CF2 Summary Report

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Domains and community interactions

Sub-groups (6 domains) with membership that achieves good representation of the associated communities of software toolkit/application developers

- Accelerator modeling (BLAST, Synergia, …)
  - Projects/support in major US and international labs, connections with Accelerator Frontier
  - Significant experience porting code and running on HPCs with accelerators
  - Many LOIs planned (~8 on different topics), some specific others more general
- Physics generators (GENIE, Pythia, Sherpa, Blackhat, …)
  - US labs/Universities. Developers, direct involvement in experiments, connections with EF, IF
  - Mostly physicists writing code, use of HPCs/ML at the level of small R&D efforts
  - At least one general LOI (including colliders) and one LOI specific to neutrinos

Domains and community interactions

- Detector/beam simulation (Geant4, Celeritas, ...)
  - US labs. Developers, direct involvement in experiments, connections with EF, IF
  - Collaboration with ECP-CompHEP on portability to HPCs at the level of a small R&D effort
  - Up to seven LOI on specific topics and one putting everything together
- Theoretical calculations - perturbative (multi-loop amplitudes, e.g. FIRE, FeynCalc, QGRAF, FORM, Reduce, Mathematica...)
  - US labs/universities. Connections to phenomenology groups.
  - Focus on better mathematical approaches for speedup, rather than on portability to modern platforms. They have special needs such as large memory, long runtime on single node, and mathematica.
  - Global LOI to emphasize precision theory and computing needs will be embedded in it

Domains and community interactions

- Theoretical calculations - LQCD/USQCD (QUDA, Grid, Chroma, MILC, QDP++.)
  - US labs/universities. Connections to various experiments, snowmass theory studies
  - Strong ties to ECP, significant experience using HPCs with accelerators
  - Many individual LOIs planned by subgroups. Have a lead USQCD LoI drawing attention to 7 white papers from last year.
- Cosmology calculations (ExaSky, …)
  - US labs/universities. Developers, direct involvement in experiments, connections with Cosmic Frontier
  - Strong ties to ECP/ASCAR, significant experience using HPCs with accelerators
  - A few LOIs focussed on different challenges: next generation system architectures, improve physics, analysis/workflow complexity (data-intensity, ML)

Classical Computing

Event generation: Physics goals are extending parton showers, higher orders. Software challenges to achieve goals, entire rewrites, technically hard. Experiments need to trust to use.

Neutrinos: interactions with nuclear physics, lots of knowledge & intellectual input built in myriad bits of code

Work needed is several orders of magnitude more to control systematic errors

Pythia: software/physics improvements can be made, adaptation to HPCs would need significant development, verification/validation effort. Some elements are parallelizable others are not.

Accelerator modelling: Portion of community using HPC, with SciDAC and ECP support. Cross over to other energy accelerators and nuclear.

Detector modelling: Prior project parallelising (part of) Geant4 (GeantV) sets scale of effort. Celeritas is the current R&D effort to adapt G4 to HPC/GPU (ORNL, FNAL, ANL). Real thing may take in excess of 10 FTE if on time for HL-LHC

Fundamental role for nuclear physicists (Geant4 models). Need to estimate systematic errors.

Continuous development and support of Geant4 toolkit demands more effort.

Theory (Lattice): Able to use HPC, with SciDAC, ECP funding which need to continue/replace/evolve, along with local cluster investment. Funded algorithms, software development programs. ASCR serves purposes well.

Theory (Perturbative) Bespoke configurations of high memory long job run computing nodes need, not typically easy on HPC sites. Mathematics & algorithms even more important than computing power. Symbolic portions challenging, phase space integrals more HPC friendly. 100TB data not uncommon.

Cosmic simulation: Strong record of efficient HPC exploitation well served by ASCR, with SciDAC and ECP funding.

Data volume a significant issue. ~500k LOC applications.

Machine learning

Detector modelling:

Use ML in ATLAS fast calorimeter ~90% of runtime. Initially PCA, more moving to GANS. Very HPC friendly. Need education programme to disseminate across all ATLAS sites as so important. Education in summer schools. Some reinforcement learning.

Calorimeter simulation time LHCb 50% : move to ML.

Cosmic simulation:

Use in preconditioning, for example where algorithms self heal; learn a good solution guess.

Education is important, and direct interactions. Encourages physicists and computer scientists to be broadly interested and educated. We should be interested in each others work.

Theory (Lattice):

Attempts to use in MCMC where algorithm self heals; learn a good proposal. Breadth and interdisciplinary engagement. ECP has 3 applied math members, JLAB & William & Mary working together particularly well. ML LOI will be written.

Quantum Computing

Many interested in the science and quantum mechanics, but practical usage looks far off.
Cosmic: nature of bulk cosmic data inappropriate.
Event generation: Neutrinos (no), colliders some color reconnection possibilities and possible advances in parton showers.
Accelerator modelling: some proposals (Ji Qiang).
Lattice: intellectual interest in addressing sign problem, neutron star phases of matter, etc..Escape Euclidean space limitations. Not expected for workhorse calculations.

Career paths
Ubiquitous problem in all sub-topics. Physicists develop the software with expert knowledge in both physics, algorithms and computing. Retention can be difficult, as often on soft money.