

USQCD WP: Computational Algorithms for LQCD

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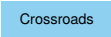

Contributors (agreed so far): Norman Christ, Will Detmold, Robert Edwards, Martin Savage, Phiala Shanahan... Thank you!

Challenges:

- Change in Hardware: BlueGene end-of-line. Intel program change. ANL Aurora pushed to 2021..
- No matter what the architecture, (local computation)/(internode bandwidth) is bad, and only will get worse. LQCD seem to be something of an outlier on this. → importance of algorithmic improvement, not only code performance. (CA solvers, Split Grid, reduced precision,.....)
- Ensemble Generation: Better control of critical slowing down if you want to go $a^{-1} \sim 3\text{Gev}$ or beyond. Also, reliability likely an increasing concern.
- Programming Model: Portability between GPU, CPU, other architectures, OpenMP/OpenACC, Kokkos, Jitify, CUDA/nvcc...

- Data reuse, Memory hierarchy :Low latency, low capacity ↔ High capacity, high latency, Asynchronous I/O, Data integrity, inline/offline (de)compression...
- New paradigm: Machine Learning, Quantum computing...

Relevant Pre-Exascale and Exascale Systems for ECP

Pre-Exascale Systems				Exascale Systems
2013	2016	2018	2020	2021-2022
 Argonne IBM BG/Q Open	 Argonne Intel/Cray KNL Open	 ORNL IBM/NVidia P9/Volta Open	 NERSC-9 LBNL TBD Open	 Argonne Intel/Cray TBD Open
 ORNL Cray/NVidia K20 Open	 LBNL Cray/Intel Xeon/KNL Unclassified			 ORNL TBD Open
 LLNL IBM BG/Q Secure	 LANL/SNL Cray/Intel Xeon/KNL Secure	 LLNL IBM/NVidia P9/Volta Secure	 LANL/SNL TBD Secure	 LLNL TBD Secure

Outline(tentative):

- Introduction and motivation
- Linear Systems and Eigensolvers (Joo, Jung)
- Gauge Generation (Joo, Christ)
- Correlation Function construction (Jung,Edwards)
- Hardware and Programming Model Considerations (Joo)
- Opportunities using Big-Data and Machine Learning (Detmold, Shanahan)
- Opportunities using Quantum Computing (Savage)
- Summary