

Introduction to Lattice QCD algorithms

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Functional integrals and QFT

- The expectation value of an operator $\mathcal{O}$ is defined non-perturbatively by the **functional integral**

$$\langle \mathcal{O} \rangle \equiv \frac{1}{Z} \int (\mathcal{D}\phi) e^{-S[\phi]} \mathcal{O}[\phi],$$

- normalisation constant Z is chosen such that $\langle 1 \rangle = 1$,
- $\mathcal{D}\phi$ is the appropriate functional measure,
- $S[\phi]$ is the action.
- In QFT there is one integration per degree of freedom:
 - we are dealing with an infinite dimensional functional integral,
 - well-defined only in Euclidean space-time using a lattice regularisation and a finite volume.

Monte Carlo methods I

- Lattice regularisation:
 - continuum limit (lattice spacing $a \rightarrow 0$) and thermodynamic limit (physical volume $V \rightarrow \infty$) are necessary,
 - still dealing with hopelessly many integrations...
- Monte Carlo integration is based on the identification of *probabilities* with *measures*:

⇒ importance sampling

- generate a sequence of random field configurations $\{\phi_1, \phi_2, \dots, \phi_N\}$ chosen from the *probability distribution*

$$P(\phi_t) \mathcal{D}\phi_t = \frac{1}{Z} e^{-S[\phi_t]},$$

Monte Carlo methods II

- measure the value of $\mathcal{O}$ on each configuration and compute the average

$$\overline{\mathcal{O}} \equiv \frac{1}{N} \sum_{t=1}^N \mathcal{O}[\phi_t].$$

- Limit of large numbers guarantees

$$\langle \mathcal{O} \rangle = \lim_{N \rightarrow \infty} \overline{\mathcal{O}}.$$

- Central limit theorem guarantees $\langle \mathcal{O} \rangle \sim \overline{\mathcal{O}} + O(\sqrt{\frac{\sigma}{N}})$,
 - where the variance of the distribution of $\mathcal{O}$ is $\sigma \equiv \langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle$.

Markov chains I

- Use Markov process to generate the correct probability distribution.
- Consider space of configurations Ω together with (ergodic) stochastic transitions $P' : \Omega \rightarrow \Omega$.
- The deterministic evolution of probability distributions $P : Q \rightarrow Q$ is a *Markov process*.
- Distribution converges to a unique fixed point:
 - Define a metric on the space of probability distributions,
 - show Markov process is a contraction mapping,
 - the sequence $Q, PQ, P^2Q, P^3Q, \dots$ is Cauchy,
 - space of probability distributions is complete, so

$$\overline{Q} = \lim_{n \rightarrow \infty} P^n Q$$

is the unique fixed point.

Markov chains II

- Suppose ergodic Markov process P with $\overline{Q}$ as its fixed point.
- Use Markov chains to sample from $\overline{Q}$:
 - start with an arbitrary state,
 - iterate the Markov process until it has converged, ('thermalised')
 - thereafter, successive configurations will be distributed according to $\overline{Q}$.
- To construct P we only need *relative probabilities* of states:
 - we don't know the normalisation of Q ,
 - can only compute ratios of integrals,
 - cannot use Markov chains to compute integral directly.

Markov chains III

- How to construct a Markov process with specified $\bar{Q}$?
 - Detailed balance $P(y \leftarrow x)\bar{Q}(x) = P(x \leftarrow y)\bar{Q}(y)$
 - $\Rightarrow$ sufficient but not necessary.
 - Metropolis algorithm $P(x \leftarrow y) = \min\left(1, \frac{\bar{Q}(x)}{\bar{Q}(y)}\right)$
 - $\Rightarrow$ sufficient but not necessary for detailed balance.
 - Other choices are possible, e.g. $P(x \leftarrow y) = \frac{\bar{Q}(x)}{\bar{Q}(y) + \bar{Q}(x)}$.
- Markov steps P_1, P_2 with the same fixed point distribution can be combined $P_1 \circ P_2$
 - $P_1 \circ P_2$ may be ergodic, even if P_1 and P_2 are not.

Hybrid Monte Carlo I

- In order to carry out Monte Carlo computations we want an algorithm which
 - updates the fields globally,
 - since single updates are expensive for non-local actions,
 - takes large steps through configuration space,
 - in order to decorrelate successive configuration
 - does not introduce any systematic errors.

Hybrid Monte Carlo II

- A useful class of algorithms with these properties is the Hybrid Monte Carlo (HMC) method:
 - introduce 'fictitious' momentum p conjugate to each dynamical degree of freedom q ,
 - find a Markov chain with fixed point $\propto \exp[-H(p, q)]$ where

$$H(p, q) = \frac{1}{2}p^2 + S(q)$$

is the 'fictitious' Hamiltonian:

- the action $S(q)$ of the underlying QFT plays the role of the potential in the 'fictitious' classical mechanics system,
 - the Hamiltonian gives the evolution of the system in a fifth dimension, 'fictitious' or MC time.
- This generates the desired distribution $\exp[-S(q)]$ if we ignore the momenta p .

Hybrid Monte Carlo III

- The HMC Markov chain alternates two Markov steps.
 - Molecular Dynamics Monte Carlo:
 - exact integration of Hamilton's equations gives a trajectory of constant 'fictitious energy'
→ equiprobable fictitious phase space configurations,
 - approximate integration must be *reversible* and *area preserving*,
 - the so produced phase space configurations have to pass a *Metropolis accept/reject step* with acceptance $\min[1, \exp(-\delta H)]$
 - (Partial) Momentum refreshment.
- Both steps have the desired fixed point.
- Together they are ergodic.

Note: the Metropolis test makes the algorithm exact even for approximate integration.

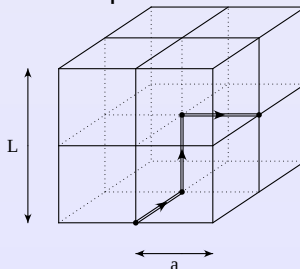
QCD on the Lattice

Quantum chromodynamics is formally described by the Lagrange density:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\not{D} - m_q)\psi - \frac{1}{4}G_{\mu\nu}G^{\mu\nu}$$

Lattice regularization: discretize Euclidean space-time

- hypercubic L^4 -lattice with lattice spacing a
- derivatives $\Rightarrow$ finite differences
- integrals $\Rightarrow$ sums
- gauge potentials A_μ in $G_{\mu\nu} \Rightarrow$ link matrices U_μ (• $\Rightarrow$ •)



QCD on the Lattice II

- Partition function $Z_{\text{QCD}} = \int (\mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi) e^{-S_{\text{QCD}}[U; \bar{\psi}, \psi]}$
- Mathematically well defined theory
- Non-perturbative, gauge invariant regularisation (low energy physics)
- Continuum limit $\Rightarrow a \rightarrow 0$
 - Poincaré symmetries are restored automatically
- Direct simulation of Grassmann fields is not feasible.
 - The problem is not that of manipulating anticommuting values in a computer.
 - It is that $e^{-S_F} = e^{-\bar{\psi} \mathcal{D} \psi}$ is not positive and thus we get poor importance sampling.

QCD on the Lattice III

- We therefore integrate out the fermion fields to obtain the fermion determinant $\int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\bar{\psi} D \psi} \propto \det(D)$:

$$Z = \int (\mathcal{D}U) \det D(U) e^{-S_G[U]}$$

- ψ and $\bar{\psi}$ always occur quadratically,
- the overall sign of the exponent is unimportant.
- Any operator $\mathcal{O}$ can be expressed in terms of the bosonic fields

$$\mathcal{O}'(U) = \mathcal{O} \left(\frac{\delta}{\delta \psi}, \frac{\delta}{\delta \bar{\psi}}; U \right) e^{-\bar{\psi} D \psi} \Big|_{\psi=\bar{\psi}=0}$$

e.g. the fermion propagator is $\langle \psi(x) \bar{\psi}(y) \rangle = D^{-1}(x, y)$.

Dynamical fermions I

- Pseudofermions:

- Represent the fermion determinant as a bosonic Gaussian integral with a non-local kernel

$$\det D(U) \propto \int \mathcal{D}\phi \mathcal{D}\bar{\phi} e^{-\bar{\phi} D^{-1}(U) \phi}.$$

- The fermion kernel must be positive definite for the bosonic integral to converge.
- The new bosonic fields are called *pseudofermions*.
- It is usually convenient to introduce two flavours of fermions and to write

$$(\det D(U))^2 = \det (D(U)^\dagger D(U)) \propto \int \mathcal{D}\phi \mathcal{D}\bar{\phi} e^{-\bar{\phi} (D(U)^\dagger D(U))^{-1} \phi}$$

Dynamical fermions II

- Introduce Gaussian momenta $P_\mu(x)$ conjugate to $U_\mu(x)$ with action $S_P = 1/2 \sum_{\mu,x} P_\mu(x)^2$.
- The new partition function is now

$$Z = \int (\mathcal{D}U \mathcal{D}\bar{\phi} \mathcal{D}\phi) e^{-S_P - S_g[U] - \bar{\phi} \frac{1}{D^\dagger(U)D(U)} \phi}$$

- Generate a sequence of $\{P, U\}$ with the correct probability distribution:
 - update $P_\mu(x)$ using Gaussian random noise,
 - update ϕ using Gaussian random noise via $\phi = D^\dagger \eta$,
 - evolve $\{P, U\}$ according to the Hamiltonian

$$\mathcal{H}[P, U] = \frac{1}{2} P^2 + S_g[U] + S_f[U]$$

- accept/reject the final configuration $\{P', U'\}$ with probability

$$P_{\text{accept}} = \min \left(1, e^{-(\mathcal{H}[P', U'] - \mathcal{H}[P, U])} \right).$$

Dynamical fermions III

- The discrete Hamiltonian equations of motion dictate the following update for U and P ,

$$\begin{aligned} T_U(\delta\tau) : \quad U &\implies e^{i\delta\tau P} U \\ T_P(\delta\tau) : \quad P &\implies P + \delta\tau \cdot F \end{aligned}$$

where F is the force due to the variation of the gauge field:

$$F = -\frac{\delta\mathcal{H}}{\delta U}.$$

- Inversions required for the equations of motion need not be exact – integration is approximate anyway.
- Inversion for the Metropolis accept/reject step needs to be 'exact'.

Dynamical fermions IV

- Are HMC trajectories reversible and area preserving?
 - Yes, if a leapfrog integration scheme is used:

$$T(\delta\tau) = T_P(\delta\tau/2)T_U(\delta\tau)T_P(\delta\tau/2).$$

- Recently, so-called Omelian integrators were suggested which are also reversible and area preserving, but appear to be more efficient.
 - The only fundamental source of irreversibility is the rounding error caused by using finite precision floating point arithmetic.
- The evaluation of the pseudofermion action and the corresponding force requires the solution of a (large) set of linear equations $(D^\dagger D)^{-1} \phi = \chi$.

Iterative methods I

- Consider a system of linear equations $Ax = b$ and the residual vector $r \equiv b - Ax_i$ for an approximate solution x_i .
- Rewriting the system as

$$(I - (I - A))x = b$$

leads to a basic iteration

$$\begin{aligned}x_i &= b + (I - A)x_{i-1} \\&= x_{i-1} + r_{i-1} \\&= x_{i-2} + r_{i-2} + r_{i-1} \\&\vdots \\&= x_0 + r_0 + r_1 + \dots + r_{i-1}.\end{aligned}$$

Iterative methods II

- Multiply $x_i = x_{i-1} + r_{i-1}$ with A from the left

$$Ax_i = Ax_{i-1} + Ar_{i-1}$$

and subtract from b

$$b - Ax_i = b - Ax_{i-1} + Ar_{i-1}$$

$$r_i = r_{i-1} - Ar_{i-1}$$

$$= (I - A)r_{i-1}$$

- So finally we have

$$\begin{aligned} x_i &= x_0 + r_0 + (I - A)r_0 + \dots + (I - A)^{i-1}r_0 \\ &= x_0 + [r_0, Ar_0, A^2r_0, \dots, A^{i-1}r_0]. \end{aligned}$$

Krylov spaces I

- This linear space defines the **Krylov subspace**

$$\mathcal{K}_n(A; r_0) \equiv \text{span}(r_0, Ar_0, A^2r_0, A^3r_0, \dots, A^{n-1}r_0).$$

- Iterative methods are based on finding an approximate solution x_n within a Krylov subspace

$\Rightarrow$ Krylov subspace methods

- Convergence is measured by the *residual* $r_n = \|b - Ax_n\|$.

Krylov spaces II

- Krylov subspace methods are often used as exact methods:
 - they require $O(V)$ iterations to find the solution,
 - they do not give the 'exact' answer in practice due to rounding errors,
 - they are more naturally thought of as methods for solving systems of linear equations in an (almost) ∞ -dimensional linear space.

Krylov spaces III

- Approximations obtained from a Krylov subspace method are of the form

$$A^{-1}b \sim x_n = x_0 + P_{n-1}(A)r_0$$

where P_{n-1} is a polynomial of degree $n - 1$

- For the simple case $x_0 = 0$ we have

$$A^{-1}b \sim P_{n-1}(A)b$$

i.e. $P_{n-1}(A)$ is a polynomial approximation of $A^{-1}b$.

- All techniques provide the same type of polynomial approximations, but the type of constraints has important effects.

Krylov spaces IV

- More specifically, we seek an approximate solution x_n in $\mathcal{K}_n$ by imposing the Petrov-Galerkin projection condition

$$r_n \equiv b - Ax_n \perp \mathcal{L}_n$$

where $\mathcal{L}_n$ is another n -dimensional subspace.

- Two broad choices:
 - $\mathcal{L}_n = \mathcal{K}_n(A; r_0)$ or $\mathcal{L}_n = A\mathcal{K}_n(A; r_0) \Leftrightarrow$ orthogonalisation
 $\rightarrow$ FOM (Arnoldi), GMRES, CG, GCR, ...
 - $\mathcal{L}_n = \mathcal{K}_n(A^\dagger; r_0) \Leftrightarrow$ bi-orthogonalisation
 $\rightarrow$ Lanczos, BCG, QMR, BiCGstab, ...
- A projection method may have different implementations $\rightarrow$ different, but mathematically equivalent algorithms.

Krylov spaces V

- For the choice $\mathcal{L}_n = \mathcal{K}_n$ one can show that $\{r_0, r_1, \dots, r_{n-1}\}$ form an orthogonal basis of $\mathcal{K}_n(A; r_0)$.
- Assume A hermitian and $r_0, \dots, r_n$ orthogonal. Then

$$\gamma_n r_{n+1} = Ar_n - \alpha_n r_n - \beta_n r_{n-1} - \delta_n r_{n-2} - \dots$$

- Requiring $(r_{n+1}, r_{n-2}) = 0$ leads to **3-term recurrence**

$$\gamma_n r_{n+1} = Ar_n - \alpha_n r_n - \beta_n r_{n-1}.$$

- Requiring $(r_{n+1}, r_{n-1}) = (r_{n+1}, r_n) = 0$ leads to

$$\begin{aligned}\alpha_n &= (Ar_n, r_n)/(r_n, r_n), \\ \beta_n &= (Ar_n, r_n)/(r_{n-1}, r_{n-1}).\end{aligned}$$

Krylov spaces VI

- In contrast to the above multi-dimensional projection methods, there also exist 1-dimensional projection processes where

$$\mathcal{K} = \text{span}(w) \quad \text{and} \quad \mathcal{L} = \text{span}(v),$$

i.e. each iteration step is completely independent of the previous one.

e.g. Minimal Residual (MR) iteration

- The best and most complete reference is

Yousef Saad, *Iterative Methods for Sparse Linear Systems*,
second edition, SIAM, 2003.

Multi-shift solvers

- Often necessary to solve $(A + \sigma)x = b$ for several shifts σ
 - for obtaining propagators at several masses, $(D + \delta m_i)^{-1}b$,
 - for calculating rational matrix functions

$$R_{n,n}(A) = \frac{P_n(A)}{Q_n(A)} = \sum_{i=1}^n \frac{c_i}{A + \sigma_i}.$$

- For Krylov subspace solvers this can be achieved by realising that [\[Jegerlehner, Frommer et al.\]](#)

$$\mathcal{K}(A + \sigma; 0) = \mathcal{K}(A; 0).$$

- the solution $(A + \sigma)^{-1}b$ can be obtained with little overhead during the construction of $A^{-1}b$,
 - only a single Krylov space is needed.
- Overall convergence usually governed by the worst conditioned $A + \sigma$.

Generalities

- Most (all) inversion methods suffer from slow convergence.
- Preconditioning is the key ingredient for the success of Krylov subspace methods.
- General strategy is to modify the original linear system which makes it easier to solve by iterative methods:
 - search for preconditioner M which approximates A^{-1} , then solve

$$M^{-1}Ax = M^{-1}b,$$

- M^{-1} should be easy to calculate.
- Polynomial preconditioners, incomplete factorisations, Schwarz alternating procedure, domain decompositions, ...
- No limits, but good preconditioners usually derived from good knowledge of the physical problem.

Even/odd preconditioning I

- Dirac operators containing only nearest-neighbour interactions can be written as

$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix}$$

where D_{ee} and D_{oo} are diagonal.

- Perform a LU-decomposition

$$D = \begin{pmatrix} D_{ee} & 0 \\ D_{oe} & 1 \end{pmatrix} \begin{pmatrix} 1 & D_{ee}^{-1} D_{eo} \\ 0 & D_{oo} - D_{oe} D_{ee}^{-1} D_{eo} \end{pmatrix} = L \cdot U.$$

Even/odd preconditioning II

- Invert D by inverting each factor separately,

$$L^{-1} = \begin{pmatrix} D_{ee} & 0 \\ D_{oe} & 1 \end{pmatrix}^{-1} = \begin{pmatrix} D_{ee}^{-1} & 0 \\ -D_{oe} & 1 \end{pmatrix},$$

$$U^{-1} = \begin{pmatrix} 1 & D_{ee}^{-1}D_{eo} \\ 0 & D_{oo} - D_{oe}D_{ee}^{-1}D_{eo} \end{pmatrix}^{-1} = \begin{pmatrix} 1 & -D_{ee}^{-1}D_{eo} \\ 0 & \hat{D}^{-1} \end{pmatrix}$$

where $\hat{D} = D_{oo} - D_{oe}D_{ee}^{-1}D_{eo}$.

- Note that $\hat{D}$ is better conditioned and hence cheaper to invert than the original D .

Low-mode preconditioning I

- The vector space on which A acts, can be split into two (bi-)orthogonal pieces using the (bi-)orthogonal projectors

$$P = \sum_k r_k l_k^\dagger, \quad P_\perp = 1 - P$$

- r'_k s and l'_k s are approximate right and left eigenvectors,
 - form a bi-orthogonal basis, i.e. $l_i^\dagger r_j = \delta_{ij}$.
- Then A yields the following block form

$$A = \begin{pmatrix} PAP & PAP_\perp \\ P_\perp AP & P_\perp AP_\perp \end{pmatrix}.$$

Low-mode preconditioning II

- Perform a LU decomposition of A

$$A = \begin{pmatrix} 1 & 0 \\ P_{\perp}AP(PAP)^{-1} & 1 \end{pmatrix} \begin{pmatrix} PAP & PAP_{\perp} \\ 0 & S \end{pmatrix} \equiv L \cdot U$$

where $S = P_{\perp}AP_{\perp} - P_{\perp}AP(PAP)^{-1}PAP_{\perp}$ is the Schur complement of A .

- Invert each factor separately,
 - L^{-1} is easy:

$$L^{-1} = \begin{pmatrix} 1 & 0 \\ -P_{\perp}AP(PAP)^{-1} & 1 \end{pmatrix}$$

- U^{-1} requires $(PAP)^{-1}$ which is easy (inversion in a small sub-space) and S^{-1}
- Note that S is better conditioned than original matrix A .

Recapitulation

- Recapitulate:

- represent the fermion determinant as a bosonic integral,

$$\det(D(U)D(U)^\dagger) = \int \mathcal{D}\phi \mathcal{D}\phi^\dagger e^{-\phi^\dagger (D(U)D(U)^\dagger)^{-1} \phi},$$

- introduce Gaussian momenta $P_\mu(x)$ conjugate to $U_\mu(x)$ with action $S_P = 1/2 \sum_{\mu,x} P_\mu(x)^2$,
- evolve P, U according to the Hamiltonian

$$\mathcal{H} = \frac{1}{2}P^2 + S_g[U] + S_f[U]$$

yielding the force

$$F = -\frac{\delta \mathcal{H}}{\delta U} = F_g[U] + F_f[U].$$

Multiple time-steps I

- One observes that $F_g[U] \gg F_f[U]$.
- Introduce two time steps:
 - a short one associated with the large, but cheap gauge force $F_g[U]$,
 - a long one associated with the small, but expensive fermionic force $F_f[U]$.
- Moreover, the fermionic force itself can be split into two or more pieces, $F_f[U] = F_f^1[U] + F_f^2[U] + \dots$ and put on different time scales according to their size.
- Split the force such that the most expensive piece contributes the least.

Multiple time-steps II

- Generically, this is achieved by splitting the fermion Dirac operator into a long-range infrared (IR) part and a short-range ultraviolet (UV) part:
 - UV part is large, but cheap,
 - IR part is small, but expensive.
- In practice, split the fermion determinant into different pieces

$$\det(M) = \det(M_1) \det(M_2) \dots$$

and use different pseudo-fermion fields on different time scales.

- How do we obtain the desired splitting?

⇒ look at the preconditionings!

Multiple time-steps III

- Mass preconditioning [Hasenbusch, Urbach et al.]

$$\det(D(m)^\dagger D(m)) = \det\left(\frac{D(m)^\dagger}{D(M_1)^\dagger} \frac{D(m)}{D(M_1)}\right) \det(D(M_1)^\dagger D(M_1))$$

where m is the physical mass, and $M > m$ the preconditioning mass:

- force from $D(M_1)^\dagger D(M_1)$ is large, but cheap,
- force from $\frac{1}{D(M_1)^\dagger} D(m)^\dagger D(m) \frac{1}{D(M_1)}$ is small but expensive.
- Tune M (or possibly $M_1, M_2, \dots$) such that the forces are optimally arranged in order to apply multiple time-steps.
- Speed-up factors can be up to 10 even in a physically relevant set-up.

Multiple time-steps III

- Polynomial filtering [Peardon et al.]

$$\det(D^\dagger D) = \det(P(D^\dagger D)) \det\left(D^\dagger D \frac{1}{P(D^\dagger D)}\right)$$

- $P(x) \approx \frac{1}{x}$ in the interval $[\mu, \lambda_{\max}(D^\dagger D)]$.
 - The approximation covers the UV part of $D^\dagger D$.
 - Only a low order polynomial is needed, since μ is large.
 - $P(x)$ is easy to invert and yields a large force contribution.
 - Correction term is still hard to invert, but yields a small force.
- Speed-up factors currently still under investigation.

Multiple time-steps IV

- Domain decomposition [Lüscher]. An ultra-local Dirac operator can be decomposed into different domains

$$D = \begin{pmatrix} D_{\Omega} & D_{\partial\Omega} \\ D_{\partial\Omega'} & D_{\Omega'} \end{pmatrix}.$$

- The preconditioning matrix is

$$D' = \begin{pmatrix} D_{\Omega} & 0 \\ 0 & D_{\Omega'} \end{pmatrix}.$$

and describes the UV physics.

- D' is easy to invert and yields a large force.
- The correction term is expensive to invert, but yields a small force.
- Again, speed up factors up to 10 can be achieved in physically relevant situations.

Multiple time-steps V

- Rational Hybrid Monte Carlo [Clark and Kennedy] writes

$$\det(D^\dagger D) = \det \left[(D^\dagger D)^{1/n} \right]^n$$

and uses a rational approximation $R(x) \approx x^{1/n}$.

- Inverse of R is also a rational function.
 - Use multi-shift solver to calculate R and R^{-1} .
 - Smallest shift is expensive, but contributes a small force.
 - Use coarser time scale for the more expensive smaller shifts.
- Improvement factors are again up to 10 in physically relevant simulation set-ups.

Conclusions

- All the different algorithmic improvements in HMC rely on multi-pseudofermion fields and multiple time scales.
- Together with the usual increase in computer time, the new developments push lattice QCD calculations into new regimes.
- Calculations are now possible which were not possible before.
- Lattice QCD is entering exciting times,
⇒ make sure you participate!