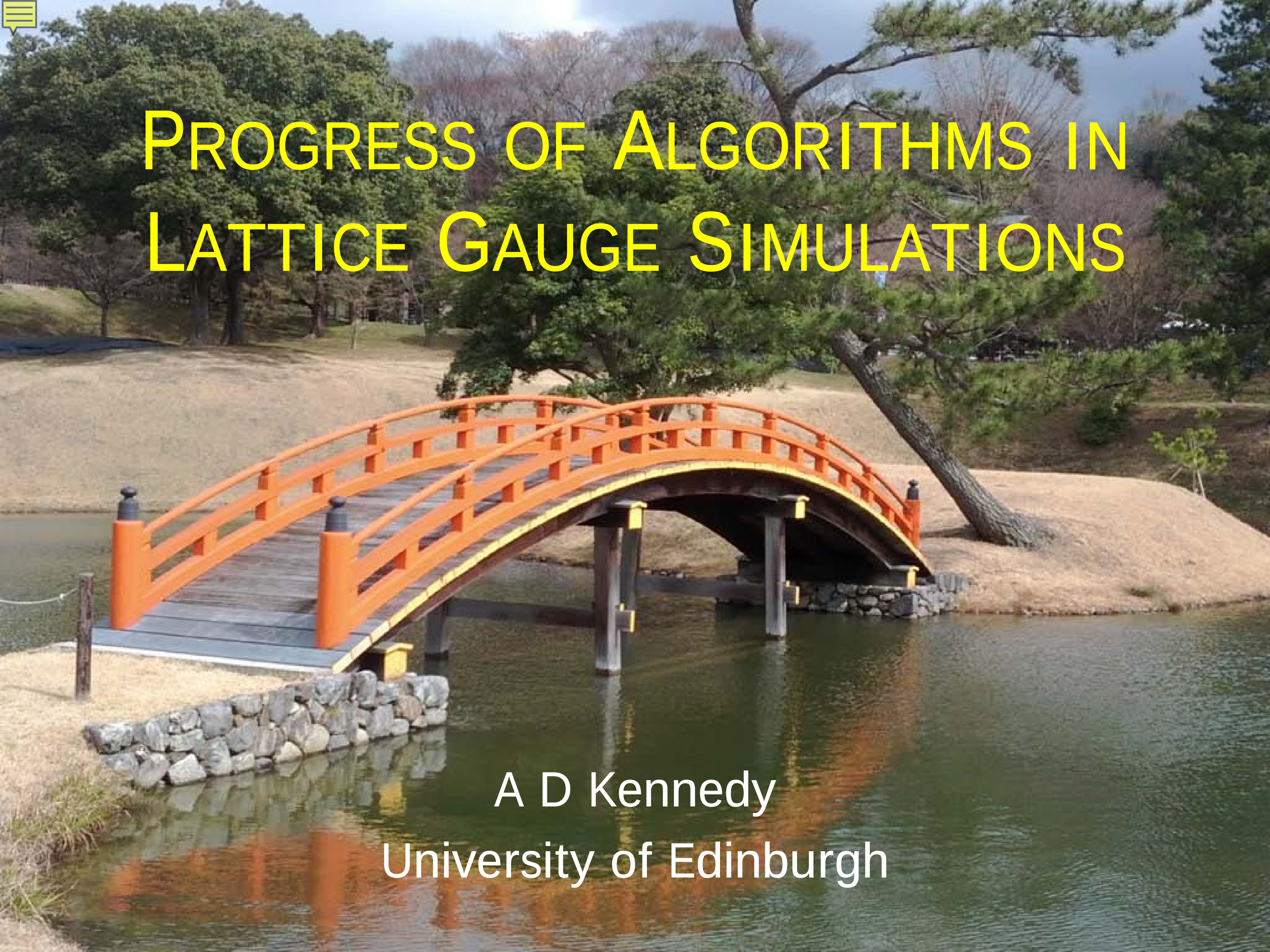

Progress of Algorithms in Lattice Gauge Simulations

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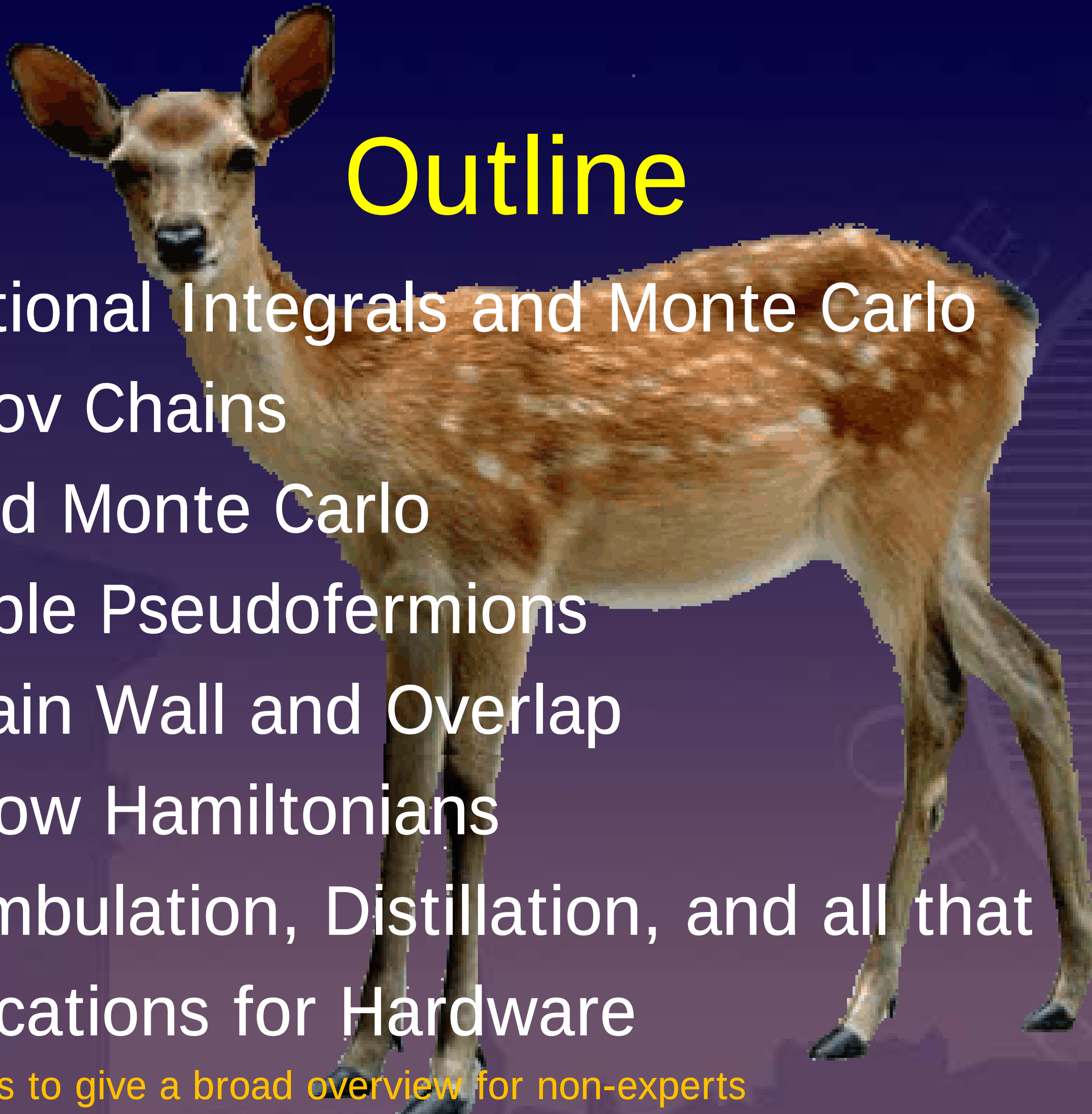
Outline



- Functional Integrals and Monte Carlo
- Markov Chains
- Hybrid Monte Carlo
- Multiple Pseudofermions
- Domain Wall and Overlap
- Shadow Hamiltonians
- Perambulation, Distillation, and all that
- Implications for Hardware
- My goal is to give a broad overview for non-experts

Introduction

- The goal of LGT is to solve quantum field theories non-perturbatively
- Not solving PDE
  - But we end up integrating Hamilton's equations anyhow
- Lots of linear algebra
- Well suited to large parallel computers

Functional Integrals

- The basic problem is just to evaluate the Feynman path integral for some interesting <u>action</u> S and <u>observable</u> □

$$\langle W \rangle = \frac{1}{Z} \square \, df \, W(f) e^{iS(f)}$$

  - This looks easy, but □ is a <u>field</u> and the integral is thus infinite dimensional

Euclidean Field Theory

- In order to make this numerically tractable we work in Euclidean space where $e^{iS} \rightarrow e^{-S}$ is real and positive
  - We will pay for this later when we want to make measurements
  - Similar to statistical mechanics

Configurations & Measurements

- Computations are split into two phases
  - Generate ensemble of field configurations
  - Make <u>measurements</u> on this ensemble

$$\overline{W} = \frac{1}{N}\sum_{n=1}^{N} W(\phi_n)$$

Monte Carlo

- The only feasible way of evaluating ∞ dimensional integrals is by Monte Carlo
- Hopeless without importance sampling
- Need to generate four dimensional field configurations with probability density

$$P(\phi)d\phi \propto e^{-S(\phi)}d\phi$$

Markov Chains

- Use ergodic Markov chain with this distribution as its fixed point
  - Ergodic means you can get from anywhere to anywhere with non-zero probability
- Fixed point $\leftarrow$ detailed balance $\leftarrow$ Metropolis
- We can mix different steps as long as they all have the same fixed point distribution
  - Individual steps do not need to be ergodic as long as a combined steps are ergodic

Hybrid Monte Carlo

- Introduce a “fictitious” Hamiltonian system with action as the potential

$$H(f,p) = \tfrac{1}{2}p^2 + S(f)$$

- Generate fields in this “phase space” with distribution

$$P(f,p) \propto e^{-H(f,p)}$$

Hamiltonian Monte Carlo

- We then use Hamilton’s equations to produce a reversible and area preserving Markov step
  - Perfect for Metropolis with acceptance probability

$$P_{\text{accept}} = \frac{P(f', p')}{P(f, p)} = e^{-dH(f, p)}$$

HMC

- To make this ergodic interleave it with a <u>momentum refreshment</u> Markov step
  - This just selects new momenta from a Gaussian heatbath
- Symmetric Symplectic Integrators
  - No step-size errors
  - Step-size just controls acceptance rate
  - Acceptance rate and trajectory length control autocorrelations
- Still interesting questions about scaling behaviour (Lüscher and Schaefer)

Fermions

- Fermions are anti-commuting (Grassmann) fields

$$Z(\eta,\bar{\eta}) = \int d\psi\, d\bar{\psi}\, e^{-\bar{\psi} M(\phi)\psi + \bar{\eta}\psi + \bar{\psi}\eta}$$

$$= \det M(\phi)\, e^{\bar{\eta} M(\phi)^{-1} \eta}$$

- This causes two <u>nasty</u> problems

Fermionic Observables

- Nasty problem #1
  - Need inverses of the fermion kernel for fermion correlators

$$\left\langle y(x)\,\bar{y}(y)\right\rangle = \frac{d^2 Z}{d\bar{h}(x)\,dh(y)} = M^{-1}_{x,y}(f)$$

Pseudofermions

- Nasty problem #2
  - Write the fermion determinant as a <u>bosonic</u> functional integral

$$\det \mathcal{M}(\phi) \propto \int d\bar{\chi}\, d\chi\, e^{-\bar{\chi}\mathcal{M}^{-1}(\phi)\chi}$$

  - These unphysical spin-half bosons are known as <u>pseudofermions</u>

Pseudofermion Heatbath

- We can easily generate pseudofermion fields from another Gaussian heatbath
- But we need to solve a linear system to update the gauge fields

$$\dot{p} = -\frac{\partial H}{\partial \phi} = -\frac{\partial}{\partial \phi}\left[S(\phi) + \bar{\chi} M^{-1}(\phi)\chi\right]$$

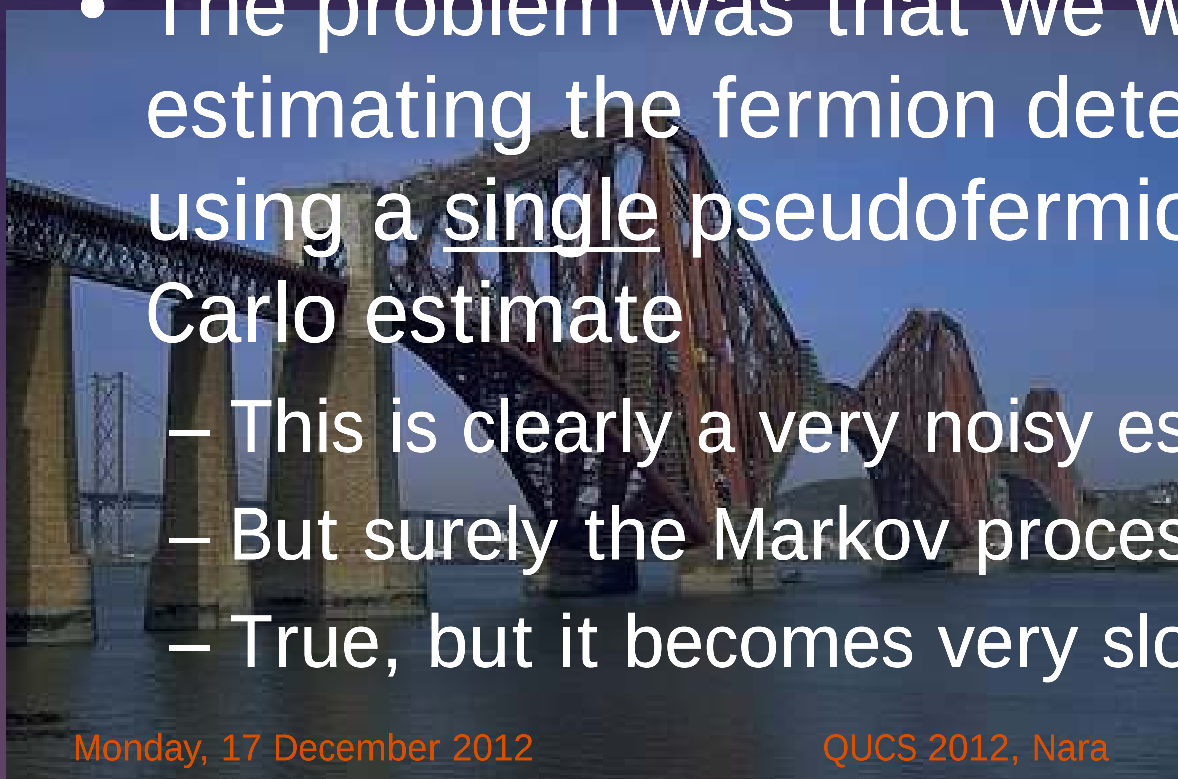
$$= -\frac{\partial S}{\partial \phi} + \bar{\chi} M^{-1}(\phi)\frac{\partial M(\phi)}{\partial \phi} M^{-1}(\phi)\chi$$

Pseudofermions Instability

- For a long time it was thought that it was prohibitively expensive to reach small (physical) quark masses
- The HMC integrator step size had to be very small for light fermions to avoid instabilities
- This was thought to be caused by the Dirac operator (fermion kernel) becoming almost singular

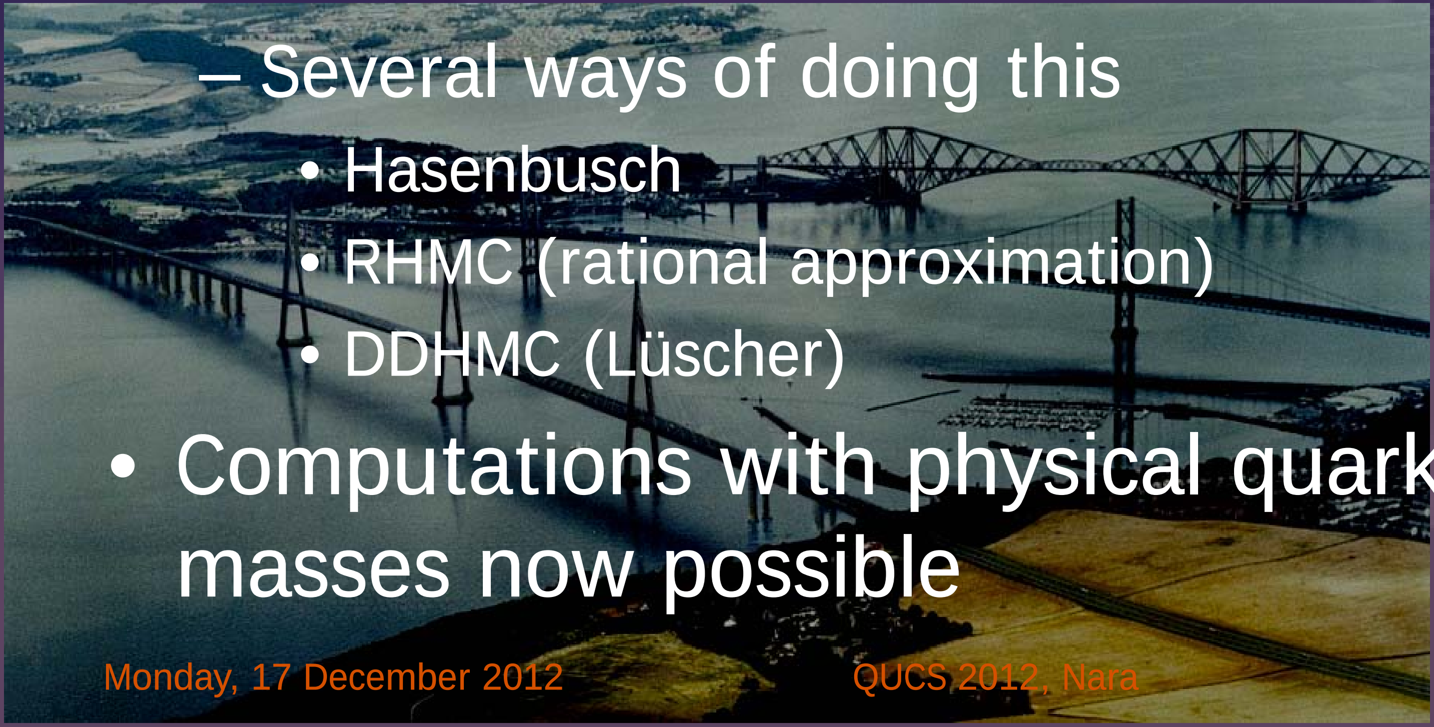
Single Pseudofermions

- But this was wrong
- The problem was that we were estimating the fermion determinant using a single pseudofermionic Monte Carlo estimate
  - This is clearly a very noisy estimate
  - But surely the Markov process is still valid?
  - True, but it becomes very slow



Multiple Pseudofermions

- The solution is to introduce multiple pseudofermion fields
  - A small number suffice
  - Several ways of doing this
    - Hasenbusch
    - RHMC (rational approximation)
    - DDHMC (Lüscher)
- Computations with physical quark masses now possible



Chiral Symmetry

- Another long-standing problem of lattice field theories was that chiral symmetry $\psi \to e^{i\alpha\gamma_5}\psi$ is explicitly broken on the lattice
  - It is violated by both Wilson and staggered discretizations of the Dirac operator
  - Only restored in the continuum limit with much fine-tuning
  - Chiral symmetry explains much low-energy phenomenology, such as the π being the Goldstone boson for spontaneously broken chiral symmetry

On-Shell Chiral Symmetry

- Replace with Lüscher’s on-shell chiral symmetry

$$y \to e^{j a g_5 (1- aD)} y, \; \bar{y} \to e^{j a (1- aD) g_5}$$

- Which leads to the Ginsparg—Wilson relation

$$g_5 D + D g_5 = 2aD g_5 D$$

Domain Wall and Overlap

- This problem has been solved by the (equivalent) Domain Wall and Overlap formulations

$$D_N = \tfrac{1}{2}\left(1 + \gamma_5 \operatorname{sgn} \gamma_5 (D_W - M)\right)$$

  - This Neuberger operator is very expensive to apply, and even more expensive to invert
  - We need to implement the sgn function
  - Most algorithms use some rational approximation and some five-dimensional Schur complement

Improvement

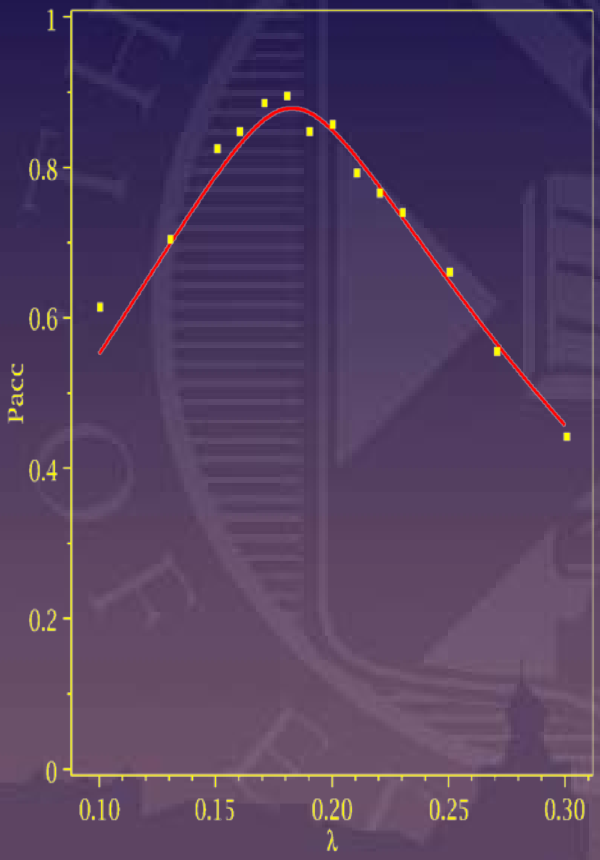
- <u>Improved actions</u> have long been popular
  - Improve discretization to better approximate continuum physics on coarse lattices

'THE GOOD NEWS IS, THERE'S ROOM FOR IMPROVEMENT.'

  - Works in context of perturbative QFT (Symanzik)
  - Sadly, improvement is an asymptotic expansion and cut-off effects fall as $a^n + e^{-c/a}$
- But improved actions are less local
  - Not a problem in principle, but maybe in practice as we work on finite lattices

Shadow Hamiltonians

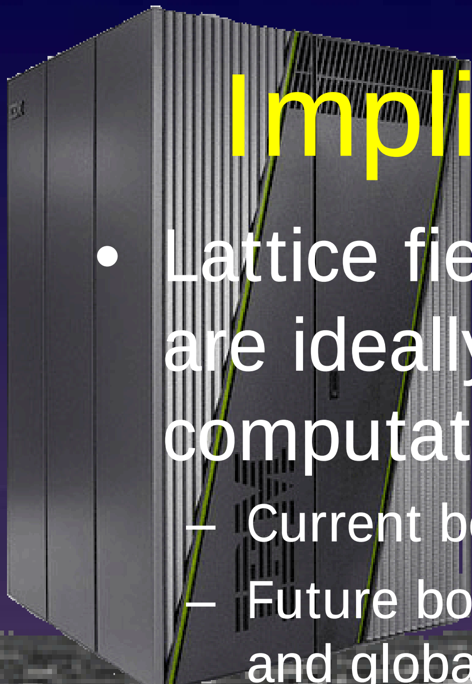
- Numerical integration of Hamilton's equations use symmetric symplectic integrators
- These exactly conserve a Shadow Hamiltonian close to the desired one
  - Again, only an asymptotic expansion
- This can be used to "automate" tuning of integrator parameters
- Higher-order integrators important for larger lattice volume?



Perambulation, Distillation, etc.

- Finding eigenstates of the Hamiltonian (Transfer Matrix)
  - Measuring correlation functions is essentially just the power method
- But the state space is very large...
  - Choice of basis
  - All-to-all solvers
  - Low modes and eigensolvers
- Multigrid and local coherence
  - Helpful for many solutions on same configuration
- Stochastic estimates
- What is a good basis for nuclei?

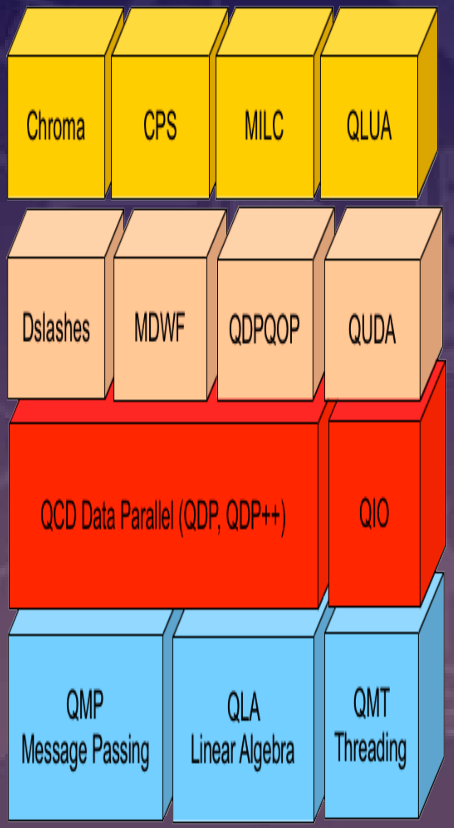
Implications for Hardware



- Lattice field theory Monte Carlo computations are ideally suited to massively parallel computation
  - Current bottlenecks are streaming memory access
  - Future bottlenecks probably 4D grid network communications and global reductions
  - Fundamental problem is getting data on/off chip
- Homogeneous or inhomogenous network?
  - Mainly a balance of cost and pain (cost usually wins)
- Multi-scale algorithms can be implemented but have lower performance

Software Matters

- Cost and delay of efficient implementation of new algorithms on awkward new machines
  - Tension between efficiency and portability
  - Inhibits experimentation and use of new techniques
- Algorithms and architecture stable enough to partition software stack into layers
  - Different people responsible for different layers
  - Cleaner interfaces between layers (HPC bytecode?)



Conclusions

- Lattice Gauge Simulations algorithms have reached a mature stage
- Changes have been incremental rather than revolutionary
  - No reason to expect this to change
- Improved methods with better volume scaling will help as lattices get larger
  - E.g., force-gradient integrators