

# Squeezing water from a stone

A brief overview of lattice QCD

**Jonas Rylund Glesaaen**  
jonas@glesaaen.com

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**A bit about me**

# Background

- **NTNU: Master's in physics**
- **Frankfurt: PhD in Lattice QCD**
- **Swansea: Postdoc Lattice QCD**
- **Oslo: Software development**

# Lattice QCD

# Quantum Chromo Dynamics

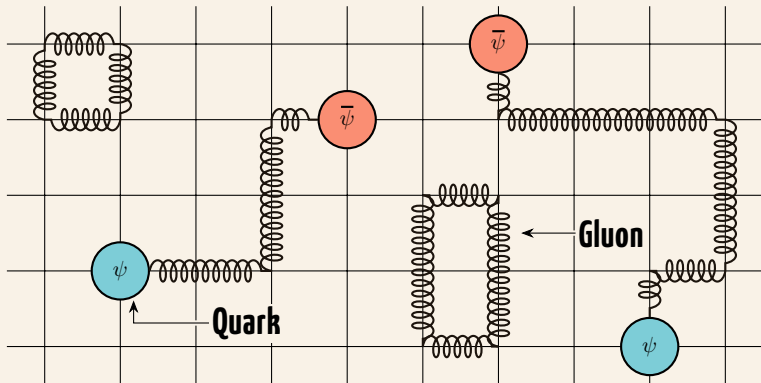
Theoretical description of the **strong nuclear force**



It binds matter together at the subatomic level

# Lattice QCD

Basically we just put on a (**HUGE**) lattice



# The important equations

$$S = \int d^4x \bar{\psi}(x) Q \psi(x) + \mathcal{L}_g[U(x)]$$

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# The important equations

$$S = \int d^4x \bar{\psi}(x) Q \psi(x) + \mathcal{L}_g[U(x)]$$

$$\mathcal{Z} = \int D\psi DU e^{-S[\psi, U]}$$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D\psi DU \mathcal{O}[\psi, U] e^{-S[\psi, U]}$$

# Discretisation

$$S \rightarrow \sum_{i,j} \bar{\psi}(x_i) Q_{i,j}[U] \psi(x_j) + \mathcal{L}_g[U(x_i)]$$

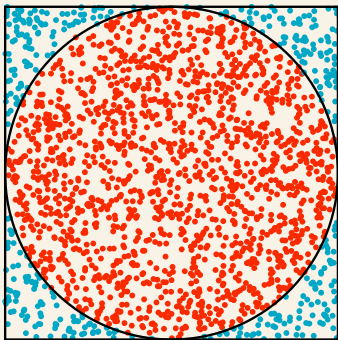
# Discretisation

$$S \rightarrow \sum_{i,j} \bar{\psi}(x_i) Q_{i,j}[U] \psi(x_j) + \mathcal{L}_g[U(x_i)]$$

$$\mathcal{Z} = \int \mathrm{D}\psi \mathrm{D}U e^{-S[\psi,U]} = \int \mathrm{D}U \det(Q) e^{-\sum \mathcal{L}_g[U(x)]}$$

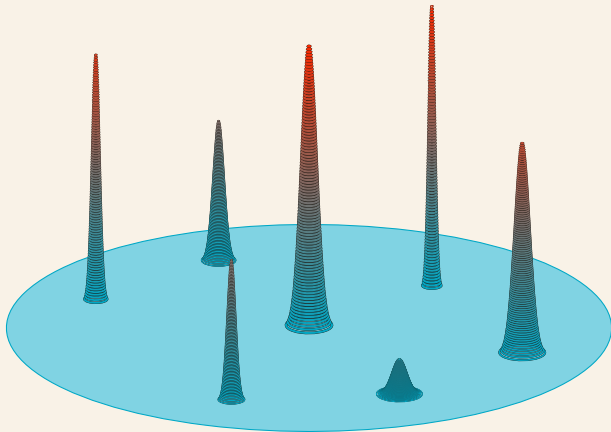
# Monte Carlo Integration

# Monte Carlo integration

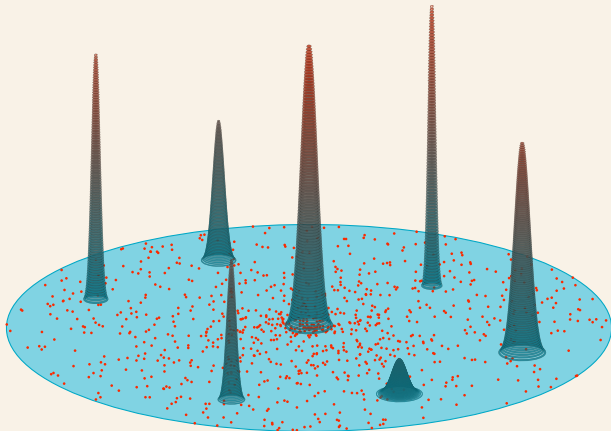


$$\pi \approx 4 \cdot \frac{1609}{2000} \\ = 3.21799$$

# The QCD Integrand



# The QCD Integrand



# Redefining the problem

$$\langle \mathcal{O} \rangle = \int \mathrm{D}U \mathcal{O}[U] \underbrace{\frac{1}{\mathcal{Z}} e^{-S[U]}}_{\text{Probability density}} = \int \mathrm{D}U \mathcal{O}[U] \mathcal{P}[U]$$

**Integral over U can be stochastically estimated.**

$$\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_k \mathcal{O}[U_k] \quad \begin{array}{c} \uparrow \\ \text{Distributed } \propto \mathcal{P} \end{array}$$



# Markov Chains

$$U_1 \xrightarrow{\propto \mathcal{P}} U_2 \xrightarrow{\propto \mathcal{P}} U_3 \xrightarrow{\propto \mathcal{P}} U_4 \xrightarrow{\propto \mathcal{P}} \dots$$

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$$p = \min\{1, \mathcal{P}[U_k'] / \mathcal{P}[U_k]\}$$

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**The distribution can be achieved with a Metropolis accept-reject step**

$$p = \min\{1, \mathcal{P}[U_k'] / \mathcal{P}[U_k]\}$$

**But the evaluation of this is very expensive...**

$$\begin{array}{c}
\text{\textit{VOL}} \times N_d \times N_c \\
\updownarrow
\end{array}
\begin{pmatrix}
D(0|0) & D(0|\hat{0}) & 0 & 0 & 0 & \dots \\
D(\hat{0}|0) & D(\hat{0}|\hat{0}) & D(\hat{0}|2\hat{0}) & 0 & 0 & \dots \\
0 & D(2\hat{0}|\hat{0}) & D(2\hat{0}|2\hat{0}) & D(2\hat{0}|3\hat{0}) & 0 & \dots \\
0 & 0 & D(3\hat{0}|2\hat{0}) & D(3\hat{0}|3\hat{0}) & D(3\hat{0}|\hat{4}\hat{0}) & \dots \\
0 & 0 & 0 & D(4\hat{0}|3\hat{0}) & D(4\hat{0}|\hat{4}\hat{0}) & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
D(\hat{1}|0) & D(\hat{1}|\hat{0}) & 0 & 0 & 0 & \dots \\
D(\hat{1}|\hat{0}) & D(\hat{0}\hat{1}|\hat{0}) & D(\hat{0}\hat{1}|2\hat{0}) & 0 & 0 & \dots \\
0 & D(2\hat{0}\hat{1}|\hat{0}) & D(2\hat{0}\hat{1}|2\hat{0}) & D(2\hat{0}\hat{1}|3\hat{0}) & 0 & \dots \\
0 & 0 & D(3\hat{0}\hat{1}|2\hat{0}) & D(3\hat{0}\hat{1}|3\hat{0}) & D(3\hat{0}\hat{1}|\hat{4}\hat{0}) & \dots \\
0 & 0 & 0 & D(4\hat{0}\hat{1}|3\hat{0}) & D(4\hat{0}\hat{1}|\hat{4}\hat{0}) & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
D(2\hat{1}|0) & D(2\hat{1}|\hat{0}) & 0 & 0 & 0 & \dots \\
D(2\hat{1}|\hat{0}) & D(\hat{0}2\hat{1}|\hat{0}) & D(\hat{0}2\hat{1}|2\hat{0}) & 0 & 0 & \dots \\
0 & D(2\hat{0}2\hat{1}|\hat{0}) & D(2\hat{0}2\hat{1}|2\hat{0}) & D(2\hat{0}2\hat{1}|3\hat{0}) & 0 & \dots \\
0 & 0 & D(3\hat{0}2\hat{1}|2\hat{0}) & D(3\hat{0}2\hat{1}|3\hat{0}) & D(3\hat{0}2\hat{1}|\hat{4}\hat{0}) & \dots \\
0 & 0 & 0 & D(4\hat{0}2\hat{1}|3\hat{0}) & D(4\hat{0}2\hat{1}|\hat{4}\hat{0}) & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
D(3\hat{1}|0) & D(3\hat{1}|\hat{0}) & 0 & 0 & 0 & \dots \\
D(3\hat{1}|\hat{0}) & D(\hat{0}3\hat{1}|\hat{0}) & D(\hat{0}3\hat{1}|2\hat{0}) & 0 & 0 & \dots \\
0 & D(2\hat{0}3\hat{1}|\hat{0}) & D(2\hat{0}3\hat{1}|2\hat{0}) & D(2\hat{0}3\hat{1}|3\hat{0}) & 0 & \dots \\
0 & 0 & D(3\hat{0}3\hat{1}|2\hat{0}) & D(3\hat{0}3\hat{1}|3\hat{0}) & D(3\hat{0}3\hat{1}|\hat{4}\hat{0}) & \dots \\
0 & 0 & 0 & D(4\hat{0}3\hat{1}|3\hat{0}) & D(4\hat{0}3\hat{1}|\hat{4}\hat{0}) & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
=
\begin{pmatrix}
\psi(0) \\
\psi(\hat{0}) \\
\psi(2\hat{0}) \\
\psi(3\hat{0}) \\
\psi(4\hat{0}) \\
\vdots \\
\psi(\hat{1}) \\
\psi(\hat{0}\hat{1}) \\
\psi(2\hat{0}\hat{1}) \\
\psi(3\hat{0}\hat{1}) \\
\psi(4\hat{0}\hat{1}) \\
\vdots \\
\psi(2\hat{1}) \\
\psi(\hat{0}2\hat{1}) \\
\psi(2\hat{0}2\hat{1}) \\
\psi(3\hat{0}2\hat{1}) \\
\psi(4\hat{0}2\hat{1}) \\
\vdots \\
\psi(3\hat{1}) \\
\psi(\hat{0}3\hat{1}) \\
\psi(2\hat{0}3\hat{1}) \\
\psi(3\hat{0}3\hat{1}) \\
\psi(4\hat{0}3\hat{1}) \\
\vdots
\end{pmatrix}
=
\begin{pmatrix}
\xi(0) \\
\xi(\hat{0}) \\
\xi(2\hat{0}) \\
\xi(3\hat{0}) \\
\xi(4\hat{0}) \\
\vdots \\
\xi(\hat{1}) \\
\xi(\hat{0}\hat{1}) \\
\xi(2\hat{0}\hat{1}) \\
\xi(3\hat{0}\hat{1}) \\
\xi(4\hat{0}\hat{1}) \\
\vdots \\
\xi(2\hat{1}) \\
\xi(\hat{0}2\hat{1}) \\
\xi(2\hat{0}2\hat{1}) \\
\xi(3\hat{0}2\hat{1}) \\
\xi(4\hat{0}2\hat{1}) \\
\vdots \\
\xi(3\hat{1}) \\
\xi(\hat{0}3\hat{1}) \\
\xi(2\hat{0}3\hat{1}) \\
\xi(3\hat{0}3\hat{1}) \\
\xi(4\hat{0}3\hat{1}) \\
\vdots
\end{pmatrix}$$

$$\begin{array}{c}
\text{\textit{VOL}} \times N_d \times N_c \\
\leftarrow \hspace{1.5cm} \rightarrow
\end{array}$$

$VOL \times N_d \times N_c$

$$\begin{pmatrix}
 D(0|0) & D(0|\bar{0}) & 0 & 0 & 0 & \dots \\
 D(\bar{0}|0) & D(\bar{0}|\bar{0}) & D(\bar{0}|2\bar{0}) & 0 & 0 & \dots \\
 0 & D(2\bar{0}|\bar{0}) & D(2\bar{0}|2\bar{0}) & D(2\bar{0}|3\bar{0}) & 0 & \dots \\
 0 & 0 & D(3\bar{0}|2\bar{0}) & D(3\bar{0}|3\bar{0}) & D(3\bar{0}|4\bar{0}) & \dots \\
 0 & 0 & 0 & D(4\bar{0}|3\bar{0}) & D(4\bar{0}|4\bar{0}) & \dots \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
 D(0|1) & D(0|\bar{1}) & 0 & 0 & 0 & \dots \\
 0 & D(1|\bar{0}) & D(1|\bar{1}) & 0 & 0 & \dots \\
 0 & 0 & D(2\bar{1}|\bar{0}) & D(2\bar{1}|1\bar{0}) & 0 & \dots \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
 D(2\bar{1}|0) & D(2\bar{1}|\bar{0}) & 0 & 0 & 0 & \dots \\
 D(2\bar{1}|0) & D(\bar{0}2\bar{1}|\bar{0}) & D(\bar{0}2\bar{1}|2\bar{0}) & 0 & 0 & \dots \\
 0 & D(2\bar{0}2\bar{1}|\bar{0}) & D(2\bar{0}2\bar{1}|2\bar{0}) & D(2\bar{0}2\bar{1}|3\bar{0}) & 0 & \dots \\
 0 & 0 & D(3\bar{0}2\bar{1}|2\bar{0}) & D(3\bar{0}2\bar{1}|3\bar{0}) & D(3\bar{0}2\bar{1}|4\bar{0}) & \dots \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
 D(3\bar{1}|0) & D(3\bar{1}|\bar{0}) & 0 & 0 & 0 & \dots \\
 D(3\bar{1}|0) & D(\bar{0}3\bar{1}|\bar{0}) & D(\bar{0}3\bar{1}|2\bar{0}) & 0 & 0 & \dots \\
 0 & D(2\bar{0}3\bar{1}|\bar{0}) & D(2\bar{0}3\bar{1}|2\bar{0}) & D(2\bar{0}3\bar{1}|3\bar{0}) & 0 & \dots \\
 0 & 0 & D(3\bar{0}3\bar{1}|2\bar{0}) & D(3\bar{0}3\bar{1}|3\bar{0}) & D(3\bar{0}3\bar{1}|4\bar{0}) & \dots \\
 0 & 0 & 0 & D(4\bar{0}3\bar{1}|3\bar{0}) & D(4\bar{0}3\bar{1}|4\bar{0}) & \dots \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
 \end{pmatrix}
 \begin{pmatrix}
 \psi(0) \\
 \psi(\bar{0}) \\
 \psi(2\bar{0}) \\
 \psi(3\bar{0}) \\
 \psi(4\bar{0}) \\
 \vdots \\
 \psi(20\bar{1}) \\
 \psi(\bar{0}2\bar{1}) \\
 \psi(2\bar{0}2\bar{1}) \\
 \psi(3\bar{0}2\bar{1}) \\
 \vdots \\
 \psi(3\bar{1}) \\
 \psi(\bar{0}3\bar{1}) \\
 \psi(2\bar{0}3\bar{1}) \\
 \psi(3\bar{0}3\bar{1}) \\
 \psi(4\bar{0}3\bar{1}) \\
 \vdots
 \end{pmatrix}
 =
 \begin{pmatrix}
 \xi(0) \\
 \xi(\bar{0}) \\
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 \xi(3\bar{0}) \\
 \xi(4\bar{0}) \\
 \vdots \\
 \xi(20\bar{1}) \\
 \xi(\bar{0}2\bar{1}) \\
 \xi(2\bar{0}2\bar{1}) \\
 \xi(3\bar{0}2\bar{1}) \\
 \vdots \\
 \xi(3\bar{1}) \\
 \xi(\bar{0}3\bar{1}) \\
 \xi(2\bar{0}3\bar{1}) \\
 \xi(3\bar{0}3\bar{1}) \\
 \xi(4\bar{0}3\bar{1}) \\
 \vdots
 \end{pmatrix}$$

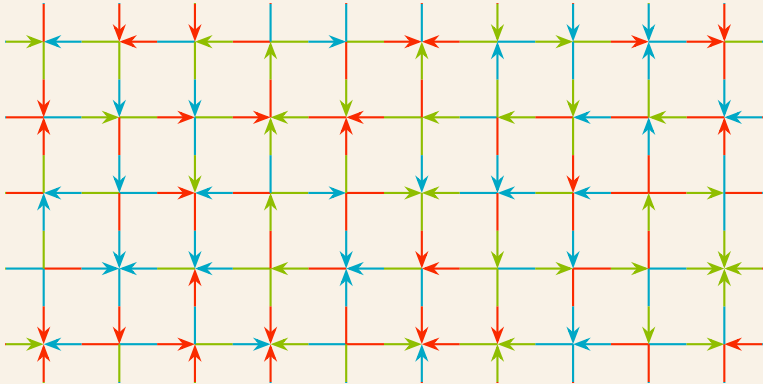
**We need to solve this matrix equation  
many many many times**

**Our low temperature lattices are:**

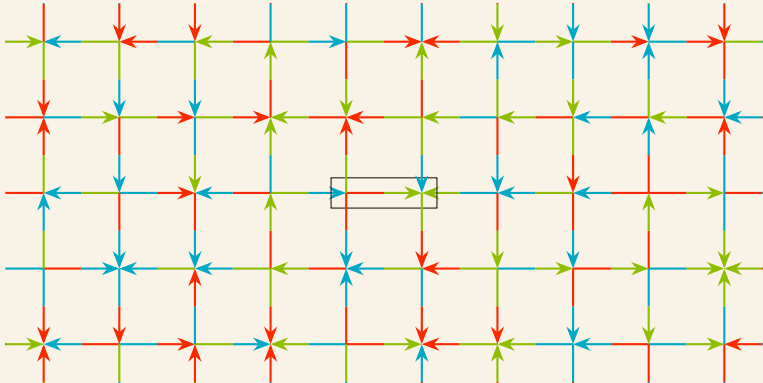
$$256 \times 32^3 \times 4 \times 3 \sim 10^8$$

$VOL \times N_d \times N_c$

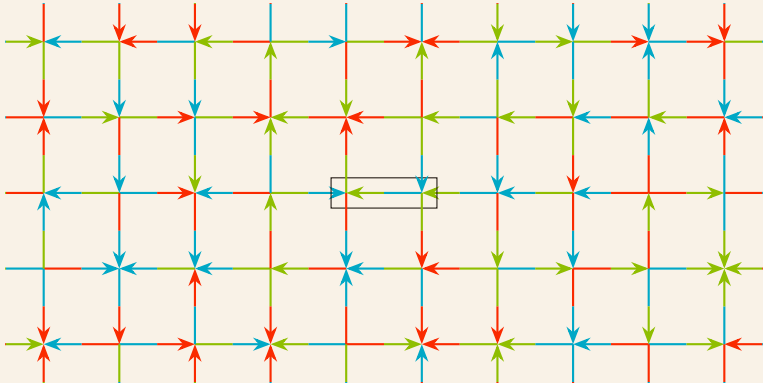
# Single link updates



# Single link updates

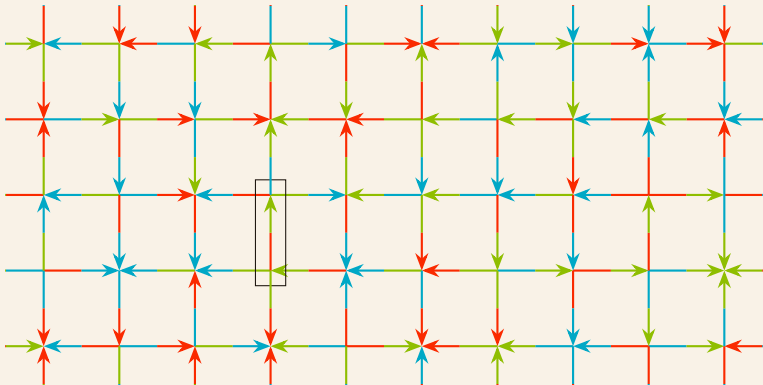


# Single link updates

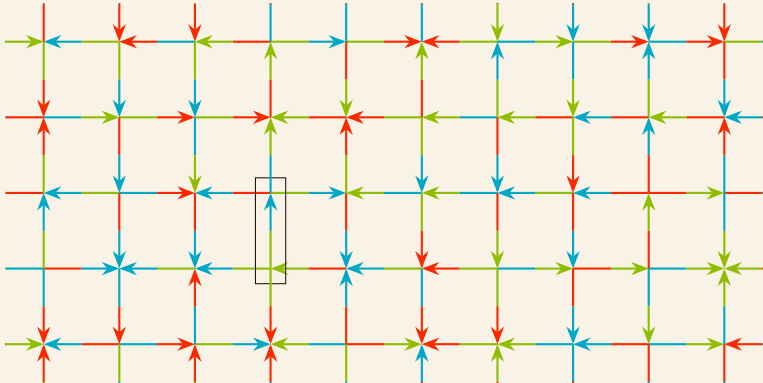




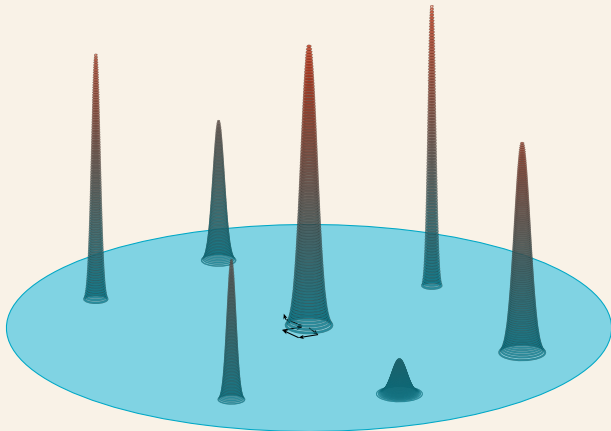
# Single link updates



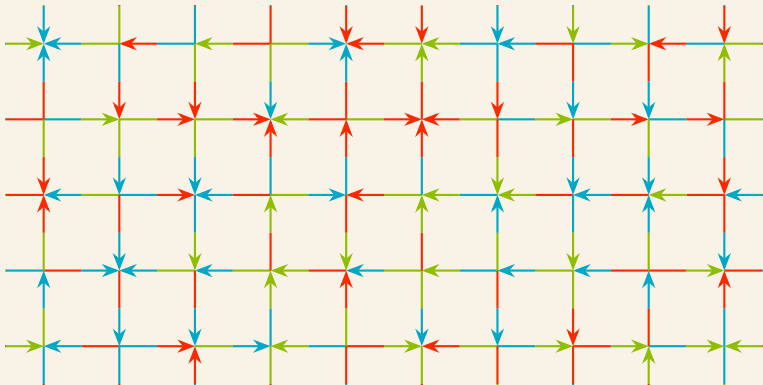
# Single link updates



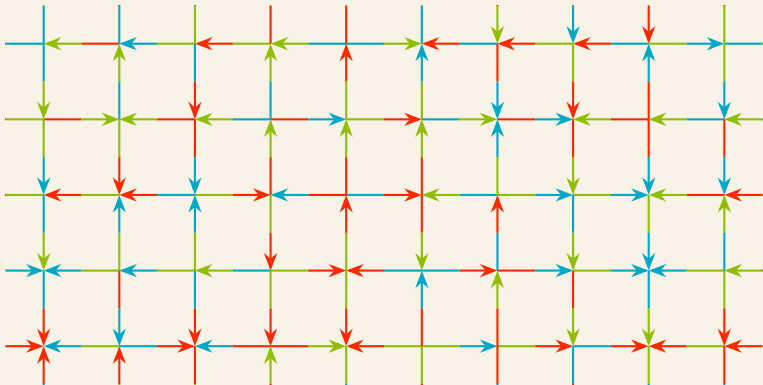
# Single link updates



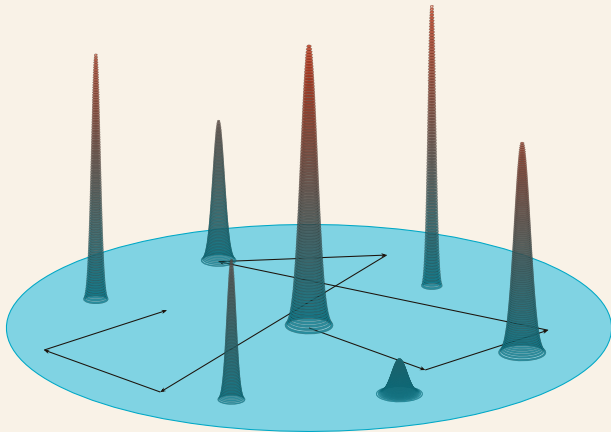
# Configuration updates



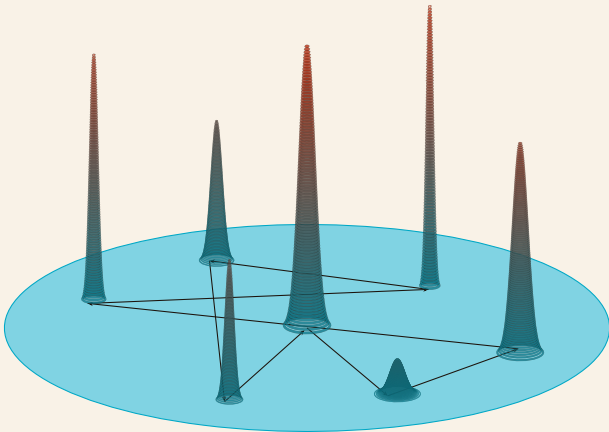
## Configuration updates



# Configuration updates (random)



# Configuration updates (directed)



# Clever algorithms

- **Langevin algorithm (1981)**

Steepest descent + Gaussian noise

- **Molecular Dynamics algorithm (1983)**

Additional stochastic variables + Hamilton's equations

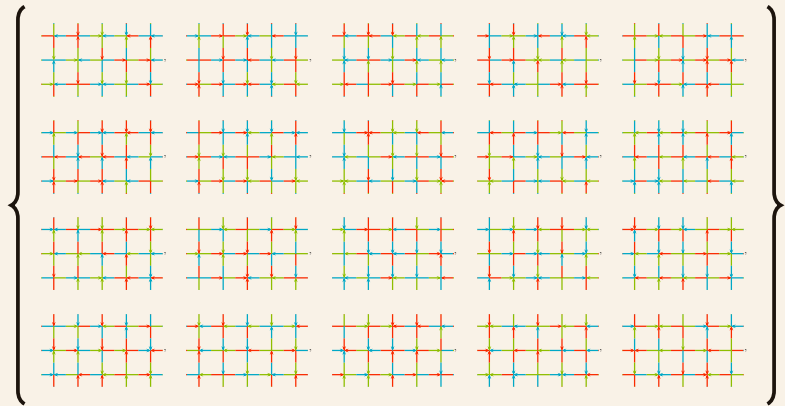
- **Hybrid Monte Carlo (1987)**

Combine Langevin and MD with Metropolis accept-reject



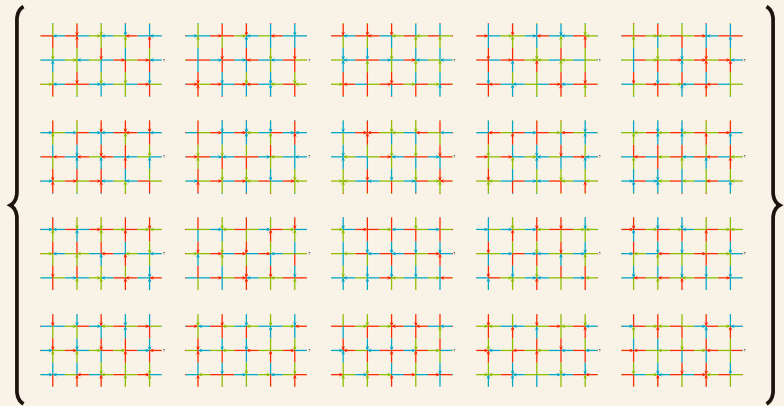
# Measurements

# Configurations



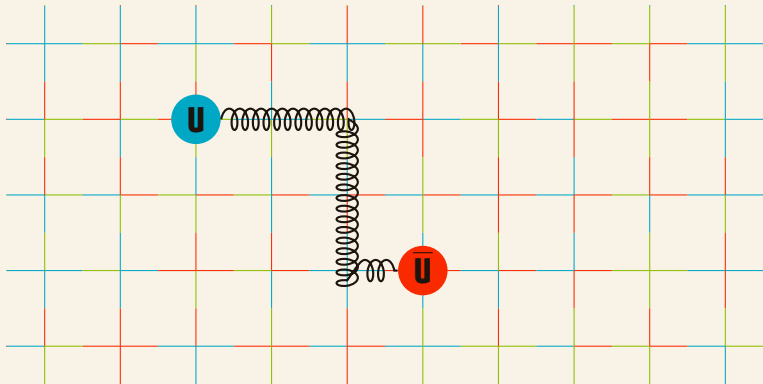
**Each configuration consists of  $(4 \cdot 18 \cdot \text{VOL})$  numbers.**

# Configurations

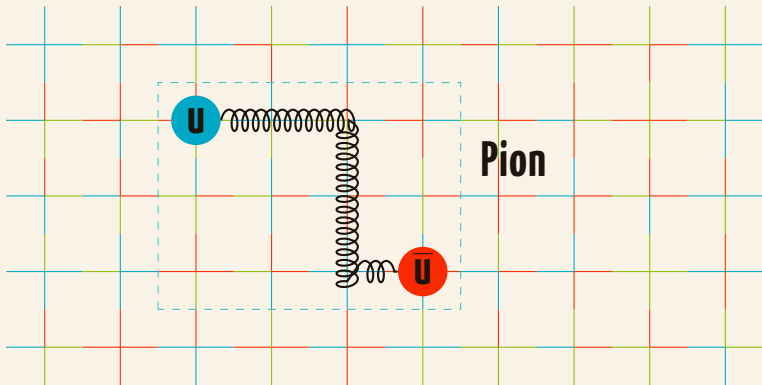


**Low temperature configuration is 4.5 GB**

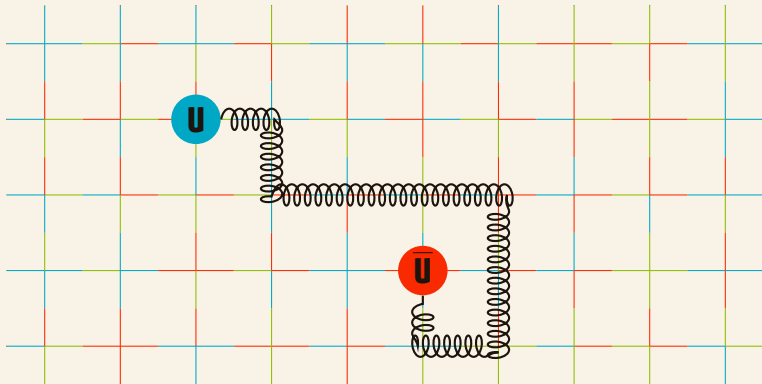
# Hadron spectroscopy



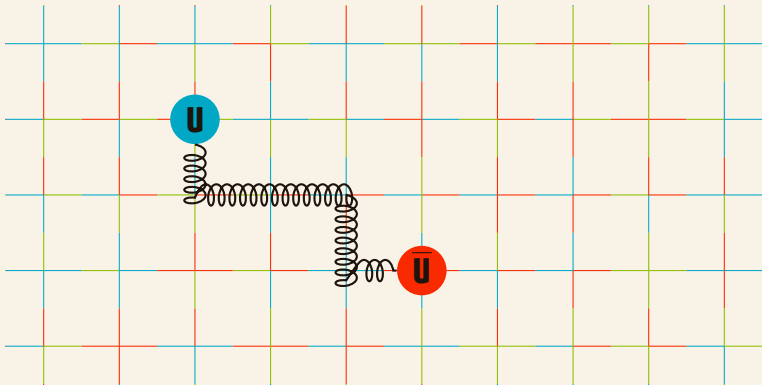
# Hadron spectroscopy



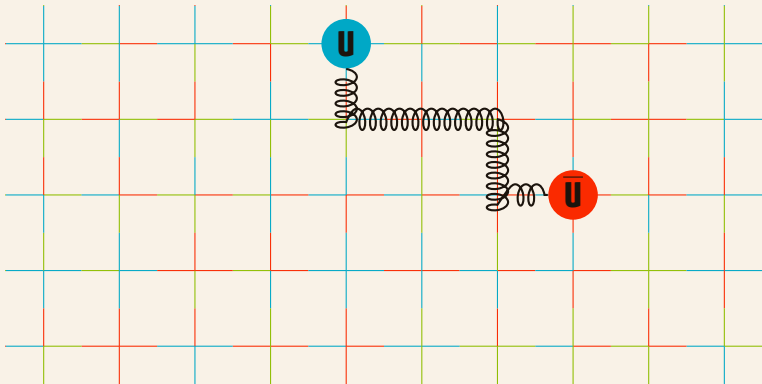
# Hadron spectroscopy



# Hadron spectroscopy

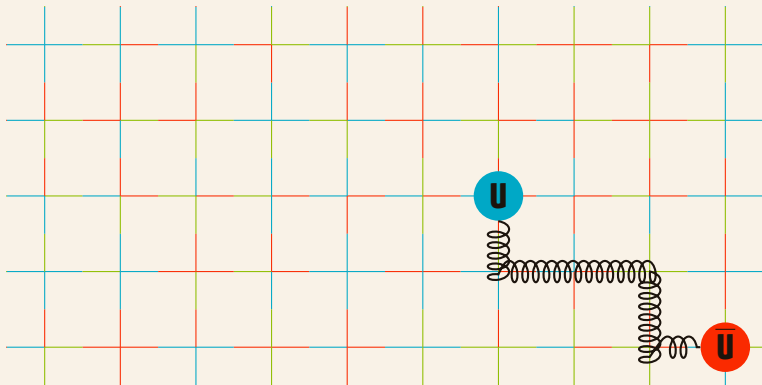


# Hadron spectroscopy

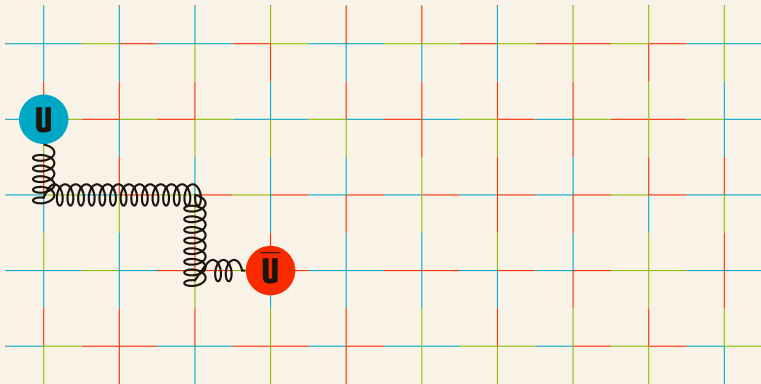




# Hadron spectroscopy

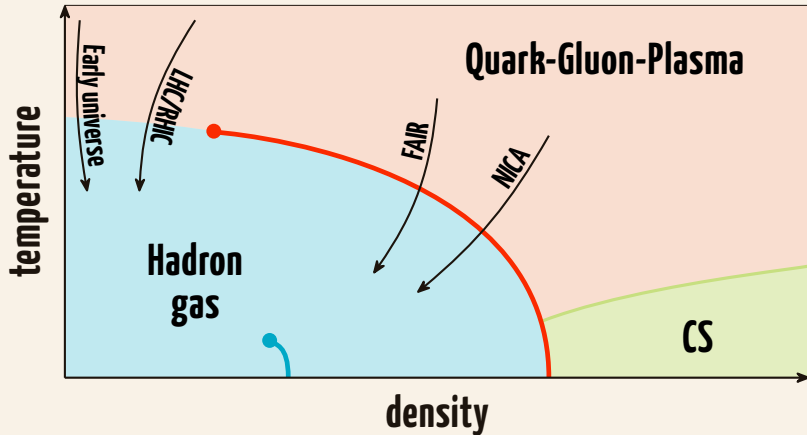


# Hadron spectroscopy



# Results

# Phase diagram of QCD



# Baryon parity breaking

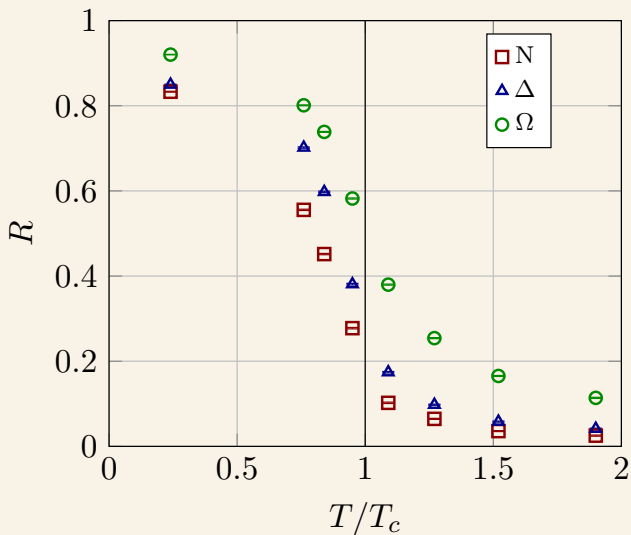


Mass: 938 MeV



Mass: 1535 MeV

# Baryon parity restoration



# Conclusion

**Questions?**