Computational challenges in lattice simulations of low–energy Quantum Chromodynamics

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Presentation Plan

- An introduction to Lattice QCD
- Computational challenges – solvers
- MG solvers for QCD systems

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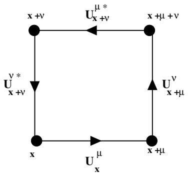
Preliminaries and notation



4d space-time becomes discrete lattice

- Gauge potentials, $A_\mu \in su(3)$, integrated over lattice links

$$U_x^\mu = \exp\left(igA_\mu(x + a\frac{\mu}{2})\right) \approx \exp\left(\int_{x+\mu}^{x} igA_\mu(x)dx\right), U_x^\mu \in SU(3)$$

- Gamma matrices: $\gamma_\mu \in \mathbb{C}^{4\times 4}$, $\mu = 1, 2, 3, 4$, $\{\gamma_\mu, \gamma_\nu\} = \delta_{\mu,\nu} I$ and $\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 = \gamma_5^*$
- $\psi_{s,c}^j$: $s = 1, 2, 3, 4,\ c = 1, 2, 3,\ j = 1, .., n_f \quad (n_f = 1)$

K. Wilson, *Confinement of Quarks*, Phys. Rev. D10, 2445 (1974)

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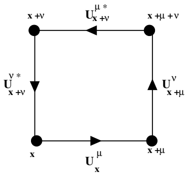

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- $\psi_{s,c}^j$: $s = 1, 2, 3, 4$, $c = 1, 2, 3$, $j = 1, .., n_f$ $\quad (n_f = 1)$
- Covariant finite differences: $\quad \frac{e^{iagA_\mu(x+a\frac{\mu}{2})}\psi(x+a\mu)-\psi(x)}{a} \approx (\partial_\mu + igA_\mu)\psi(x)$
- Plaquette variables: $U_p = U_x^\mu U_{x+\mu}^\nu U_{x+\nu}^{\mu *} U_x^{\nu *}$

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Lattice QCD path integral

$$\langle \Omega[U] \rangle = \frac{1}{Z} \int \Omega[U] \det(M[U]) e^{-S_g[U]} [dU], \quad [dU] = \prod_{x,\mu} dU_{x,\mu}$$

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  - Interpret $\det(M[U])e^{-S_g[U]}$ as a *Boltzman* weight and use importance sampling to generate $\{U_k\}$: $P(U_k) \propto \frac{1}{Z} \det(M[U])e^{-S_g[U]}$

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- Approximating $\det(M[U])$ (pseudu-fermions):

$$\det(M[U]) = \int e^{-\phi^* M^{-1}[U]\psi} [d\phi^*][d\psi] := \int e^{-S_f(U,\phi^*,\psi)} [d\phi^*][d\psi]$$

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Dirac PDE

$$(\gamma_\mu D_\mu + m)\psi \quad = \quad \sum_\mu \sum_s (\gamma_\mu e_s) \otimes (D_\mu \psi_s) + m(e_s \otimes \psi_s)$$

where $\psi_s : \mathbb{R}^4 \mapsto \mathbb{C}^3$ and $e_s \in \mathbb{C}^4,\ s = 1, .., 4$

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Wilson's discretization adds a scaled Laplacian term, $a\Delta_a$:

$$(M\psi)_x = \sum_\mu P_\mu^+ \otimes U_x^\mu \psi_{x+\mu} + P_\mu^- \otimes U_{x-a\mu}^{\mu *} \psi_{x-\mu} + m_q \psi_x,$$

where $P_\mu^\pm = \frac{1}{2a}(I \pm \gamma_\mu)$ and $m_q = m + \frac{4}{a}$

- Breaks chiral symmetry, $[\gamma_5, M] \neq 0$

The Overlap Operator

$$
\begin{aligned}
N_M &= I + M(M^*M)^{-1/2} \\
&= \gamma_5(\gamma_5 + sign(Q)) \\
&= \gamma_5 N_Q
\end{aligned}
$$

- $Q = \gamma_5 M \Rightarrow Q^* = Q$
- $sign(Q) = V\,sign(\Lambda)V^*$
- $sign(Q) = Q\left(Q^2\right)^{-1/2}$

- Represented by a dense matrix $\Rightarrow$ cannot be determined explicitly. Instead use a nested iteration for

$$(\gamma_5 + sign(Q))\,\psi = \phi$$

  - *outer* iteration: MVM with N_Q
  - *inner* iteration: approximate $sign(Q)v$ in $N_Q v$

Rational approximation of the Overlap Operator

Idea: Approximate

$$sign(t) \approx r(t) = \sum_{i=1}^{m} \omega_i \frac{t}{t^2 + \tau_i} \in R_{2m-1,2m}$$

Then

$$sign(Q)b \approx r(Q)b = \sum_{i=1}^{m} \omega_i Q \left(Q^2 + \tau_i I\right)^{-1} b$$

Known: spec$(Q) \subseteq [-b, -a] \cup [a, b]$, $0 < a < b$

Can solve all these m systems *in one stroke*
('Multishift CG') since

$$K_m(Q^2, b) = K_m(Q^2 + \tau_i I, b),\ i = 1, 2, \ldots, m$$

On the best approximation

Theorem (Zolotarev)

The (l_∞-) best approximation to sign(t) on $[-b/a,-1]\cup[1,b/a]$ *from* $R_{2m-1,2m}$ *is*

$$r(t) = ts(t^2) \quad \textit{where} \quad s(t) = D\frac{\prod_{i=1}^{m-1}(t+c_{2i})}{\prod_{i=1}^{m}(t+c_{2i-1})},$$

where

$$c_i = \frac{\mathrm{sn}^2\left(iK/(2m); \sqrt{1-(b/a)^2}\right)}{1-\mathrm{sn}^2\left(iK/(2m); \sqrt{1-(b/a)^2}\right)},$$

K complete elliptic integral

D determined through

$$\max_{t\in[1,(b/a)^2]}\left(1-\sqrt{t}s(t)\right) = -\min_{t\in[1,(b/a)^2]}\left(1-\sqrt{t}s(t)\right)$$

Tasks in Lattice Simulations

1. Discretize gauge and fermion actions to preserve symmetries of the continuum
   - Least squares formulation – w/ BU & CU
2. Generate gauge configurations according to QCD Lagrangians
   - Multi-scale updates based on Compatible Monte Carlo Sweeps – w/ BU, Yale, & UCLA
3. Generate quark propagators for each gauge configuration: Solving $Mx = b$
   - Multi-scale preconditioners – all
4. Write the lattice form of operators which represent observables (e.g., two-point correlation functions for mass)
5. Calculate those operators (which involve quark propagators) for each configuration, approximating $(M^{-1})_{ij}$, $\det(M)$, $\mathrm{trace}(M^{-1})$
   - unbiased multi-scale variance reduction of stochastic trace estimators – w/ BU
6. Analyze data by averaging over various configuration

Multigrid for QCD circa 2000

R. Ben-Av et al, *Fermion simulations using parallel transported multigrid*, Phys. Lett. **B253** (1991), pp. 185–192.

R. Ben-Av, M. Harmatz, S. Solomon, and P. G. Lauwers, *Parallel transported multigrid for inverting the dirac operator: Variants of the method and their efficiency*, Nucl. Phys.**B405** (1993), pp. 623–666.

A. Brandt, *Multigrid methods in lattice field computations*, Nucl Phys. Proc. Suppl. **26** (1992), pp. 137–180.

R. C. Brower, T. Ivanenko, A. R. Levi, and K. N. Orginos, *Chronological inversion method for the dirac matrix in hybrid monte carlo*, Nucl. Phys. **B484** (1997), pp. 353–374.

R. C. Brower, E. Myers, C. Rebbi, and K. J. M. Moriarty, *The multigrid method for fermion calculations in quantum chromodynamics*, (1993), Print-87-0335, IAS,PRINCETON.

R. C. Brower, K. J. M. Moriarty, C. Rebbi, and E. Vicari, *Multigrid propagators in the presence of disordered u(1) gauge fields*, Phys. Rev. **D43** (1991), pp. 1974–1977.

R. C. Brower, C. Rebbi, and E. Vicari, *Projective multigrid for propagators in lattice gauge theory*, Phys. Rev. Lett. **66** (1991) pp. 1263–1266.

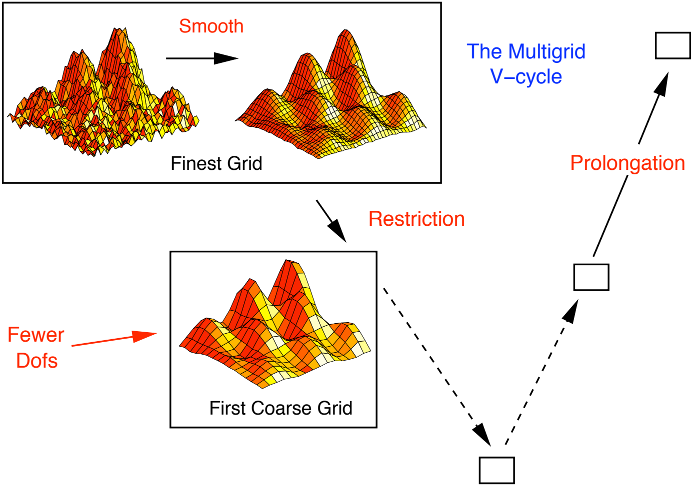
R. C. Brower, et. al., *Projective multigrid for Wilson fermions*, Nucl. Phys. **B366** (1991), pp. 689–705.

P. Hasenfratz, *Prospects for perfect actions*, Nucl. Phys. Proc. Suppl. **63** (1998), pp. 53–58.

A. Hulsebos, J. Smit, and J. C. Vink, *Multigrid inversion of the staggered fermion matrix with u(1) and su(2) gauge fields*, in Juelich 1991, Proceedings, Fermion algorithms (QCD161:W573:1991), pp. 161-168.

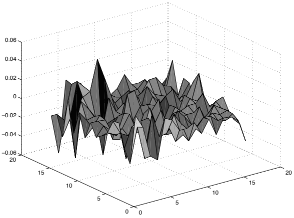
Many others ...

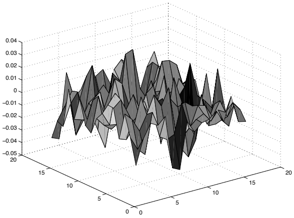
Basic MG components



Multigrid for QCD circa 2000 ...

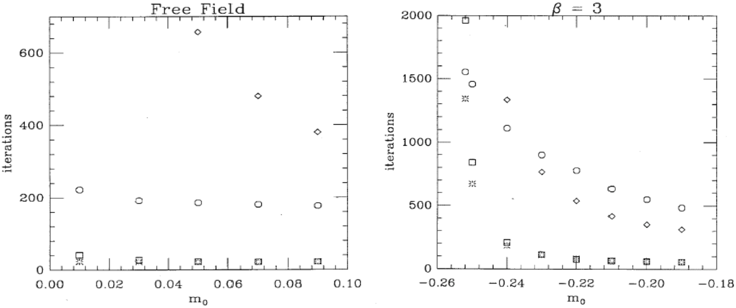
- Gauge field U is not geometrically smooth $\Rightarrow$ near kernel is locally oscillatory





- Constant preserving (algebraic) multigrid methods completely fail
- Overall, Lattice QCD and MG have long and painful history, e.g.,
  - Parallel Transport MG, *Lauwers et al*: attempt to define coarse-scale fields consistent with fine-scale
  - Renormilization Group approaches, *de Forcrand et al*: smooth out the fields within gauge field equivalence classes (gauge invariance) to generate systems more amenable to constant preserving MG techniques
  - Projective (adaptive) MG, *Brower et al*: semi-adaptive methods that solve local eigenvalue problems to characterize near kernel and and define a coarse-scale basis

Multigrid for QCD circa 2000 ...



Jacobi (Diamond), CG (circle), MG V-cycle (square), W-cycle (star)

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Solver challenges:

- Systems are nearly singular
- Non-hermitian and positive real or hermitian and maximally indefinite
- Near kernel is unknown: highly oscillatory with oscillations dependent upon fluctuations in background gauge fields $\leftarrow$ heterogeneity of covariant derivatives
- Large near kernel dependent upon on topology

Multi-scale iterative solvers in lattice computations

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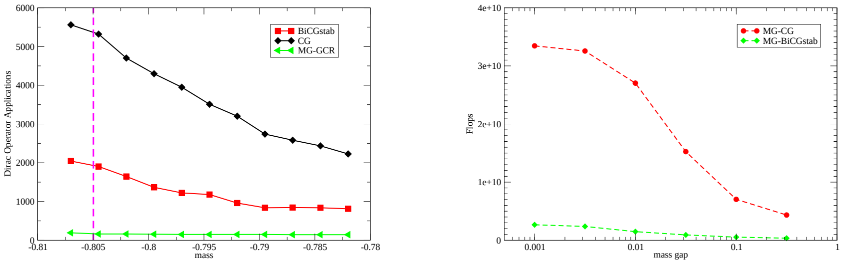
What is needed? A method that can

- Approximate several "arbitrary" kernel components to within desired level of accuracy
- Extract the components from the algebraic problem
- Automatically construct coarse–level basis

Results: 4D Dirac–Wilson system

- Adaptive smoothed aggregation MG for M
- $M \in \mathbb{C}^{N\times N}, \quad N = 32^3 \cdot 64 \cdot 12$
- $\beta = 5.6$, typical configuration



Number of applications of M (left) and flops (right) needed to reduce relative residual by $O(10^{10})$

Adaptive MG Algorithm for Lattice QCD J. Brannick, R. Brower, M. Clark, J. Osborne, and C. Rebbi, PRL-100(4), 2007, The removal of critical slowing down, —, Lattice 08 Proc.

Outlook

- Solver development effort yielding optimal methods for M and thus for N_M
- Currently focused on optimizing performance in first assembly language implementation for BG/P
- Implementing MG solver on GPU's
- Beginning with development of multi-scale methods for HMC and trace calculations used in disconnected diagram calculaitons
- Long-term: finite element model for QCD Lagrangian

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Funding for two postdoc positions and several PhD students (ANL-ALCF: sum. prog., BU: ECE, Physics, PSU: Math)