PanDA engagement with theoretical community via SciDAC-4

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Executive Summary

- In late 2016 BigPanDA got contacted by two collaboration of theorists who were preparing SciDAC proposals and who where interested in using PanDA for workload management of their simulations
    - USLQCD Collaboration
    - CRUNCH Collaboration
- After initial discussions agreed to join both proposals

- We engaged both collaborations about 1.5 year ago as part of BigPanDA beyond ATLAS activities
    - Discussions with P. Petreczky at BNL (LQCD)
    - BigPanDA presentation at the MADAI (future CRUNCH) collaborations meeting at MSU

- DOE NP-ASCR(SciDAC-4) call for proposals,. Support for cutting edge computational nuclear theory on LCFs and DOE .
- 5 year projects
- Letters of intent submitted Jan. 2017
- Proposals submitted Feb. 2017
- Decisions are expected mid-summer 2017

LQCD

- Projects title: "Computing the Properties of Matter with Leadership Computing"
- Lead PI: Robert Edwards TJLab
- ~20 collaborators from BNL, MIT, LANL, MSU, GWU, UNC, TJLAb, W&M, PNNL, Intel, nVidia
- Lattice QCD calculations in support of TJlab, RHIC, LHC-HI physics programs, future electron – ion collider

CRUNCH

- Project Title: "Calculating Rigorous Uncertainties for Nuclear Collisions of Heavy ions (CRUNCH)"

- Lead PI Michael Strickland – Kent State U.

- ~10 collaborators from BNL, Duke, MSU, OSU, LNLL, Minnesota, Rutgers

- Modeling of heavy ion collisions in support of RHIC, LHC-HI

Computing aspects. LQCD example

- Lattice QCD – 170M hours allocation on LCFs in 2016 through INCITE and SciDAC
- HTC like computing in many cases. Below based on BNL's LQCD group workflow on Titan
  - Many ,MPI wrapped, independent ,GPU enabled, single node jobs,
  - ~5 hours run time, that sets the number of ranks on Titan
  - Currently direct, by hand submission, ~2 small, 2 big jobs per week
- USLQCD uses several LCFs, plans to work on next-gen machines (Sierra, Aurora, …). GPU and PHI optimized codes. nVidia and Intel are collaborators on the proposals.
- Very suitable for automation by PanDA
- We expect that PanDA will allow to automate job submission, increase volume of submitted jobs, automatic resubmission, monitoring, data movement
- Meeting in early April 2017 with Robert Edwards to start the discussion about detailed requirements and implementation details