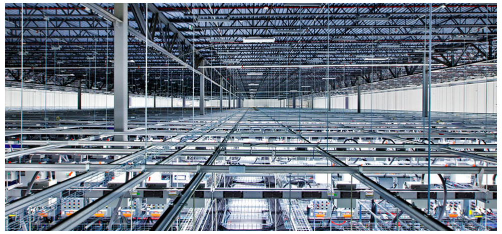
Astrophysical Research and Next-Generation Computing

Salman Habib

CPS and HEP Divisions
Argonne National Laboratory
The University of Chicago
Northwestern University

Supercomputer

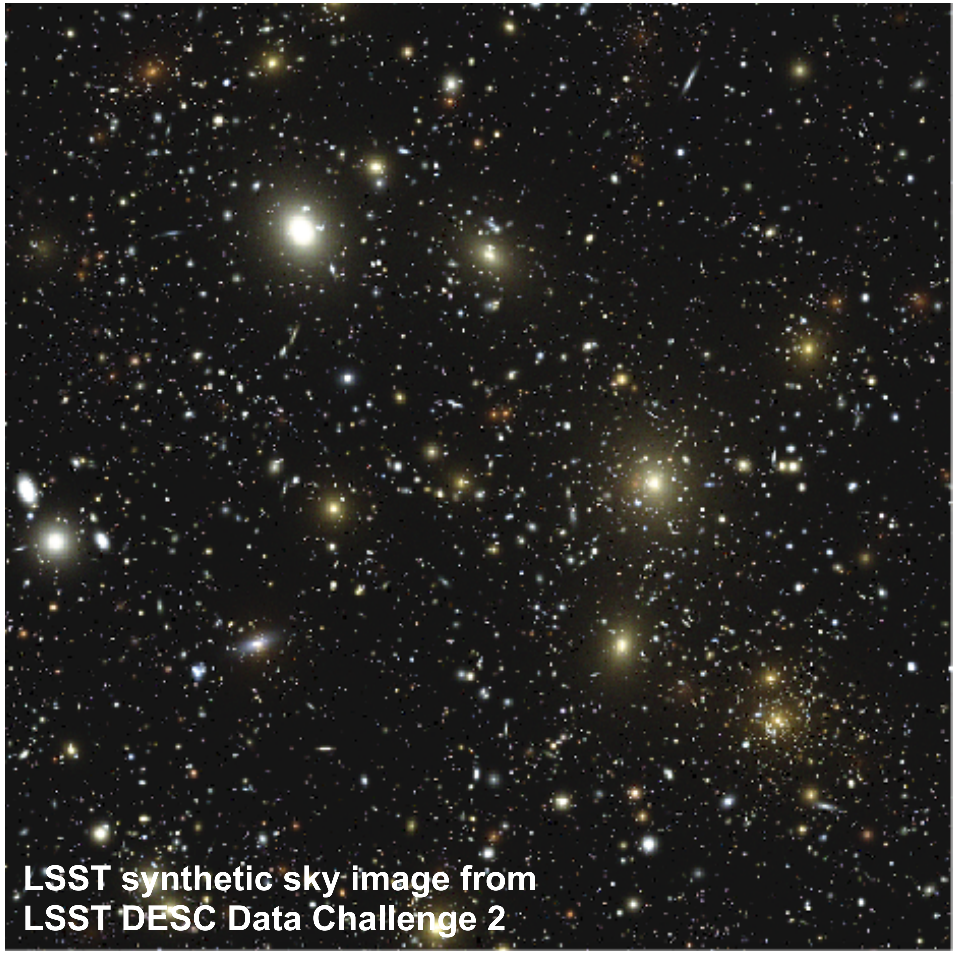


Cloud Resources

Institutional cluster

Access to distributed computing and data resources

Remote 'power' workstation



LSST synthetic sky image from
LSST DESC Data Challenge 2

Astro 2020
Panel on Enabling Foundation for Research
Feb 3, 2020

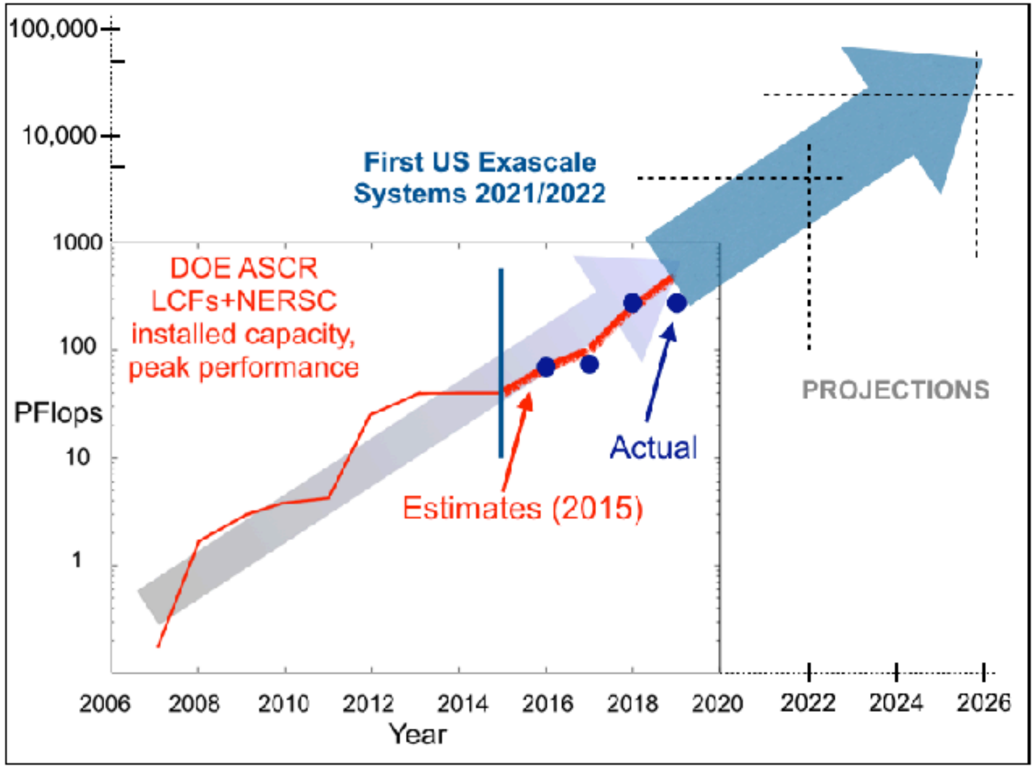
Wide Set of Computational Requirements

- Laptop to local workstation — usual workload, do not foresee major evolution
- Challenges to confront in HPC and HTC systems: changes in architecture driven by power limitations and commercial interests (AI/ML)
- Next-generation HPC systems are accelerated, e.g., CPU+GPU, or require highly vectorized code (ARM)
- HPC: winning programming model has yet to emerge, meantime difficult to extract performance from the new architectures (communication/flops imbalance)
- Astro community getting used to productivity languages (Python, Julia), plus has problem of moving legacy code
- Nontrivial to scale-up code from laptop to HPC system
- **Challenge:** performant high-level programming paradigm for HPC systems
- HTC tasks well-suited to cloud paradigm (whether “science” or commercial cloud)
- **Challenge:** Getting agencies to fund “science cloud” facilities with associated data repositories
- Note: Can also run HTC tasks on HPC platforms, albeit at lower efficiency

HPC and HTC Futures

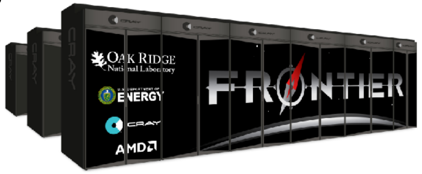
Major Growth in DOE HPC Facilities:

- By 2022, the LCFs (Argonne/ORNL) and NERSC (LBNL) will have ~Eflops of compute power, by mid 2020’s, tens of Eflops (NSF systems will also grow, but more conservatively)
- HPC systems now designed around three usage models: compute-intensive, data-intensive, and AI/ML
- HTC systems in commercial space will increasingly go in the AI/ML direction; architecture has possibilities for astro/science exploits (e.g., NumPy ports)
- DOE Exascale Computing Project tasked with moving science code to new systems (~30 projects) supported by software technology teams; performance portability is an important concern
- **Challenge:** HPC-based research is becoming more and more complex and specialized, no longer the realm of the lone “renaissance scientist”



Public Specs on Aurora and Frontier:

- Performance: >1EF
- Compute node: CPU+GPU
- System Memory: ~10PB
- Storage: >200PB at ~10TB/s
- # Cabinets: ~100+



Career Tracks

Training and Career Path for Next-Generation Computational Astrophysicists:

- First, internalize seriousness of problem — very few graduating PhD students in the US have a solid computational/modern CS background
- Training must take place at undergrad/grad levels but not with blunt tools, good place for collaboration with national laboratories and universities
- Scale and complexity of computational astro problems make it necessary for work to be carried out in reasonably large teams, “single professor” model will break down with time (look to industry); lack of sustainable model for software development
- Departments need to rethink their hiring and teaching philosophies

Diversity in the Workforce:

- Serious problem in the entire area of computation
- More support structures to promote diversity (two-body problems, family leave, flextime, etc.)
- Lack of peer groups at all levels is a major challenge
- Cultural change in how research groups function