

Event-Chain Monte Carlo for pure gauge lattice QCD

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Pure gauge lattice QCD

- Lattice of SU(3) links
- We use the path integral formalism with the **Wilson action** to compute observables
- We sample gauge configurations according to a **Boltzmann probability distribution**

Wilson action

$$S[U] = \frac{\beta}{3} \sum_{n \in \Lambda} \sum_{\mu < \nu} \text{ReTr} [\mathbb{1} - U_{\mu\nu}(n)] \quad (1)$$

Probability distribution of the configurations

$$d\pi(U) = \frac{e^{-S[U]} \mathcal{D}U}{\int e^{-S[U]} \mathcal{D}U} \quad (2)$$

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.

- Autocorrelation of observables grows $\approx a^{-z}$ (z is a **critical exponent**)
- The **topological charge** Q is especially sensible to the CSD

Algorithm	$z(Q^2)$
Heatbath	≈ 5.7 [1]
HMC	≈ 5 (+1 for the decreasing step size) [2]

Event-Chain Monte Carlo (ECMC)

Introduced in 2010 by Bernard, Krauth, Wilson [3], **eliminated CSD** in 2d/3d spin systems [4], hard/soft sphere systems [3], $O(3)$ 2d lattice fields [5], $SU(3)\times SU(3)$ principal chiral model [5]

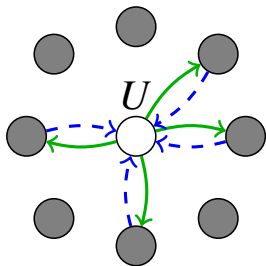
It is a **factorized** MCMC algorithm with the following particularities :

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

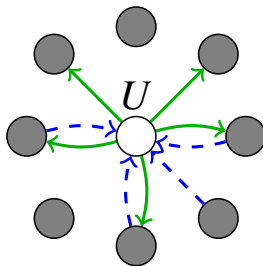
Global balance

Global Balance

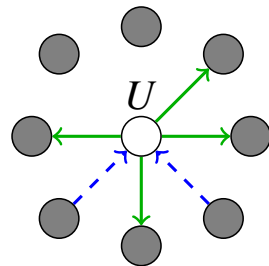
$$\sum_{U' \in \mathcal{C}} \pi(U') p^{\text{acc}}(U' \rightarrow U) = \pi(U) = \sum_{U' \in \mathcal{C}} \pi(U) p^{\text{acc}}(U \rightarrow U') \quad (3)$$



(a) Detailed



(b) Partially irreversible



(c) Maximally irreversible

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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** [6] :

XY-embedding

$$U_\mu(n) \rightarrow U_\mu(n)' = X(\theta)U_\mu(n), \quad X(\theta) = Re^{i\theta\lambda_3}R^\dagger \quad (4)$$

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 :

$$p^{\text{acc}}(U \rightarrow U') = \min \left(1, \frac{\pi(U')}{\pi(U)} \right) = \min \left(1, e^{-\Delta S} \right) \quad (5)$$

$$\text{with } \Delta S = \frac{\beta}{3} \text{ReTr} \left[(e^{i\theta\lambda_3} - \mathbb{1}) R^\dagger U_\mu(n) V(n, \mu) R \right] \quad (6)$$

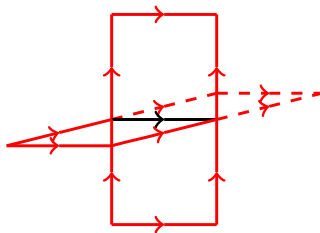


Figure 2 – A link (black) and its surrounding staples (red) in a 3D lattice

Factorization

- We use the **factorized** Metropolis acceptance probability

$$\text{Non factorized} : p^{\text{acc}}(U \rightarrow U') = \min \left(1, \frac{\pi(U')}{\pi(U)} \right) = \min \left(1, e^{-\Delta S} \right) \quad (7)$$

$$\text{Factorized} : p^{\text{fact}}(U \rightarrow U') = \underbrace{\min \left(1, e^{-\Delta S_1} \right)}_{\text{Plaquette 1}} \times \underbrace{\min \left(1, e^{-\Delta S_2} \right)}_{\text{Plaquette 2}} \times \dots \quad (8)$$

- 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 :

$$\epsilon = \begin{cases} 1 & \rightarrow \text{we increase } \theta \\ -1 & \rightarrow \text{we decrease } \theta \end{cases} \quad (9)$$

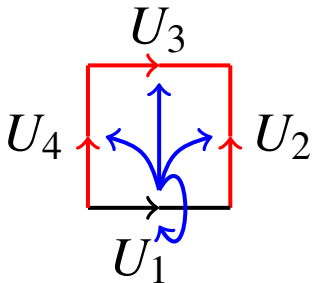
$$X(\theta) = Re^{i\epsilon\theta\lambda_3} R^\dagger \quad (10)$$

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

Reflective lifting

Lifting probability

$$P(U_1 \rightarrow U_i) = \frac{|\partial_\theta S_i^j(0)|}{\sum_{l \in P^j} |\partial_\theta S_l^j(0)|}, \quad \epsilon \rightarrow -\text{sign}(\partial_\theta S_i^j(0)), \quad \partial_\theta S_i^j(0) = \frac{\beta}{3} \text{ReTr} \left[i\lambda_3 R^\dagger U_i V_i^j R \right].$$



Pros :

- Easily adaptable to any action

Cons :

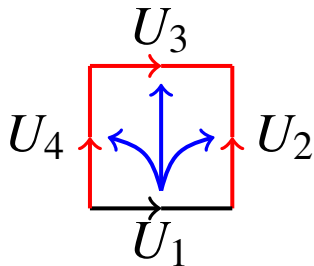
- Computationally heavy (staples computation)
- Allows backtracking

Forward lifting

Lifting probability

$$P(U_1 \rightarrow U_i) = \frac{1}{3},$$

and we change ϵ, R according to table 1.



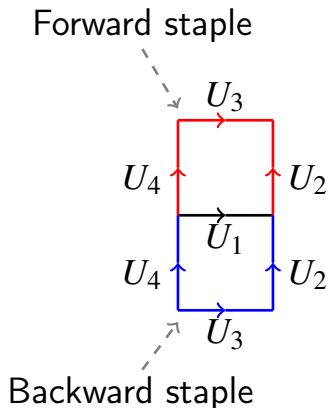
Pros :

- 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

$$dp_i^{\text{acc}}(0 \rightarrow \epsilon\theta_r) = \max(0, f(\epsilon\theta_r))d\theta_r, \quad f(\epsilon\theta) = \frac{-\epsilon}{\pi(0)} \frac{\partial\pi}{\partial\theta} \Big|_{\theta=\epsilon\theta_r}. \quad (11)$$

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

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

Event-driven approach

- In practice, we need to solve

Reject generation equation

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

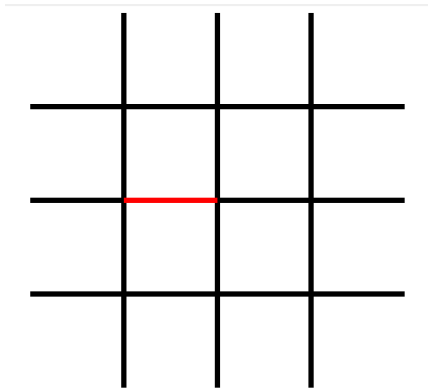
with $S(\theta) = \text{ReTr} \left[(e^{i\theta \lambda_3} - \mathbb{1}) R^\dagger U_\mu(n) S_j(n, \mu) R \right] .$

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

$$\exp\left(\frac{\beta}{3}\right) = \int_0^{\theta_r} [-A \sin(\epsilon \theta) + B \cos(\epsilon \theta)]^+ d\theta. \quad (12)$$

→ This can be solved analytically !

Summary

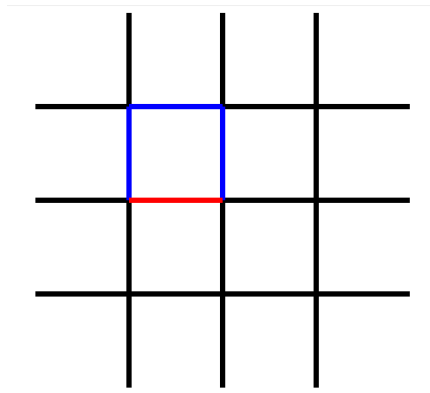


We update the red link until a reject occurs



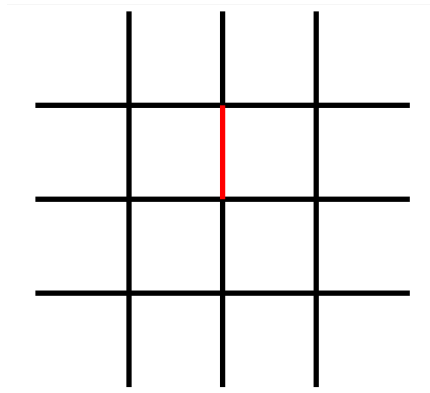
We generate a reject angle θ_r for each plaquette and choose the lowest (event-driven approach)

Summary



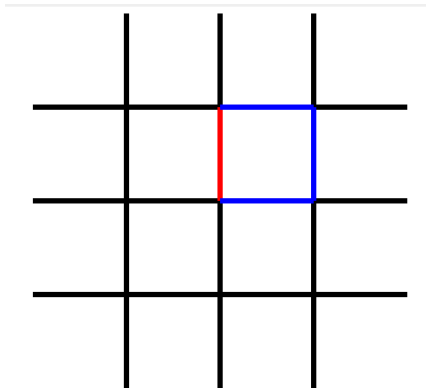
... One of the two attached staples refused a move...

Summary



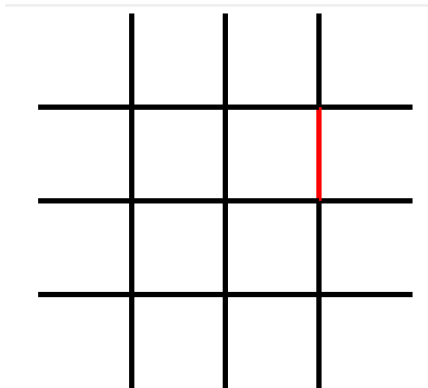
... so we change the updated link to another link of the plaquette (lift)...

Summary



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

Summary



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

Plan

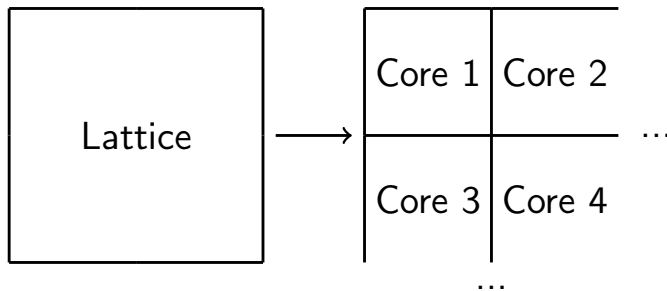
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Parallelization

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

Problem

How can we parallelize the ECMC algorithm ?



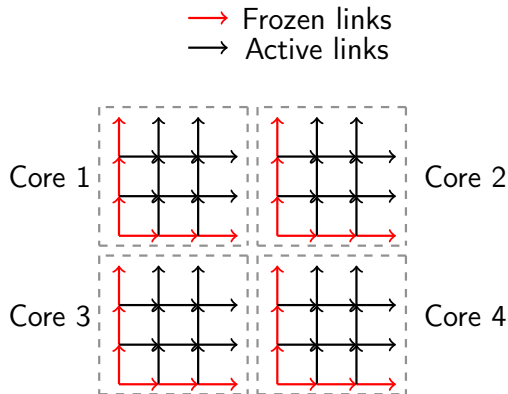
We **freeze** the boundary links (cf. [7]) $\rightarrow$ the Event-Chain **bounces** on frozen links

Pros :

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

Cons :

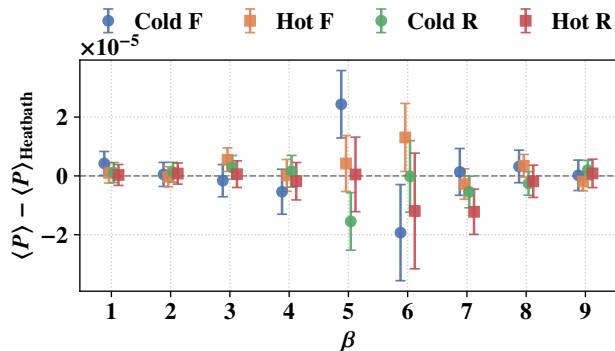
- Introduces **backtracking** (backtracking rate decreases when the lattice is large)
- $\frac{\text{Nb. Active links}}{\text{Nb. Total links}} = (1 - 1/L_{\text{core}})^3$



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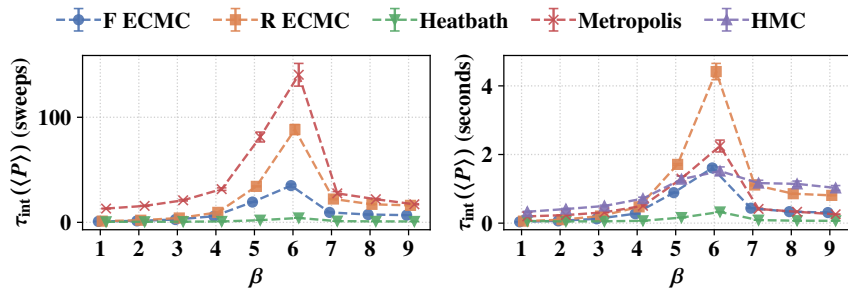
Results – Correctness



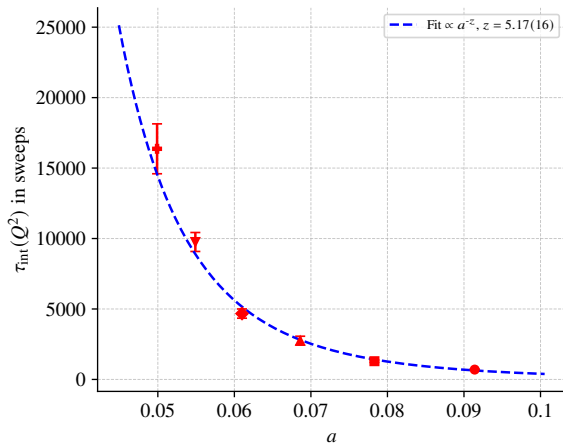
- No visible bias
- Agreement up to $\times 10^{-5}$, standard

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

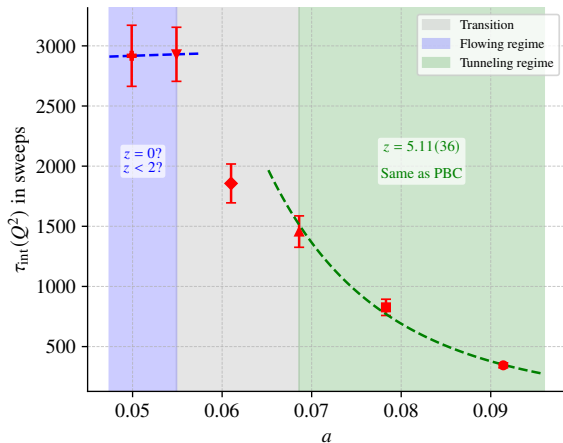
Results – Autocorrelation and comparison



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

Results – $z(Q^2)$ PBC, Forward ECMC (Preliminary)

- Runs at constant physical volume of $V \approx 1.2\text{fm}$ with periodic boundary conditions
- ECMC **scales slightly better** than Heatbath and HMC but with greater constant coefficient $\rightarrow$ overrelaxtion?
- Effects of parallelization and ECMC **parametrization** has to be investigated

Results – $z(Q^2)$ OBC, Forward ECMC (Preliminary)

- Runs at constant physical volume of $V \approx 2.4\text{fm}$ with open boundary conditions
- Hints to a better flowing regime than HMC → need more data at finer lattice spacing (Finite Size Scaling?)
- Effects of parallelization and ECMC parametrization has to be investigated

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Conclusion

- New class of algorithms to explore for quenched 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^2 and Wilson loops in Periodic/Open Boundary conditions, with overrelaxation, with different parallelizations/ECMC parametrizations
- Full characterization of the CSD for this algorithm

Thanks for your attention !

Références I

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