

Lattice QCD at the Intelligence Frontier

Genesis Phase II project





Project Overview

Broad program to address application of AI/ML to lattice QCD computations and develop the necessary data and computing infrastructure

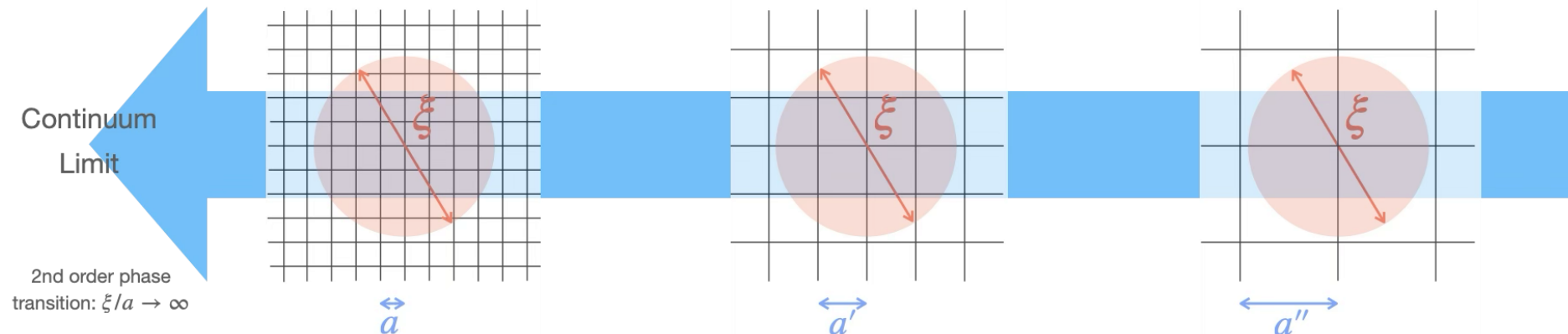
- **Area 14C:** “Partner domain expertise with data science and industry to develop AI methods and techniques capable of **drawing robust scientific insight from increasingly complex and/or petabyte-scale datasets**. Enable deeper insights by directly connecting datasets with theoretical parameters for uncertainty-aware reasoning to leverage the high- dimensionality of particle physics datasets. **Scope will address the critical slowdown problem in Lattice QCD, automate big-data analysis, achieve new levels of experimental precision and theoretical calculation,”**
- **Combine**
 - **AI innovation in core research**
 - **Agentic AI for HPC workflow orchestration**
 - **Agentic AI for HPC code development, porting and optimization**
 - **Data preparation and computational infrastructure integration and development**
- **Enabling new insights across strong interaction physics**

MIT LQCD is the leading effort on this very specific topic

Critical slowing down in LQCD

Lattice QCD is a **sampling problem**

- Markov chain used to sample QCD partition function and evaluate physical quantities via importance sampling
- Continuum field theory emerges as a limit of vanishing lattice spacing where physical length scales diverge in lattice units
 - Updates to samples in the Markov chain are typically **quasi-local**
 - Updates should change the sampled gluon fields on physical scales so become **rapidly more costly in this limit**: critical slowing down (CSD)
- Most promising method to ameliorate CSD
 - **Normalizing flows** (AI/ML) as maps from simple distribution to a complicated target distribution [Albergo, Kanwar, Shanahan, 2019]



USQCD Collaboration

<http://usqcd.github.io>

- National grouping of lattice field theory researchers
 - ~200 researchers across universities and 8 DOE labs
- Supports broad program of research in nuclear and high-energy physics
 - Quark & lepton flavor physics
 - Strong interactions beyond the SM
 - Hadronic and nuclear spectroscopy
 - Hadronic structure
 - QCD in extreme conditions
 - QIS for QFT
- Hosts a computational platform optimized for LQCD calculations
- Provides software infrastructure for the community (SciDAC program: 2001-now)
- Runs a national traineeship program educating students in QCD, HPC and AI/ML and preparing them for technical workforce at labs and in industry

Executive Committee

Tom Blum (UConn, chair)
Will Detmold (MIT, deputy chair)
Peter Boyle (BNL)
Martha Constantinou (Temple)
Carleton DeTar (Utah)
Robert Edwards (JLab)
Andreas Kronfeld (FNAL)
Huey-Wen Lin (MSU)
Kostas Orginos (William&Mary)
Anna Hasenfratz (Colorado)
Stefan Meinel (Arizona)

Proposal team

MIT: Will Detmold (NP), Phiala Shanahan (NP), Saman Amarasinghe (CSAIL)

Columbia: Norman Christ (HEP)

MSU: Huey-Wen Lin (NP),
Alexei Bazavov (CSE)

UConn: Tom Blum (HEP)

UIUC: Aida El Khadra (HEP)

William & Mary: Kostas Orginos (NP),
Andreas Stathopoulos (ASCR)



FNAL: Andreas Kronfeld* (HEP), Mike
Wagman (HEP), George Fleming (HEP)

BNL: Peter Boyle (HEP/ASCR),
Chris Kelly (ASCR)

JLab: Robert Edwards (NP)

ANL: James Osborn (ASCR)

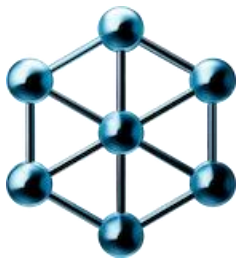
LBNL: Andre Walker-Loud (NP), Aydin
Buluc (ASCR), Sherry Li (ASCR)



NVIDIA: Kate Clark, Balint Joo,
Evan Weinberg

Google DeepMind: TBC





Proposal team

- Combines strong **academic, lab and industry** groups across the country
 - Builds on partnerships forged through 24 years of SciDAC projects and the Exascale Computing Project
- Industry connections are **deep, long-standing and intellectually rich**
 - NVIDIA: partner in LQCD software development since 2010
 - Google DeepMind: multiyear collaboration with Phiala on “the critical slowdown problem in lattice QCD”
 - No Genesis funds are planned to go to industry partners
- Team built across NP, HEP and ASCR supported groups
 - Strength in domain science and in AI/ML in HPC
- Brings **necessary computing resources** to the project (LQCD facilities at JLab, FNAL and BNL) and **early access to new hardware** through our partnerships

Phase II proposal

- We have **demonstrated Phase II readiness** through FemtoMind American Science Cloud project (FNAL, JLab, BNL, ANL; <https://amsc.energy.gov>)
- DOE HEP/NP & ASCR program managers have all told us this explicitly
 - Jeremy Love (HEP): “USQCD is very well positioned to submit a phase-2 application”
- **MIT leadership is critical to success** as we “own” the explicitly highlighted “critical slowdown problem in lattice QCD”
 - Astrid Morreale (NP): “that sentence is there for you guys”
 - **IAIFI-alignment** on this topic is also very strong
 - Other groups vying to lead project too
- Still waiting on details of the Phase 2 call (this week)
 - Lol: April 28. Proposal: May 19th. Budget: \$2–5M/y for 3y
- Overall budget ~\$3–4M/year supporting students, postdocs and research staff at partner institutions (similar in scale to LQCD SciDAC awards)



Deliverables & Metrics

Exact plans are still developing across the consortium but major thrusts will focus on

1. MIT, UIUC & Columbia: “**critical slowdown problem in lattice QCD**”

Eg:(MIT, year 1): Implementation of correlated sampling using normalizing flows for a broad class of observables. Expected AI/ML advantage >10x precision vs baseline based on preliminary work [[2603.02984](#)]

2. Fermilab & JLab: extensions of FemtoMind work on **agentic tools for HPC environments**
3. BNL, MIT, NVIDIA: **agentic approaches to HPC code development and optimization**
4. JLab, MIT, MSU: **distributed petascale dataset inference and insight**

We are seeking to support the whole USQCD community so a call is out for input. Provided there is cohesion, additional topics may be included

Workforce Development

USQCD has long history of training in physics and HPC

- **LGT4HEP DoE HEP Traineeship Program: 2022-now**
 - Students at MSU (PI), MIT, UIUC, UConn, UMd, Colorado
 - 2 semester online class taught by faculty across program
 - Summer internship at DOE lab
 - <http://lgt4hep.github.io>
- Under Genesis we would expand access to more institutions
- Proposal will also emphasize **strong pipeline from LQCD to computing and AI companies** dating back to the 90s
 - Many LQCD PhDs now working at NVIDIA, Intel, ...
 - Many also work at DOE & NNSA labs

