Dynamical fermion algorithms and many flavor simulations on the lattice

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Lattice Gauge Theory for LHC Physics

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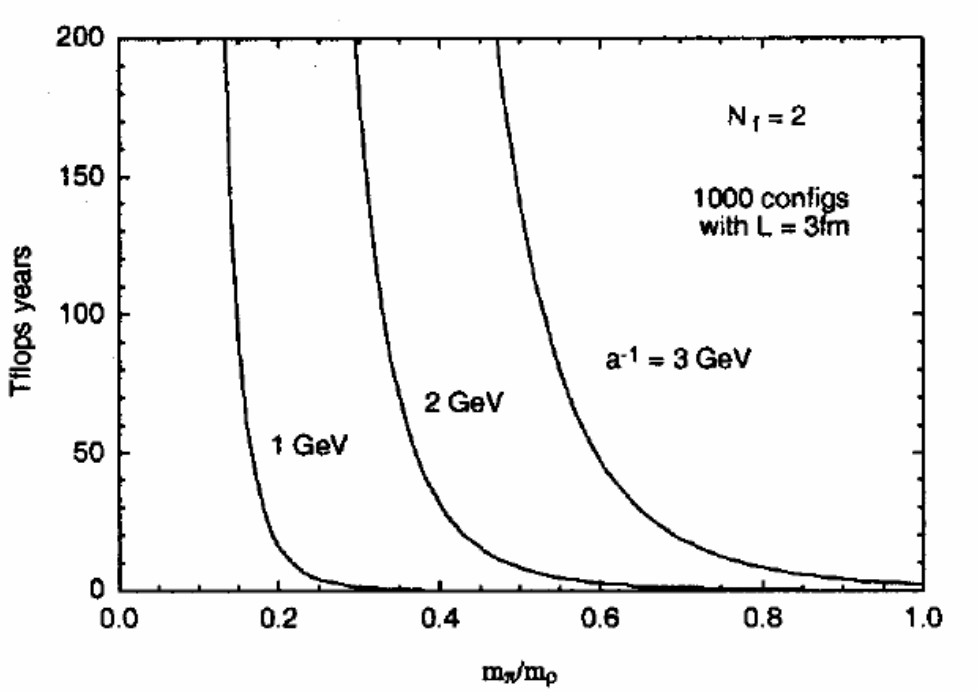
Contents

- Lattice QCD with Dynamical Fermions
- Hybrid Molecular Dynamics
- RHMC
- Multiple time scales and Hasenbusch pre-conditioning.
- Advanced integrators
- Gap DWF

The Berlin Wall



Ukawa (Lattice 2001) – Improved Wilson quarks

$$\mathbf{Cost} \sim \mathbf{L}^{5} \left(\frac{\mathbf{1}}{\mathbf{m}_{\pi}}\right)^{\mathbf{5-6}} \mathbf{a}^{\mathbf{7-8}}$$

The situation at Lattice 2001 (Berlin)

Cost for generating gauge configurations with dynamical fermions scales like a large power of the pion mass.

Despite exponential increase of CPU power, lattice simulations with realistic quark masses appeared out of reach in near future.

Where is the problem?

$$\mathbf{Cost} \sim \mathbf{L}^{5} \left(\frac{\mathbf{1}}{\mathbf{m}_{\pi}}\right)^{5-6} \mathbf{a}^{7-8}$$

Main problem comes with severe scaling with m_l (m_π)

1. One factor of $\left(\frac{1}{m_\pi} a\right)^{1-2}$ from critical slowing down.
2. Factor of $\frac{1}{m_l a} \sim \left(\frac{1}{m_\pi a}\right)^{2}$ from condition number of fermion matrix
3. Factor $\frac{1}{m_l a} \sim \left(\frac{1}{m_\pi a}\right)^{2}$ for step-size dependence on light quark mass.

Sampling the Gauge Fields

$$\ln Z = \int [\mathcal{D}U][\mathcal{D}\bar{\psi}][\mathcal{D}\psi] \exp\left(-S_g(U) + \sum_q \bar{\psi}_q M_q \psi_q\right)$$

Integrate out the fermion fields:

$$\ln Z = \int [\mathcal{D}U] \prod_q Det(M_q(U)) \exp\left(-S_g(U)\right)$$

- Want to sample gauge fields, *U* with given Boltzmann weight.
- *Det(M_q(U))* is costly to calculate.
- Quenched approximation → Omit fermion determinant (neglect quark loops) → Incorrect equilibrium distribution.
- Require method that incorporates fermion determinant

Hybrid Molecular Dynamics

- Old single-link updating used for pure gauge theory insufficient:
  - Local update, but fermion determinant is non-local.
  - Random walk exploration of phase space too slow.
- Hybrid Molecular Dynamics (**HMD**) – **Duane & Kogut, Gottlieb, et. al.** (mid 1980s)
- Use molecular dynamics to change all gauge link variables simultaneously to produce a new configuration.
- Directed march through phase space → more efficient phase space exploration.
- Dominant mode for dynamical fermion calculations for next 15 years.

HMC Φ Algorithm

Idea: Introduce pseudo-fermion field (Φ field) and fictitious momentum to create Hamiltonian:

$$\mathbf{H} = \sum_{\mathbf{i}} \frac{\mathbf{p_i^2}}{\mathbf{2}} + \mathbf{S_g(U)} + \phi_{\mathbf{i}}^{\dagger} \left(\mathbf{M^{\dagger}(U)M(U)}\right)_{\mathbf{ij}}^{\mathbf{-1}} \phi_{\mathbf{j}} = \sum_{\mathbf{i}} \frac{\mathbf{p_i^2}}{\mathbf{2}} + \mathbf{V(U)}$$

Evolve all fields in fictitious time with Hamilton's EOM using numerical "leapfrog" integrator.

$$\begin{aligned} \mathbf{p_i(t + \Delta t/2)} &= \mathbf{p_i(t - \Delta t/2)} + \frac{\delta \mathbf{V}}{\delta \mathbf{U}}\mathbf{(t)\Delta t} \\ \mathbf{U_i(t + \Delta t)} &= \mathbf{exp\left(ip_i(t + \Delta t/2)\right) U_i(t)} \end{aligned}$$

Hamiltonian conserved up to $\mathbf{O(\delta t^2)}$ step-size errors. Apply Metropolis test to enforce detailed balance.

However, only works for 2 flavor Wilson, 4 flavor staggered!

R Algorithm

For staggered fermions, fermion matrix is naturally 4-flavored.
Take roots of fermion determinant to approximate fewer flavors:

$$\mathbf{N_f\ flavors} \approx \left(\mathbf{det}(\mathbf{M^\dagger_{stag} M_{stag}})\right)^{\mathbf{N_f/4}} = \mathbf{exp}\left(\frac{\mathbf{N_f}}{\mathbf{4}}\mathbf{tr\ ln}(\mathbf{M^\dagger_{stag} M_{stag}})\right)$$

Can no longer introduce Φ field. Hamiltonian becomes:

$$\mathbf{H} = \sum_{\mathbf{i}} \frac{\mathbf{p_i^2}}{\mathbf{2}} + \mathbf{S_g(U)} - \frac{\mathbf{N_f}}{\mathbf{4}}\mathbf{tr\ ln}\left(\mathbf{M^\dagger(U) M(U)}\right)^{\mathbf{-1}}$$

Must calculate contribution from fermions stochastically → detailed balance is spoiled → can't apply Metropolis.

R Algorithm introduces $\mathbf{O(\delta t^2)}$ errors to equilibrium ensemble.
Must use many different step sizes and extrapolate, or extremely small step size.

Rational Hybrid Monte Carlo (RHMC)

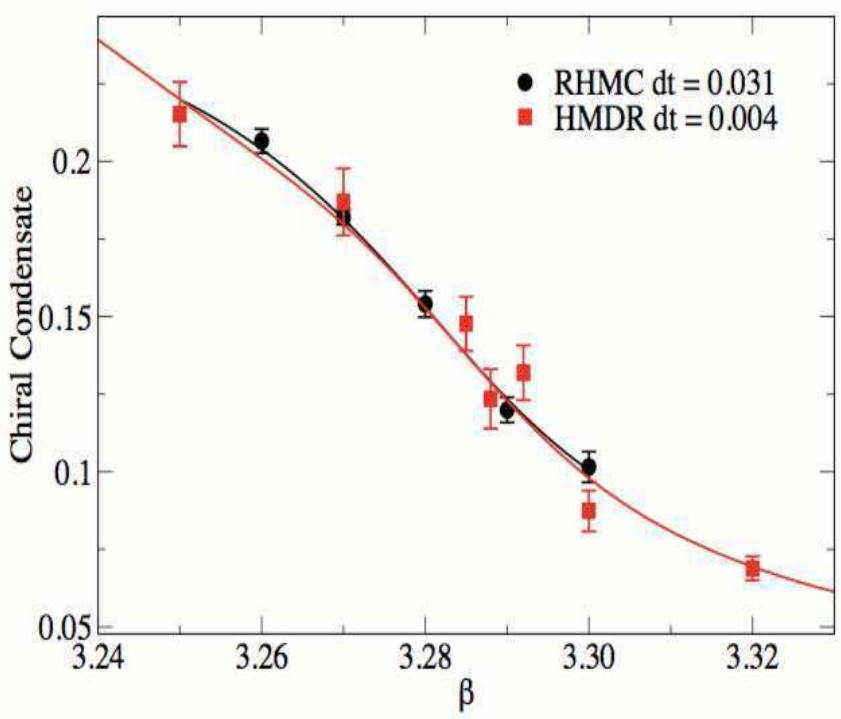
- R Algorithm necessary for realistic 2+1 flavors, but is inexact.
- RHMC (**Clark + Kennedy**) → Exact algorithm usable with any number of flavors.
- Problem with R Algorithm: No explicit form for $\left(\mathbf{M}^\dagger\mathbf{M}\right)^{-\mathbf{1/n}}$
- Solution: Use Rational Approximation.

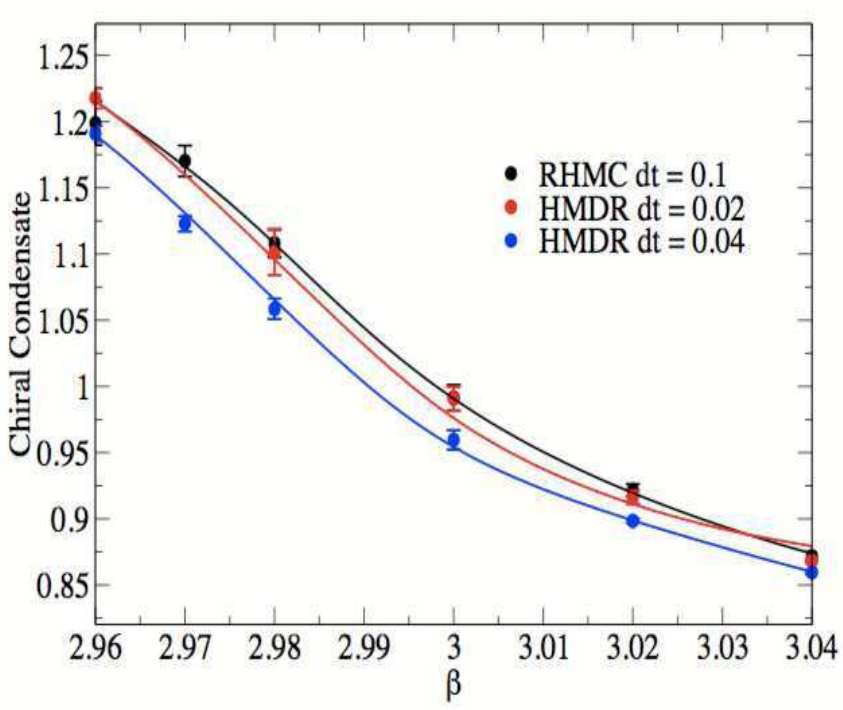
$$\mathbf{Det}\left(\mathbf{M}^\dagger\mathbf{M}\right)^{\mathbf{1/n}} = \int [\mathcal{D}\phi^\dagger][\mathcal{D}\phi]\ \mathbf{exp}\left(\phi^\dagger \mathbf{R^2}(\mathbf{M}^\dagger\mathbf{M})\ \phi\right);\ \mathbf{R}(\mathbf{x}) = \mathbf{x}^{-\mathbf{1/2n}}$$

Partial fraction expansion: $\mathbf{R}(\mathbf{x}) = \sum_{\mathbf{i=1}}^{\mathbf{m}} \frac{\alpha_\mathbf{k}}{\mathbf{x}+\beta_\mathbf{k}}$

Φ field can be introduced as in HMC Φ, Hamiltonian conserved during molecular dynamics evolution. No need to extrapolate to δt → 0, just apply Metropolis test.

R vs. RHMC





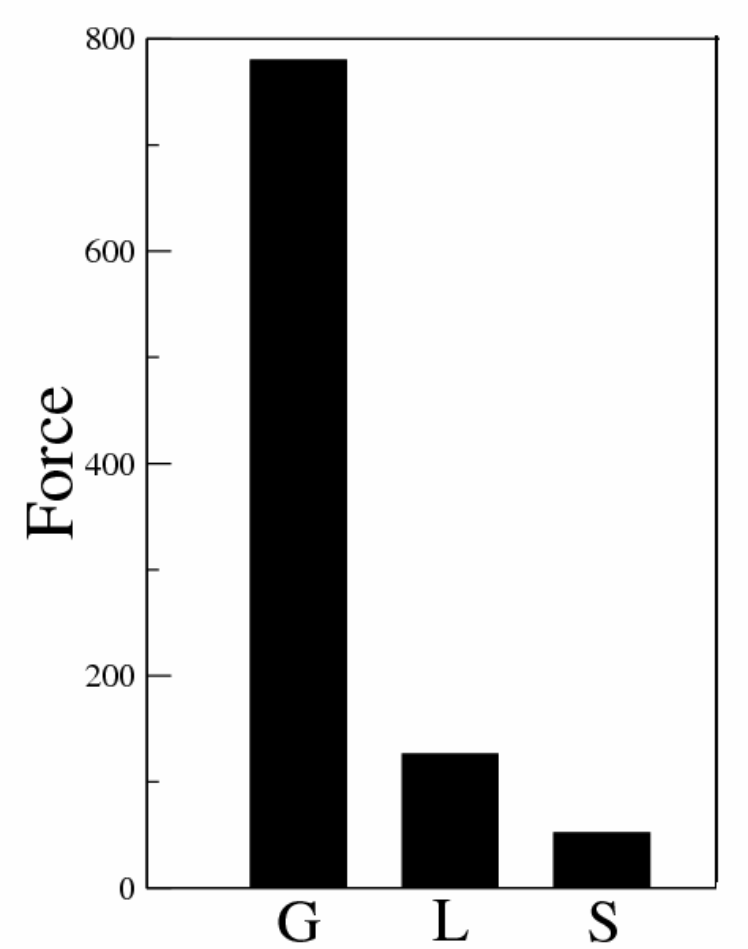
8^3x4 p4 staggered fermions, Nf = 3, ma = 0.01 (left), ma = 0.1 (right),

Much larger δt usable with RHMC than R, Step size dependence much weaker than 1/ma.

The Molecular Dynamics Integrator

- What limits the step size, δt?
- Need δH of reasonable size otherwise Metropolis step will not accept often enough.
- If $\mathbf{F} = \frac{\delta \mathbf{V}}{\delta \mathbf{U}}$ is too large, F δt is a poor approximation for the correct energy-conserving time evolution.
- $\mathbf{F}_{\mathbf{gauge}} \gg \mathbf{F}_{\mathbf{fermions}}$ - but cost of calculating fermion force much greater than gauge force.
- Multiple time-scales (**Sexton & Weingarten**)

$$\mathbf{F}_{\mathbf{gauge}} \delta \mathbf{t}_{\mathbf{gauge}} \sim \mathbf{F}_{\mathbf{fermion}} \delta_{\mathbf{fermion}}$$



Closer look at Fermion Force

- Calculation of fermion force is most expensive part of HMD evolution because it requires a matrix inversion.
- Idea: Spectrum of Dirac operator is dominated by UV modes which are insensitive to m_q. However, it is the relatively few IR modes sensitive to m_q that drive up the condition number of M.
- UV modes contribute most to the $F_{fermion}$, but it is IR modes which make cost of molecular dynamics ~ $1/m_q$
- Separate UV from IR so that the IR modes (which costs most but has relatively small force) can be done less often.
- Many ideas:
  - Hasenbusch “mass preconditioning”
  - Luscher “domain decomposition”
  - Peardon & Sexton “Polynomial Filtering”
  - Deflation, Multi-Grid

Hasenbusch mass preconditioning

Consider fermion determinant for a light quark flavor:

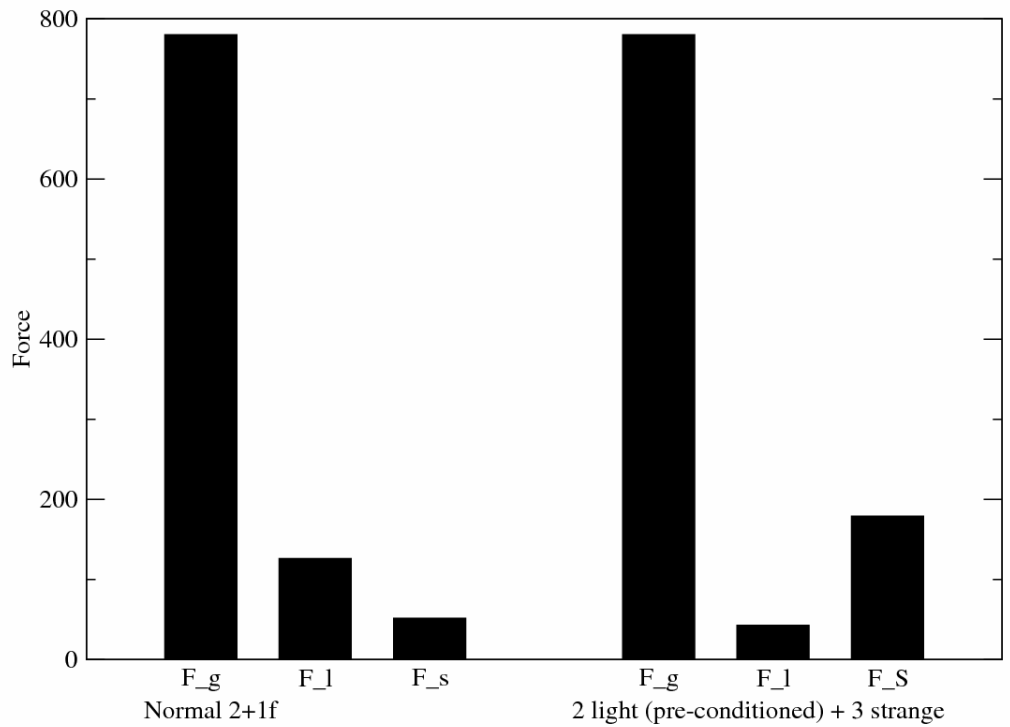
$$\mathbf{Det}\left(\mathbf{M}^{\dagger}(\mathbf{m_l})\mathbf{M}(\mathbf{m_l})\right) = \mathbf{Det}\left(\mathbf{M}^{\dagger}(\mathbf{m_{pre}})\mathbf{M}(\mathbf{m_{pre}})\right)\mathbf{Det}\left(\frac{\mathbf{M}^{\dagger}(\mathbf{m_l})\mathbf{M}(\mathbf{m_l})}{\mathbf{M}^{\dagger}(\mathbf{m_{pre}})\mathbf{M}(\mathbf{m_{pre}})}\right)$$

$m_{pre} > m_l$: UV modes are relatively insensitive to quark mass, so dividing with $\mathbf{M}^{\dagger}(\mathbf{m_{pre}}\mathbf{M}(\mathbf{m_{pre}})$ effectively removes UV modes from Term 2, leaving only IR modes. Term 1 easier to invert.

$$\mathbf{lnZ} = \int [\mathcal{D}\phi_{\mathbf{i}}^{\dagger}][\mathcal{D}\phi_{\mathbf{i}}]\mathbf{exp}\left(\phi_{\mathbf{1}}^{\dagger}\frac{\mathbf{1}}{\mathbf{M}^{\dagger}(\mathbf{m_{pre}})\mathbf{M}(\mathbf{m_{pre}})}\phi_{\mathbf{1}} + \phi_{\mathbf{2}}^{\dagger}\frac{\mathbf{M}^{\dagger}(\mathbf{m_{pre}})\mathbf{M}(\mathbf{m_{pre}})}{\mathbf{M}^{\dagger}(\mathbf{m_l})\mathbf{M}(\mathbf{m_l})}\phi_{\mathbf{2}}\right)$$

Calculate force from Φ_1 with time step δt_1, Φ_2 with time step δt_2 so that $F_1\ \delta t_1 \sim F_2\ \delta t_2$

Hasenbusch mass preconditioning



- Hasenbusch preconditioning effectively removes most of the force contribution from the light quark part of the action
- Need extra (easier) inversions of the strange quark part.

Integrators

Hamiltonian: $\mathbf{H} = \sum_{\mathbf{i}} \frac{\mathbf{p_i^2}}{\mathbf{2}} + \mathbf{S_g(U)} + \mathbf{S_F(U)} = \mathbf{T(p)} + \mathbf{V(U)}$

Define: $\hat{\mathbf{Q}}(\mathbf{t}) = \mathbf{exp}\left(\mathbf{tT'(p)}\frac{\partial}{\partial \mathbf{U}}\right)$; $\hat{\mathbf{P}}(\mathbf{t}) = \mathbf{exp}\left(-\mathbf{tV'(U)}\frac{\partial}{\partial \mathbf{p}}\right)$

$$\hat{\mathbf{Q}}(\mathbf{\Delta t})\mathbf{U(t)} = \mathbf{U(t+\Delta t)}; \quad \hat{\mathbf{P}}(\mathbf{\Delta t})\mathbf{p(t)} = \mathbf{p(t+\Delta t)}$$

Arbitrary symplectic integrators can be made from combinations of $\hat{\mathbf{Q}}, \hat{\mathbf{P}}$

Leapfrog (PQP) integrator:

$$\hat{\mathbf{G}}_{\mathbf{LF}}(\mathbf{t}) = \left(\hat{\mathbf{P}}(\delta \mathbf{t}/\mathbf{2})\hat{\mathbf{Q}}(\delta \mathbf{t})\hat{\mathbf{P}}(\delta \mathbf{t}/\mathbf{2})\right)^{\mathbf{t}/\delta \mathbf{t}}$$

Omelyan Integrator

Omelyan Integrator (**Omelyan, de Forcrand, Takaishi**):

$$\hat{\mathbf{G}}_{\mathbf{Omelyan}}(\mathbf{t}) = \left(\hat{\mathbf{Q}}(\lambda\delta\mathbf{t})\hat{\mathbf{P}}(\delta\mathbf{t}/\mathbf{2})\hat{\mathbf{Q}}((\mathbf{1}-\mathbf{2}\lambda)\delta\mathbf{t})\hat{\mathbf{P}}(\delta\mathbf{t}/\mathbf{2})\hat{\mathbf{Q}}(\lambda\delta\mathbf{t})\right)^{\mathbf{t}/\delta\mathbf{t}}$$

λ is a tunable parameter. Empirically, for DWF $\lambda \approx \mathbf{0.22}$

Like leapfrog, Omelyan is also second-order integrator, i.e. corrections of $\mathbf{O}(\delta\mathbf{t}^{\mathbf{2}})$, but tuned to give small corrections.

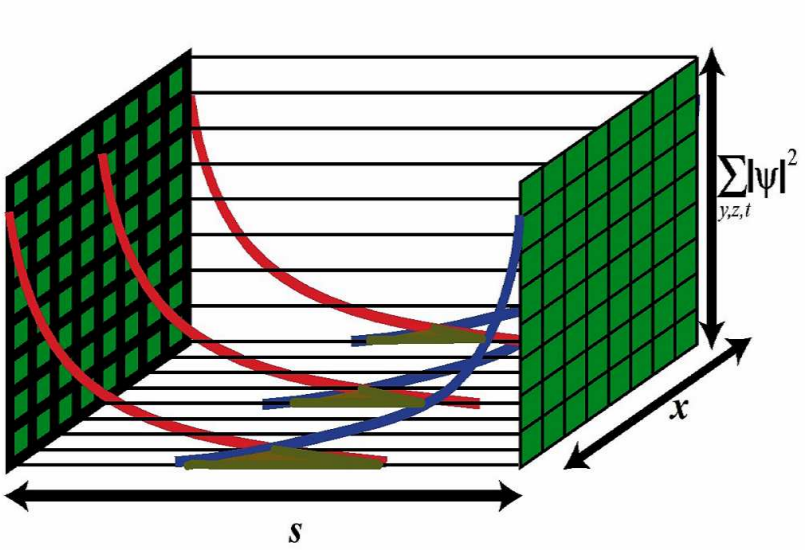
δH for Omelyan integrator about order of magnitude smaller than leapfrog at fixed δt, but extra force calculation.

Net effect is approximately 50% gain in CPU cost.

Same formalism can be used for higher order integrators: $\mathbf{O}(\delta\mathbf{t}^{\mathbf{n}})$

Domain Wall Fermions

- Domain Wall Fermions – more expensive than Wilson, staggered, but preserve exact chiral symmetry as Ls → ∞
- Four-dimensional chiral states bound to domain walls, mixing of chiral states suppressed by 5-D extent
- At strong coupling, residual chiral symmetry breaking is dominated by localized “lattice dislocations” – not well suppressed by increasing Ls.



Lattice dislocations correspond to near-zero modes of 4-D Wilson operator, $D_{Wilson}(M_5)$

Gap DWF

- Gap DWF (**Vranas**) – Explicitly Suppress these localized modes by adding extra term to Boltzmann weight:

$$\mathbf{Det}(\mathbf{M_{DWF}})\mathbf{exp}\,(-\mathbf{S_g}) \rightarrow \mathbf{Det}(\mathbf{D^2_{Wilson}}(\mathbf{M_5})\ \mathbf{Det}(\mathbf{M_{DWF}})\mathbf{exp}\,(-\mathbf{S_g})$$

- States with small λ (which spoil chiral symmetry) are given an additional weight of λ^2 from added term $D_{Wilson}(M_5)$
- Introduction of 4-D Wilson Dirac Operator does not affect physics – heavy quark mass only renormalizes bare parameters.
- Unfortunately, these same states drive topology change.
- Results in an infinite energy barrier for low-lying eigenstates to make zero-crossings that change topology.
- Need method that controls residual chiral symmetry breaking, but does not completely eliminate topological tunneling.

Twisted Gap?

Augment Boltzmann weight using twisted-mass Wilson fermions:

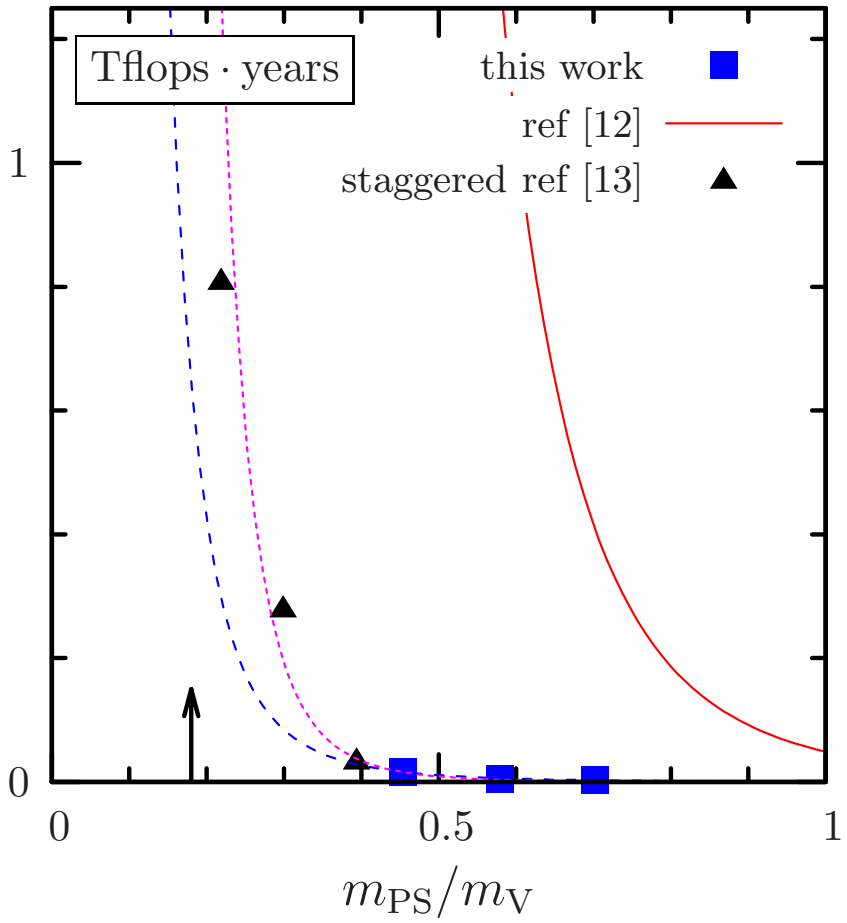
$$\mathbf{Det}(\mathbf{M_{DWF}})\mathbf{exp}\,(-\mathbf{S_g}) \rightarrow \mathbf{Det}(\frac{\mathbf{D_W^2}(\mathbf{M_5})+\epsilon^{\mathbf{2}}}{\mathbf{D_W^2}(\mathbf{M_5})+\delta^{\mathbf{2}}})\ \mathbf{Det}(\mathbf{M_{DWF}})\mathbf{exp}\,(-\mathbf{S_g})$$

- Choose ε small (but non-zero) so that small eigenvalue modes are suppressed but not completely eliminated → residual chiral symmetry breaking is under control, but topology changes is not eliminated.
- Choose δ > ε so that high-momentum modes are not affected.
- Currently under investigation by RBC
- May be useful for many flavor simulations where added fermions push the bare parameters to stronger coupling.

Scaling with N_f

- Lattice calculations with many flavors more difficult than normal QCD calculations.
- More flavors → larger fermion forces that require the use of smaller step sizes with HMC: $\delta t \sim N_f^{-3/2}$
- To see "walking" behavior in many flavor QCD → two dynamically generated scales. Need a very large lattice box to correctly show behavior at both scales without significant distortion
- Recent proposal by LSD Collaboration:
  - ~2 TFlops for exploratory studies at $N_f = 4, 6$
  - Estimate of ~10 TFlops for careful study of finite volume effects, simulations with more flavors…

The Berlin Wall (revisited)



Plot from **Jansen, et. al.** with improved Wilson fermions.

Recent work by RBC suggests

(**Christ** Lattice 2007):

$$\mathbf{Cost} \sim \mathbf{L}^{4} \frac{\langle \bar{\mathbf{q}}\mathbf{q} \rangle}{\mathbf{m_l}}$$

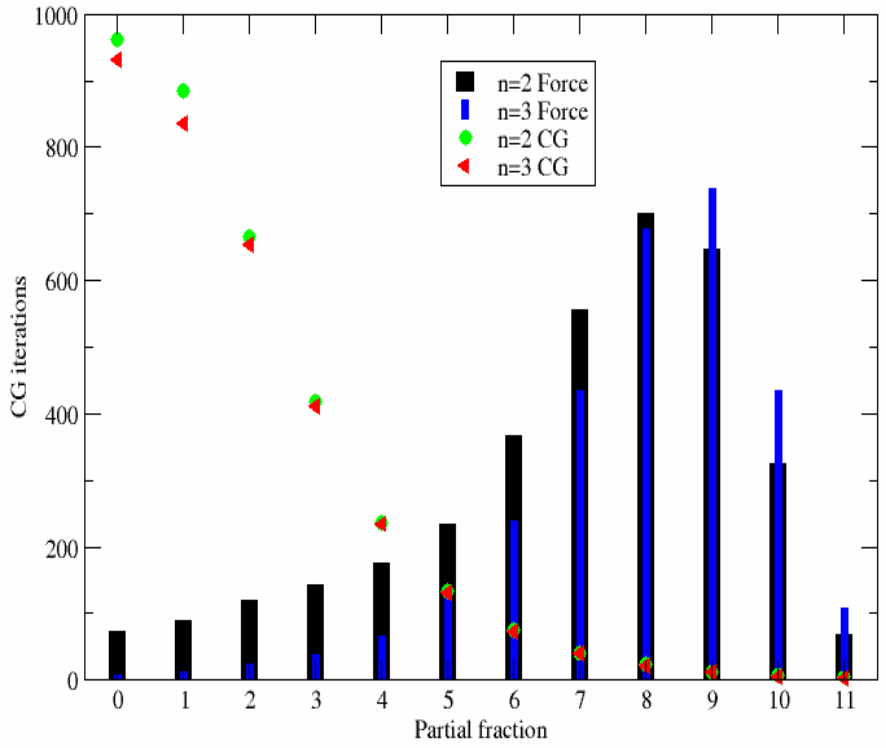
Calculations with realistic parameters feasible now with already-existing computational resources.

Conclusions

- Pessimistic estimates from 2001 did not account for algorithmic improvements.
- Severe scaling with quark masses is largely ameloriated with new techniques.
- Separation of scales: IR modes are computationally most costly, but were actually not the limiting factor for HMC.
- Many new techniques (mass preconditioning, domain decomposition, deflation) effectively separate IR and UV modes, allowing more “intelligent” HMC.
- Other methods (integrators, Gap DWF) also help.
- Arsenal of algorithms → on the cusp of realistic lattice calculations now, rather than 5-10 years from now,

BACKUP

Even Further…



Partial Fraction Expansion:

$$\mathbf{R(x)} = \sum_{\mathbf{i=1}} \mathbf{m} \frac{\alpha_{\mathbf{k}}}{\mathbf{x} + \beta_{\mathbf{k}}}$$

Terms with lightest poles (smallest β_k) are hardest to invert, convert relatively little to force.

Solve CG for lightest poles with less precision → small error in force for great CPU savings.