

Dear Colleague,

We are contacting you to ask for your assistance in preparing for a jointly sponsored DOE ASCR/HEP Exascale Requirements Review. The aim of the review is to assess current computing and data related usage and trends in HEP as they connect to ASCR resources and to project these requirements out into the exascale future.

The ASCR context of this process is that the ASCR Leadership Class Computing Facilities, Oak Ridge National Laboratory Leadership Computing Facility (OLCF), Argonne Leadership Computing Facility (ALCF), and the National Energy Research Scientific Computing (NERSC) Center are working on identifying mission-critical computational science objectives within the Office of Science leading up to the 2020 -- 2025 time frame, to assure that the ASCR facilities will be able to properly support the scale of the projected scientific enterprise. The ASCR/HEP review is the first of a series that ASCR is conducting with other program offices.

We request each of you to either contribute to writing a section of our overall white paper (3 pages to a section) in your area of expertise or to prepare an individual case study. Please see below for your name in the detailed outline to identify where we would like you to focus.

In the case of the white papers, we ask you to describe where the research field is today – and to project out the science and compute/data needs on the 2020/2025 timescale, assuming the existence of exascale computational resources. By exascale resources we mean HPC platforms in the Exaflops class and an environment that has appropriate software, storage, networking, and data analytics support. (It's also fine if you don't actually need exascale resources!) We are not expecting surgical precision in carrying out this exercise; the information will be used as a basis for discussions in the review. The important point is to emphasize the overarching importance of your science and the key challenges you will face in terms of computation and data-related matters. Please feel free to enlist the help of others in putting these short documents together to get more than one opinion in cases where the answers are not clear.

For the case studies, we would like to convey a more detailed “flavor” of how a particular field works/operates at the computational level to our ASCR colleagues. Again, we are not expecting a comprehensive document, but more of a rough snapshot.

We would like to have your final results back to us no later than May 15. We will set up a protected repository so documents can be viewed when in their intermediate stages.

Thank you for your help with this important activity.

Salman and Rob

Plans for White Papers for ASCR/HEP Exascale Workshop

White Paper topic Format – 3 pages total, roughly evenly distributed among the following questions:

- What is the current situation of science+compute in your area?
- Where does the associated community/group want to be on the 2020/2025 timescale (science+compute)?
- What are your broad compute/data/services needs in 2020/2025?
- What do you see as your biggest computational/data challenges between now and 2020/2025?

The final 30-page document is outlined below. Each bullet in the outline of the main document below is one of the white papers mentioned above, along with the name of the lead author(s).

1.0 Executive Summary – Salman/Rob

2.0 Traditional HPC use cases

- Accelerator Modeling – Jim Amundson/Robert Ryne (C. Ng, P. Spentzouris, J.-L. Vay)
- Cosmological Simulations – Katrin Heitmann/Ann Almgren (S. Habib, P. Nugent)
- Lattice QCD – Richard Brower/Steven Gottlieb (S. Sharpe, D. Toussaint)

3.0 Non-Traditional HPC use cases

- Energy Frontier experiment – Ken Bloom/Chip Brock (M. Asai, L. Bauerdick, B. Bockelman, T. LeCompte, R. Mount, H. Newman, T. Wenaus)
- Energy/Intensity Frontier Theory (non-lattice) – Stefan Hoeche
- Intensity Frontier experiment – Brett Viren/Malachi Schram (A. Gaponenko, R. Roser, C. Tull)
- Cosmic Frontier experiment – Anders Borgland/Nikhil Padmanabhan (D. Bard, J. Borrill, D. Petravick, P. Nugent)

4.0 Evolution of HEP Facilities

- Compute Engines – Stu Fuess
- Data movement and storage – Gene Olenyk/Frank Wurthwein

Individual Case Studies will be based on a table format (template attached).

These Case Studies should provide a taste of how each sub-field works and to give a more fine-grained view of the potential requirements. We are looking at a subset of representative examples, without trying to be comprehensive. Except where marked, these topics are mainly restricted to work that is already running at the production level on ASCR resources.

- EF theory – Sherpa (Stefan Hoeche),
- EF experiment – ATLAS (Tom LeCompte)

- IF Experiment **(Projections)**
 - LBNE/DUNE (Maxim Potekhin)
 - Mu2e (Andrei Gaponenko)

- Lattice QCD (Doug Toussaint)
- Cosmic Frontier simulations
 - ART – (Nick Gnedin)
 - HACC – (Adrian Pope/Nick Frontiere)

- Cosmic Frontier Experiment
 - Optical surveys – DES (Don Petravick)
 - CMB – Planck (Julian Borrill)

- Accelerator Modeling
 - Electromagnetics – ACE3P (Cho Ng)
 - Beam dynamics – BeamBeam3D (Ji Qiang)

