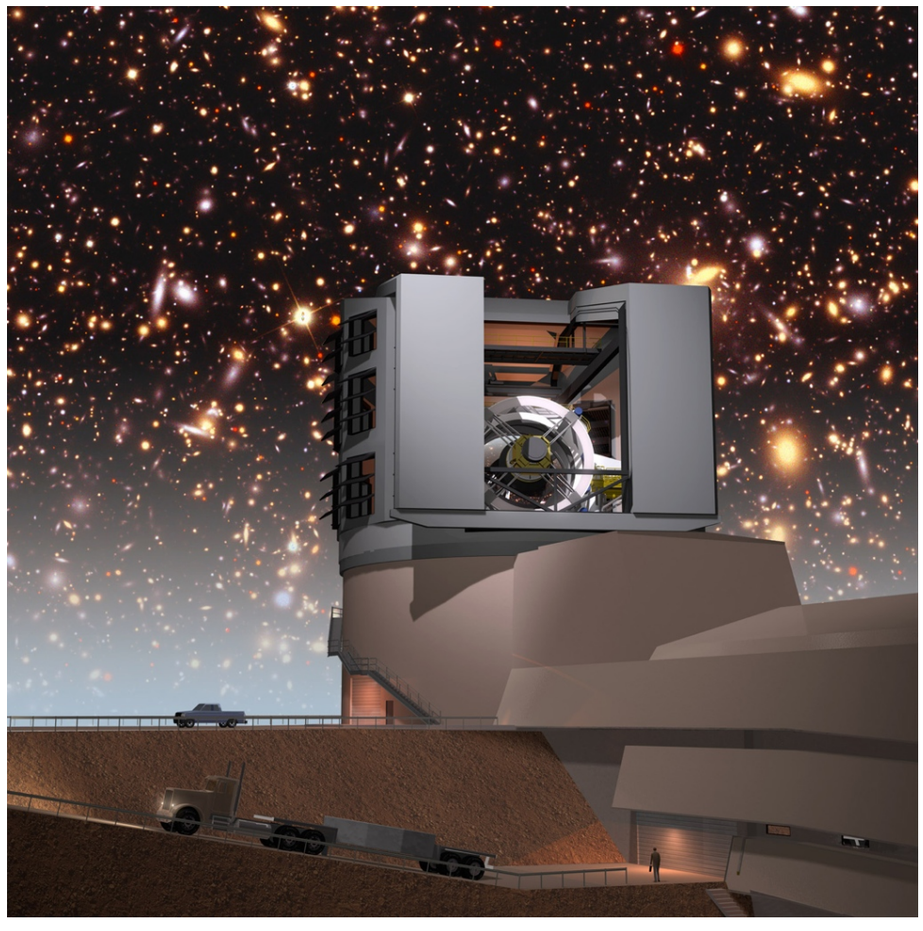
- Gnedin under a different SciDAC grant (joint with other HEP Labs) is developing ART (Adaptive Refinement Tree) massively-parallel framework for "full physics" cosmological computing that runs efficiently (scales to > 100,000 cores) on modern supercomputing platforms at ALCF and elsewhere.
  - Applications include simulations for current and future cosmological surveys, studies of systematics of future CMB experiments, baryon effects on measurements of matter clustering, etc.
- Part of multi-lab effort to cooperate in cosmological computing (successful SciDAC proposal & ASCR Leadership Computing Challenge proposal).



Cosmological computing: *Data analysis*

- Fermilab astrophysicists worked with Scientific Computing Division to define and develop software analysis frameworks enabling science application deployment and scheduling at HPC centers.
- **CosmoSIS**: Designed by theorists & Combined Probes Working Group in DES (Dodelson, co-convener).
  - Software framework empowers multiple users to develop and share code, combine analyses, and produce tight and robust constraints on dark energy and cosmological parameters.
  - Used by DES, gaining broad traction (breakout workshop in May; talks at DESI, LSST, FNAL Users' meeting).
- **LSST Software Framework** built on CosmoSIS
  - Extended to LSST tools and workflows.
  - Collaboration with LSST Dark Energy Science Collaboration Software WG and all analysis WGs.
  - Demo at SuperComputing14.





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