Event-Chain Monte Carlo for pure gauge lattice QCD

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Workshop : Progress in algorithms and numerical tools for QCD

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Plan

Lattice QCD

- A numerical way to compute observables in QCD non-perturbatively
- Space-time is discretized with lattice spacing a (UV regulator)
- Fermion fields are site variable while gauge fields are links variables

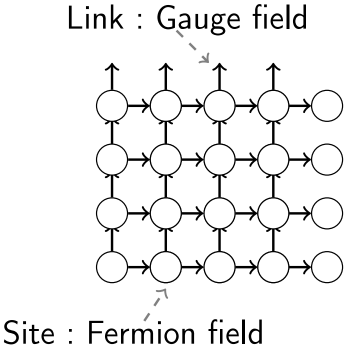


Figure 1 – A 1+1 dimensional lattice

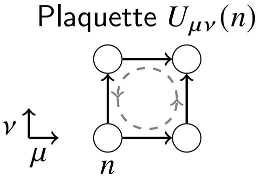


Figure 2 – A plaquette

Pure gauge lattice QCD

- In our case : only the gauge field $\longrightarrow$ no fermions
- We have a lattice of links (gauge transporters), each link is a SU(3) matrix
- We use the path integral formalism with the Wilson action to compute observables

Path integral formalism

$$\langle O \rangle = \frac{1}{Z} \int O[U] \mathrm{e}^{-S[U]} \mathcal{D}U, \qquad Z = \int \mathrm{e}^{-S[U]} \mathcal{D}U. \tag{1}$$

Wilson action

$$S[U] = \frac{\beta}{3} \sum_{n \in \Lambda} \sum_{\mu < \nu} \mathrm{ReTr} \left[\mathbb{1} - U_{\mu\nu}(n) \right] \tag{2}$$

Pure gauge lattice QCD

- In order to compute efficiently observables, we need to sample gauge configurations following a specific probability distribution

Probability distribution of the configurations

$$\mathrm{d}\pi(U) = \frac{\mathrm{e}^{-S[U]}\mathcal{D}U}{\int \mathrm{e}^{-S[U]}\mathcal{D}U} \tag{3}$$

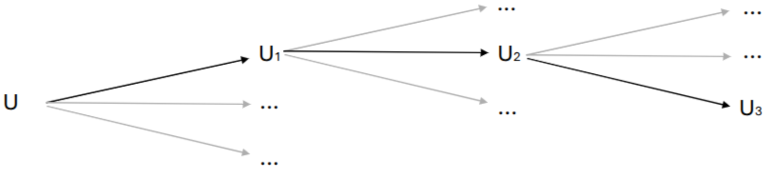


Figure 3 – Markov Chain

Critical slowing down (CSD)

Problem

When the lattice spacing a becomes very small ($a \lesssim 0.04$ fm), it becomes increasingly difficult to generate independent configurations with MCMC algorithms.

- Why ? Because when a becomes small enough, we resolve large-scale "patterns" (instantonic configurations)
- The links become more largely spatially correlated
- Numerical cost $\approx a^{-z}$ (z is a critical exponent)

Critical slowing down (CSD)

The topological charge Q is especially sensible to the CSD with $z \approx 5/6$:

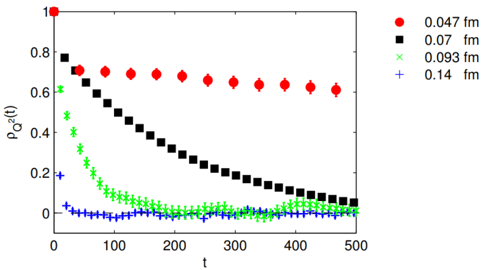


Figure 4 – Autocorrelation of Q^2 at different lattice spacings using molecular dynamics [1].

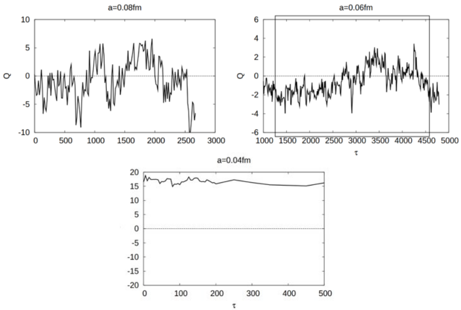


Figure 5 – Monte Carlo history of Q at different lattice spacings [1].

→ Long standing issue in lattice QCD, no optimal solution found yet

Event-Chain Monte Carlo (ECMC)

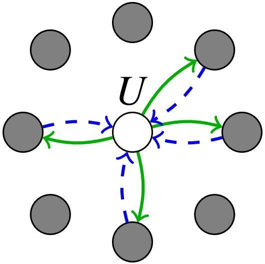
Introduced in 2010 by Bernard, Krauth, Wilson [2] to tackle CSD in hard-spheres systems. It is a factorized MCMC algorithm with the following particularities :

- Local $\longrightarrow$ One link is updated at a time
- In continuous time $\longrightarrow$ No need to discretize computer time steps
- Reject-free $\longrightarrow$ When a reject occurs, we still move in a bigger space, the *lifted* state space
- Irreversible $\longrightarrow$ We do not fulfill the *detailled* global balance

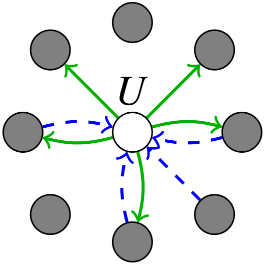
Global balance

Global Balance

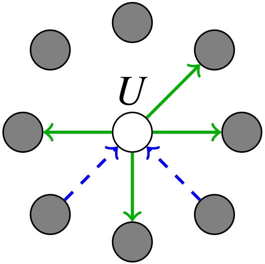
$$\sum_{U' \in C} \pi(U') p^{\mathrm{acc}}(U' \to U) = \pi(U) = \sum_{U' \in C} \pi(U) p^{\mathrm{acc}}(U \to U') \tag{4}$$



(a) Detailled



(b) Partially irreversible



(c) Maximally irreversible

Plan

ECMC for pure gauge lattice QCD

First, we need to find a parametrization of SU(3) compatible with the Event-Chain principle. We use the XY-embedding [3] :

XY-embedding

$$U_\mu(n) \to U_\mu(n)' = X(\theta)U_\mu(n), \qquad X(\theta) = Re^{i\theta\lambda_3}R^\dagger \tag{5}$$

with R a random SU(3) matrix and λ_3 the Gell-Mann matrix.

- ✓ Single parameter to update at a time
- ✓ $X(\theta_1)X(\theta_2) = X(\theta_1 + \theta_2)$ (necessary for the event-driven approach)
- ✓ Periodic boundary conditions on θ (necessary for the event-driven approach)
- ✓ Regular refreshes of R ensure ergodicity on SU(3)

Factorization

Metropolis probability of acceptance :

$$p^{\mathrm{acc}}(U \to U') = \min\left(1, \frac{\pi(U')}{\pi(U)}\right) = \min\left(1, \mathrm{e}^{-\Delta S}\right) \tag{6}$$

$$\text{with } \Delta S = \frac{\beta}{3}\mathrm{ReTr}\left[(\mathrm{e}^{i\theta\lambda_3} - \mathbb{1})R^{\dagger}U_{\mu}(n)V(n,\mu)R\right] \tag{7}$$

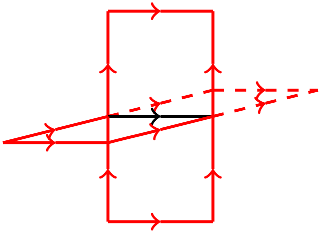


Figure 7 – A link (black) and its surrounding staples (red) in a 3D lattice

Factorization

- We use the factorized Metropolis acceptance probability

$$\text{Non factorized} \quad : p^{\text{acc}}(U \to U') = \min\left(1, \frac{\pi(U')}{\pi(U)}\right) = \min\left(1, \mathrm{e}^{-\Delta S}\right) \tag{8}$$

$$\text{Factorized} \quad : p^{\text{fact}}(U \to U') = \underbrace{\min\left(1, \mathrm{e}^{-\Delta S_1}\right)}_{\text{Plaquette 1}} \times \underbrace{\min\left(1, \mathrm{e}^{-\Delta S_2}\right)}_{\text{Plaquette 2}} \times \ldots \tag{9}$$

- Veto system : We accept the move iff all the factor plaquettes accept it

- When a reject occurs, we change to another link in the factor that refused the move.

Lifting

- When a reject occurs, we want to change the updated link while fulfilling global balance.
- We need to add a new parameter :

$$\epsilon = \begin{cases} 1 & \longrightarrow \text{we increase } \theta \\ -1 & \longrightarrow \text{we decrease } \theta \end{cases} \tag{10}$$

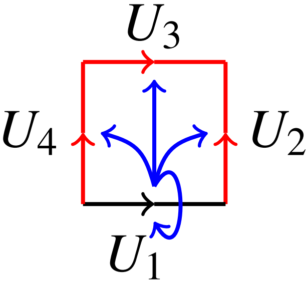
$$X(\theta) = R e^{i\epsilon\theta\lambda_3} R^\dagger \tag{11}$$

- Two possibilities : $\begin{cases} \text{Forward lifting} \\ \text{Reflective lifting} \end{cases}$

Reflective lifting

Lifting probability

$$P(U_1 \to U_i) = \frac{|\Delta S_i^j|}{\sum_{l \in P^j} |\Delta S_l^j|}, \qquad \epsilon \to -\text{sign}(\Delta S_i^j), \qquad \Delta S_i^j = \frac{\beta}{3}\text{ReTr}\left[i\lambda_3 R^\dagger U_i V_i^j R\right].$$



Pros :

- Easily adaptable to any action

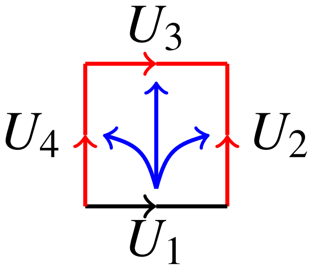
Cons :

- Computationally heavy (staples computation)
- Allows backtracking

Forward lifting

Lifting probability

$$P(U_1 \to U_i) = \frac{1}{3},$$ and we change ϵ, R according to table 1.



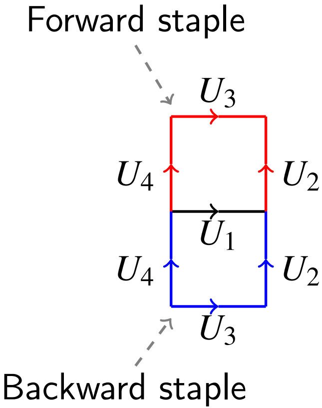
Pros :

- No backtracking
- Computationally light

Cons :

- Depends on the form of the action (traces of closed loops)

Forward lifting



	Forward		Backward	
k	R_k	ϵ_k	R_k	ϵ_k
2	$U_1^\dagger R$	$-\epsilon$	$U_3^\dagger U_4 R$	ϵ
3	$U_4^\dagger R$	ϵ	$U_4 R$	ϵ
4	R	ϵ	$U_4 R$	$-\epsilon$

Table 1 – Forward lifting rules for R_k and ϵ_k depending on the plaquette type and the link k position.

Event-driven approach

- How "high" can θ go until a reject happens ?

Probability distribution of rejects

$$\mathrm{d}p_i^{\mathrm{acc}}(0 \to \epsilon\theta_r) = \max(0, f(\epsilon\theta_r))\mathrm{d}\theta_r, \qquad f(\epsilon\theta) = \frac{-\epsilon}{\pi(0)} \frac{\partial \pi}{\partial \theta}\bigg|_{\theta=\epsilon\,\theta_r}. \tag{12}$$

- We want to sample this distribution $\longrightarrow$ Inverse CDF sampling method.
- We want θ_r such that

$$\mathbf{rand}(0,1) = \int_0^{\theta_r} [f(\epsilon\theta)]^+ \,\mathrm{d}\theta, \qquad [x]^+ = \max(0, x)$$

Event-driven approach

- In practice, we need to solve

Reject generation equation

$$-\frac{\beta}{3}\ln(\mathbf{rand}(0,1)) = \int_0^{\epsilon\,\theta_r} \left[\partial_\theta S(\epsilon\theta)\right]^+ \mathrm{d}\theta,$$

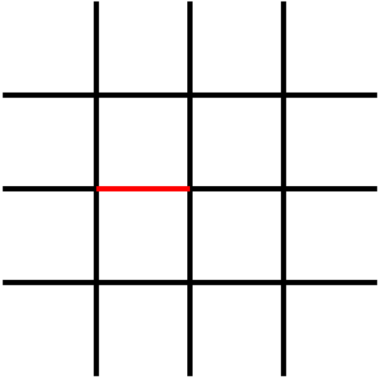
$$\text{with } S(\theta) = \mathrm{ReTr}\left[(\mathrm{e}^{i\theta\lambda_3} - \mathbb{1})R^\dagger U_\mu(n) S_j(n,\mu) R\right].$$

- Thanks to the XY-embedding and λ_3, this translates to

$$\mathbf{exp}\left(\frac{\beta}{3}\right) = \int_0^{\theta_r} \left[-A\sin(\epsilon\theta) + B\cos(\epsilon\theta)\right]^+ \mathrm{d}\theta. \tag{13}$$

$\rightarrow$ This can be solved analytically !

Summary

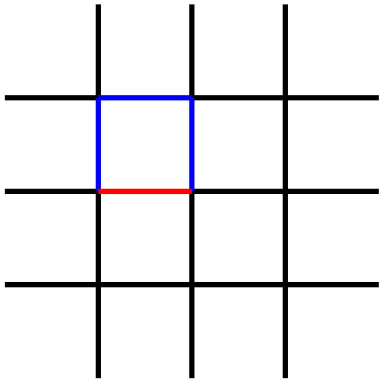


We update the red link until a reject occurs

$\Leftrightarrow$

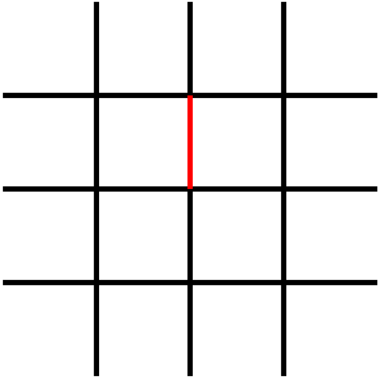
We generate a reject angle θ_r for each plaquette and choose the lowest (event-driven approach)

Summary



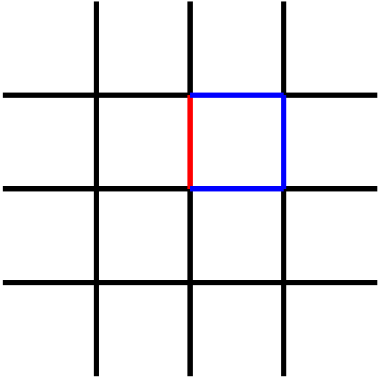
... One of the two attached staples refused a move...

Summary



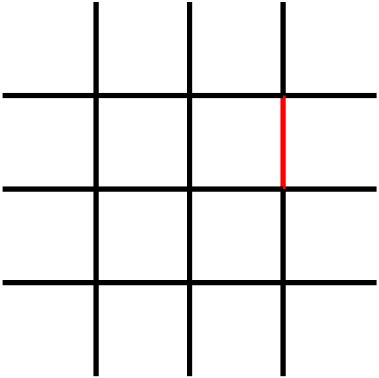
... so we change the updated link to another link of the plaquette (lift)...

Summary



... and we update it until another refusal occurs...

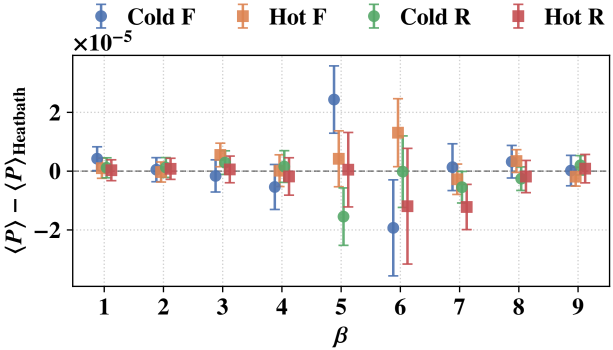
Summary



... and so on until a sample is generated.

Plan

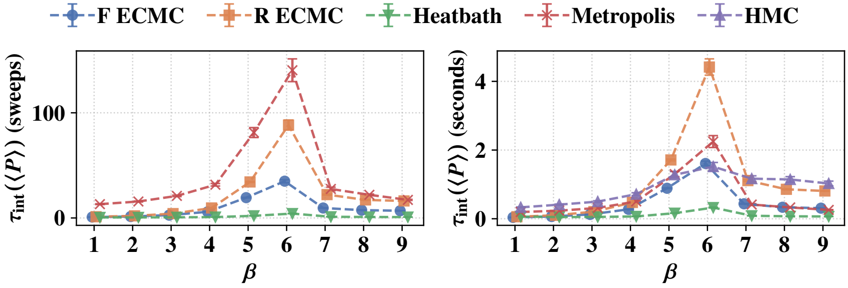
Results – Correctness



- No visible bias
- Agreement up to $\times 10^{-5}$, standard

$$\langle P \rangle = \frac{1}{18V} \sum_{\text{plaquettes}} \mathrm{ReTr}\left[U_{\text{plaquette}}\right]$$

Results – Autocorrelation and comparison



Algorithm	CPU time per sweep (in units of 1 Heatbath sweep)
Heatbath	1
Reflective ECMC	0.64
Forward ECMC	0.58
Metropolis	0.19

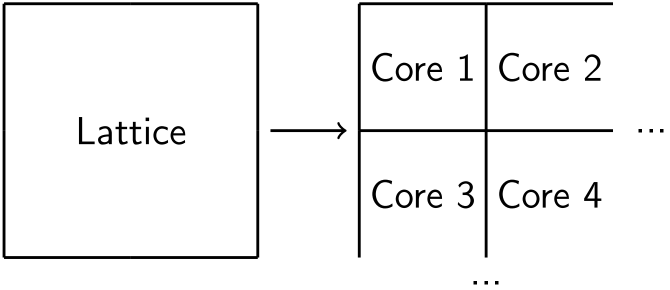
Plan

Parallelization

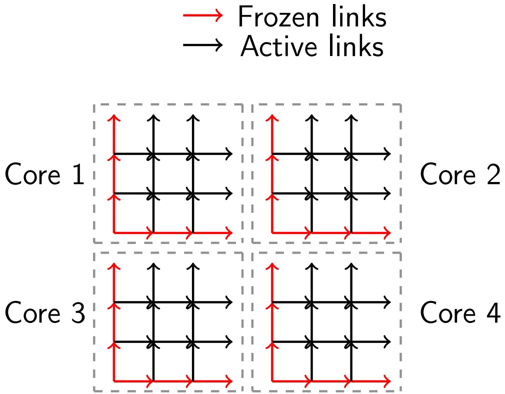
- The topological charge is a non local and extensive observable $\rightarrow$ we need large lattices

Problem

How can we parallelize the ECMC algorithm ?



We freeze the boundary links (cf. [4]) → the Event-Chain bounces on frozen links



Pros :

- Still fulfills global balance
- Still ergodic because we shift the frozen links
- No deadlocks, inactive cores or communication overhead

Cons :

- Introduces backtracking (backtracking rate decreases when the lattice is large)
- $\frac{\text{Nb. Active links}}{\text{Nb. Total links}} = (1 - 1/L_{\text{core}})^3$

Plan

Conclusion

- We adapted the ECMC algorithm to pure gauge lattice QCD
- Works for any gauge group SU(N) and any lattice dimension d
- Can be parallelized and thus generate large lattices
- ECMC yields better decorrelation of short-distance observables than Metropolis and HMC

Coming next :

- Computation of the critical exponent of Q in Periodic/Open Boundary conditions
- Characterization of the CSD for this algorithm

Thanks for your attention !

Références I

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[2] E. P. Bernard et al. “Event-Chain Monte Carlo Algorithms for Hard-Sphere Systems”. In : *Physical Review E* 80.5 (2009), p. 056704.

[3] G. Mana et al. “Multi-Grid Monte Carlo via \$XY\$ Embedding. II. Two-Dimensional \$SU(3)\$ Principal Chiral Model”. In : *Physical Review D* 55.6 (1997), p. 3674-3741.

[4] M. Lüscher. *Schwarz-Preconditioned HMC Algorithm for Two-Flavour Lattice QCD*. arXiv.org. 2004. url : `https://arxiv.org/abs/hep-lat/0409106v1` (visité le 04/06/2026).