High Performance Computing and Aspects of Computing in Lattice Gauge Theories

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RESEARCH•TECHNOLOGY•INNOVATION

EuroPLEx School
Lecture 02 – 4th November 2020

Refresh – computational intensity

Recall the definitions of kernel and machine intensities

- Kernel: floating-point rate, I/O rate, kernel intensity I_k

$$\beta_{FP} = \frac{N_{FP}}{\bar{T}} \qquad \beta_{IO} = \frac{N_{IO}}{\bar{T}} \qquad I_k = \frac{N_{FP}}{N_{IO}}$$

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- Machine: peak floating-point rate (γ_{FP}), I/O rate (γ_{IO}), and machine intensity I_m

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- Machine: peak floating-point rate (γ_{FP}), I/O rate (γ_{IO}), and machine intensity $\mathrm{I_m}$

$$\mathrm{I_m} = \frac{\gamma_{\mathrm{FP}}}{\gamma_{\mathrm{IO}}}$$

- Compute-bound, bandwidth- (or memory-) bound, balanced
  - $\mathrm{I_k} \gg \mathrm{I_m}$: Compute bound
  - $\mathrm{I_k} \ll \mathrm{I_m}$: Memory bound
  - $\mathrm{I_k} \simeq \mathrm{I_m}$: Balanced

Practical

Matrix-matrix multiplication

- Consider the multiplication:

$$C_{M\times K} = A_{M\times N} B_{N\times K} \rightarrow C_{mk} = \sum_{n=0}^{N-1} A_{mn} B_{nk}$$

- A straight- forward implementation

```
for(int m=0; m<M; m++) {
  for(int k=0; k<K; k++) {
    C[m][k] = 0;
    for(int n=0; n<N; n++) {
      C[m][k] += A[m][n]*B[n][k];
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$$N_{IO} = w(MN + NK + MK)$$

$$I_k = \frac{2}{w} \frac{1}{\frac{1}{N} + \frac{1}{K} + \frac{1}{M}}$$

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E.g. on Juwels, for double-precision (w=8 bytes), this kernel is memory-bound for $M \lesssim 200$, and compute-bound for $M \gtrsim 200$

Practical

Complex “axpy” operation

- $y_i = ax_i + y_i$, $i=0,\ldots,N-1$, with x, y, complex arrays, a complex scalar

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_Complex double x[N];
_Complex double y[N];
_Complex double a;
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- Write real and imaginary part of left-hand-side explicitly

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$$I_k = \frac{4}{3w}$$ Memory-bound (on most architectures)

Outline – 4th Nov.

Computational aspects of lattice gauge theories

- Gauge theories on the lattice
  - Path integral formulation
  - Typical workflow
- Challenges
  - Errors, systematic uncertainties
  - Computational resource requirements
- Overview of some common methods and their impact
  - Sparse linear systems, multigrid solvers, Hybrid Monte Carlo
  - Impact on current state-of-the-art in lattice QCD
- Practical/technical aspects of implementing LGT
  - Computational intensity of the Schwinger fermion matrix

Gauge Theories on the Lattice

Introduction

- Action and Lagrangian:

$$S = \int d^4x \mathcal{L}(x), \quad \mathcal{L} = \bar{\psi} \underbrace{(i\not{D} - m)}_{M} \psi - \frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu}$$

where

$$F^a_{\mu\nu} = \partial_\mu G^a_\nu - \partial_\nu G^a_\mu - g f_{abc} G^b_\mu G^c_\nu$$

- Fermion fields: ψ
- Gauge (Gluon) fields: G

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- Gauge (Gluon) fields: G
- Feynman path integral formulation:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U]\mathcal{D}[\bar{\psi}]\mathcal{D}[\psi]\mathcal{O}(U, \psi, \bar{\psi}) e^{iS[U,\psi,\bar{\psi}]}$$

- Where we have introduced the *link variables* $U_\mu(x_1;x_0)$:

$$U_\mu(x_1; x_0) \equiv e^{-ig \int_{\mathcal{C}} dx G^c_\mu(x) T_c}$$

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- Integration over field variables U and ψ via Monte Carlo:
  - ✗ Fermion fields are Grassmann-valued
  - ✗ Exponent (probability) is complex

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- **Observables**: N-point correlation functions of fermions → functions of the inverse of the fermion matrix M (Wick's theorem/Wick contractions):

$$\langle \psi_{j_1}\psi_{j_2}...\bar{\psi}_{i_1}\bar{\psi}_{i_2}... \rangle = \langle (-1)^p M^{-1}_{i_1 j_1} M^{-1}_{i_2 j_2} ... + \text{all permutations} \rangle_U$$

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  - ✗ Non-local

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- Inversion of M
  - ✓ M is sparse $\Rightarrow M\phi$ is $\mathcal{O}(N)$ operations
  - ✓ $M^{-1}\phi$ via iterative methods: $\mathcal{O}(n)$ applications of $M\phi$, $n \ll N$

Gauge Theories on the Lattice

Introduction

- Discretization. *Link variables* and *gauge action*:

$$U_\mu(x_1; x_0) \equiv e^{-ig\int^C dx G^c_\mu(x) T_c} \rightarrow U_\mu(x_n) \equiv e^{-iagG^c_\mu(x_n)T_c}$$

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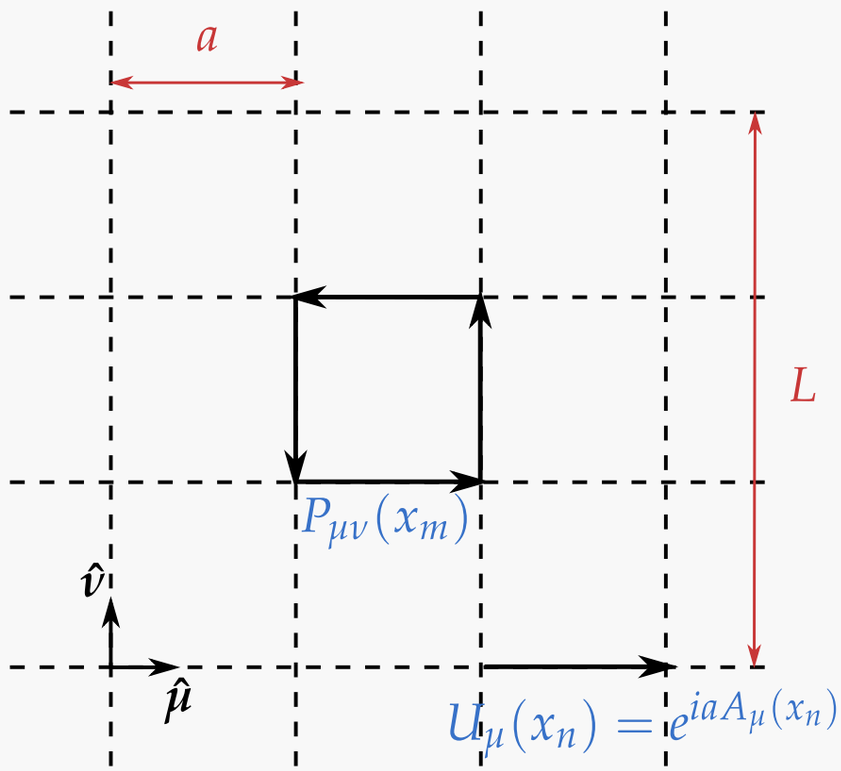

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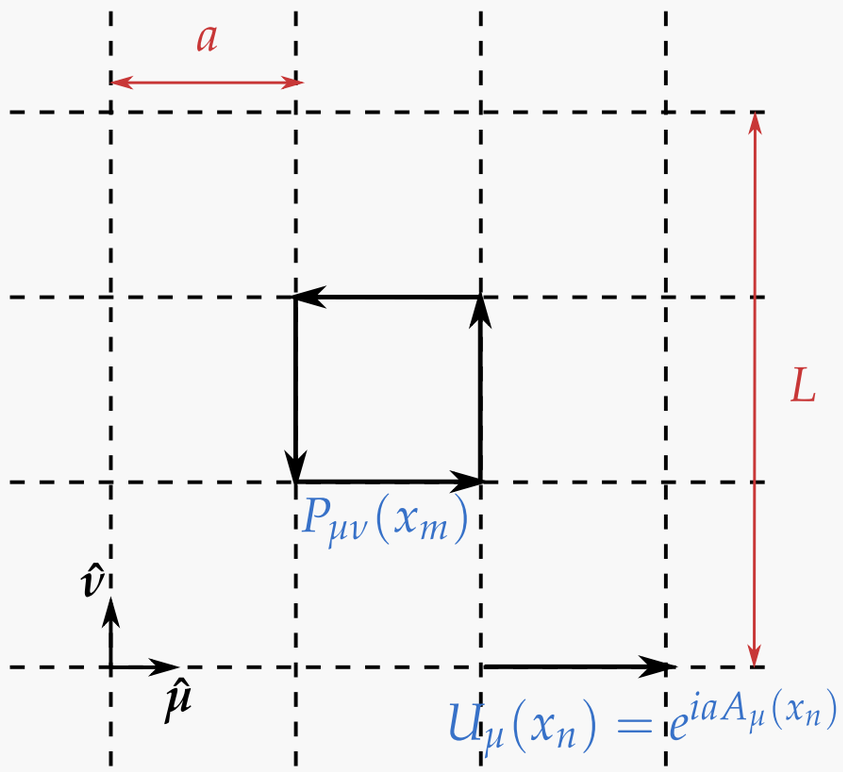
- Space-time lattice with **lattice spacing** a.



Gauge Theories on the Lattice

Introduction

- Fermion action written in terms of covariant derivatives, e.g. for Wilson fermions

$$S_F = \bar{\psi} M \psi \to -a^4 \sum_{x,\mu} \frac{1}{2a} [\bar{\psi}(x) U_\mu(x)(r-\gamma_\mu)\psi(x+a\hat{\mu}) + \bar{\psi}(x)(r+\gamma_\mu)U_{-\mu}(x)\psi(x-a\hat{\mu})]$$
$$+ a^4 \sum_x (m + \frac{4}{a} r)\bar{\psi}(x)\psi(x)$$

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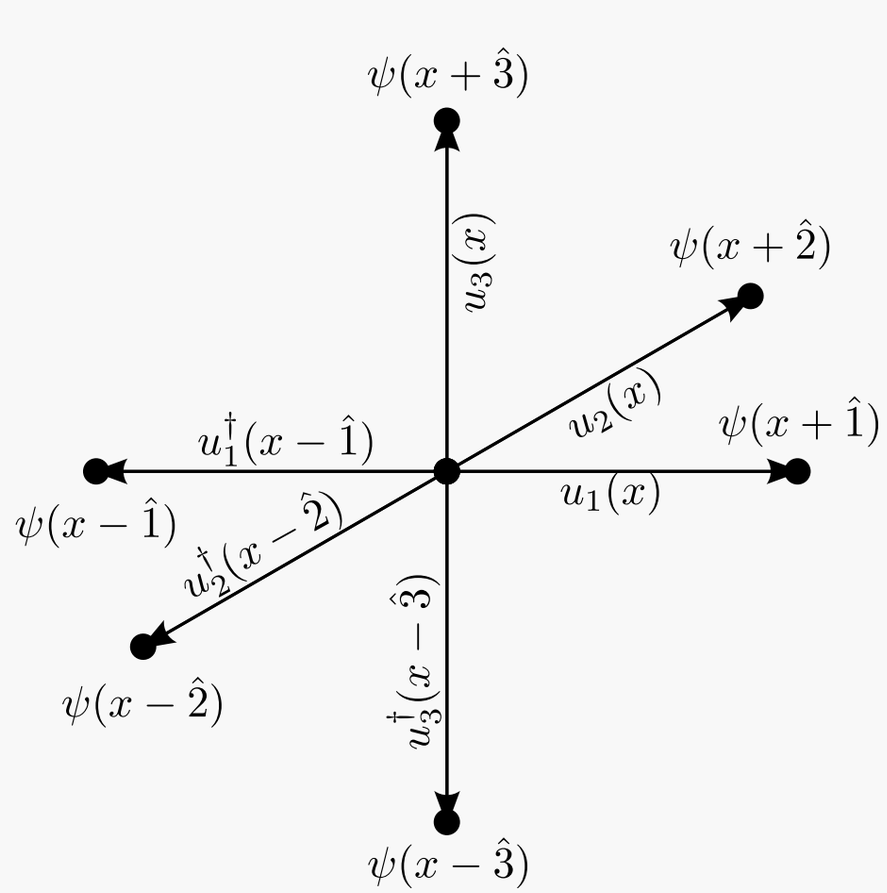

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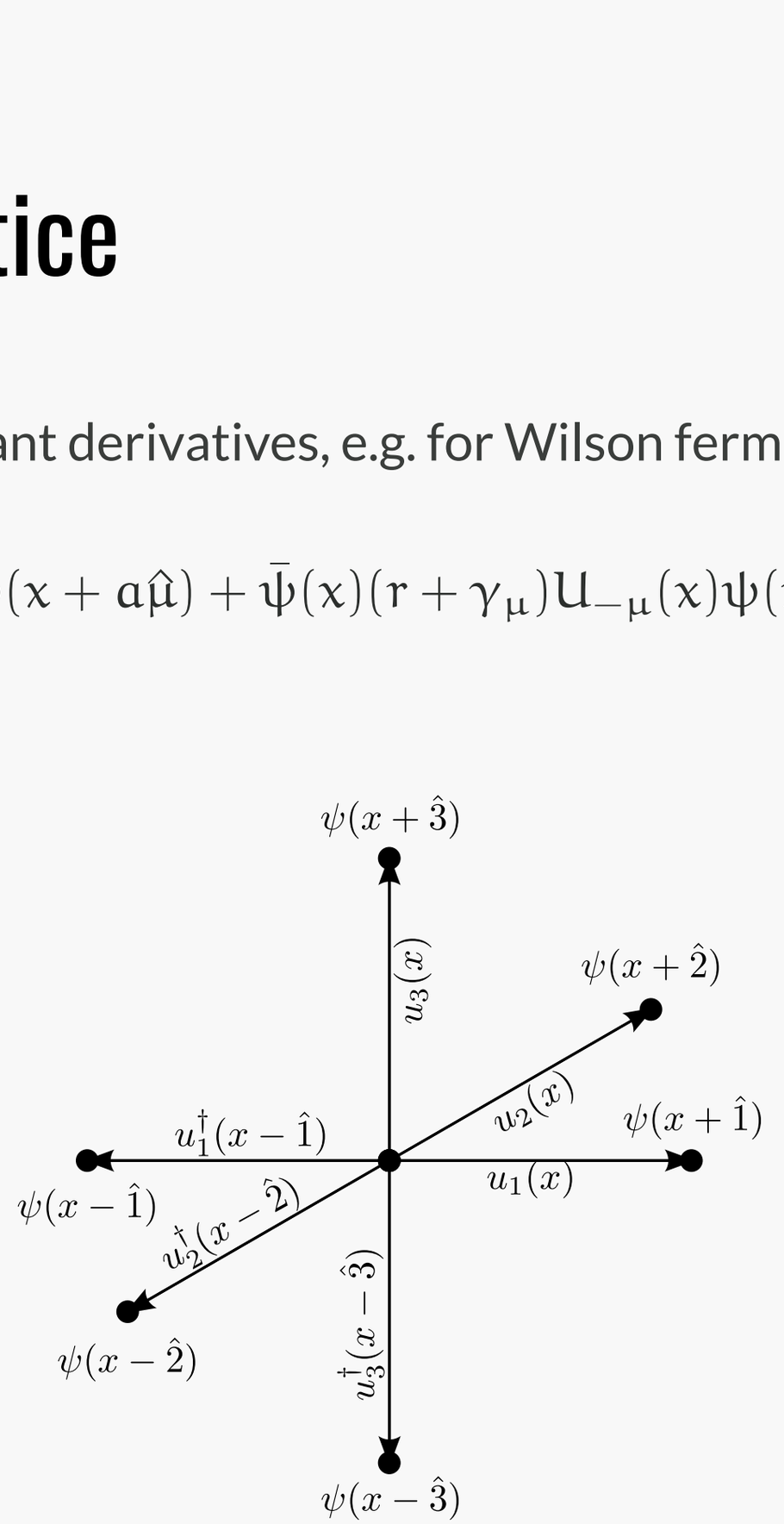
- 4-dimensional stencil
- Nearest neighbours in ψ
- In terms of covariant derivative:

$$\frac{1}{a}[U_\mu(x)\psi(x + a\hat{\mu}) - \psi(x)]$$



Gauge Theories on the Lattice

Freedom in choice of bare parameters:

- fermion masses (heavier is cheaper)
- lattice spacing/coupling a (larger is cheaper)
- lattice volume $L^3 \times T$ (smaller is cheaper)

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Eventually, all schemes must agree:

Limits: $a \to 0;\ L \to \infty; m \to m_{phys}$

Gauge Theories on the Lattice

The typical workflow

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U]\mathcal{D}[\bar{\phi}]\mathcal{D}[\phi]\mathcal{O} e^{-S_G[U] - \bar{\phi}(M^+M)^{-1}\phi}$$

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  - **Markov-chain Monte Carlo (MCMC) process:** Generate representative configurations of the gauge fields U with probability:

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- Inversions of the Dirac matrix M
  - Needed during MCMC: $\phi(M^+M)^{-1}\phi$
  - Needed during "measurements"

Gauge Theories on the Lattice

Current state-of-the-art in lattice QCD

- Typical problem sizes
  - Box length L ~ 5 – 7 fm
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Current state-of-the-art in lattice QCD

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  - A typical implementation may require two gauge-fields plus $\mathcal{O}(10)$ vectors

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    ⇒For an ensemble of 1000 configurations, storage can reach $\mathcal{O}(1)$ PBytes

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Computational characteristics

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  - Markov-chain Monte Carlo; statistical errors scale as: $1/\sqrt{\mathrm{N}_{stat}}$
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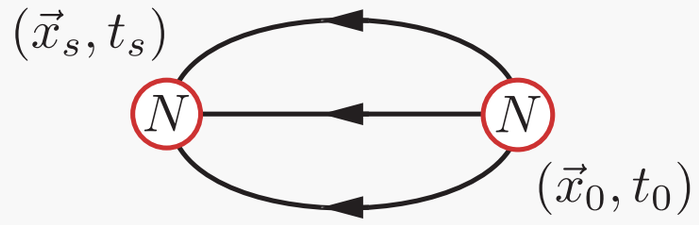

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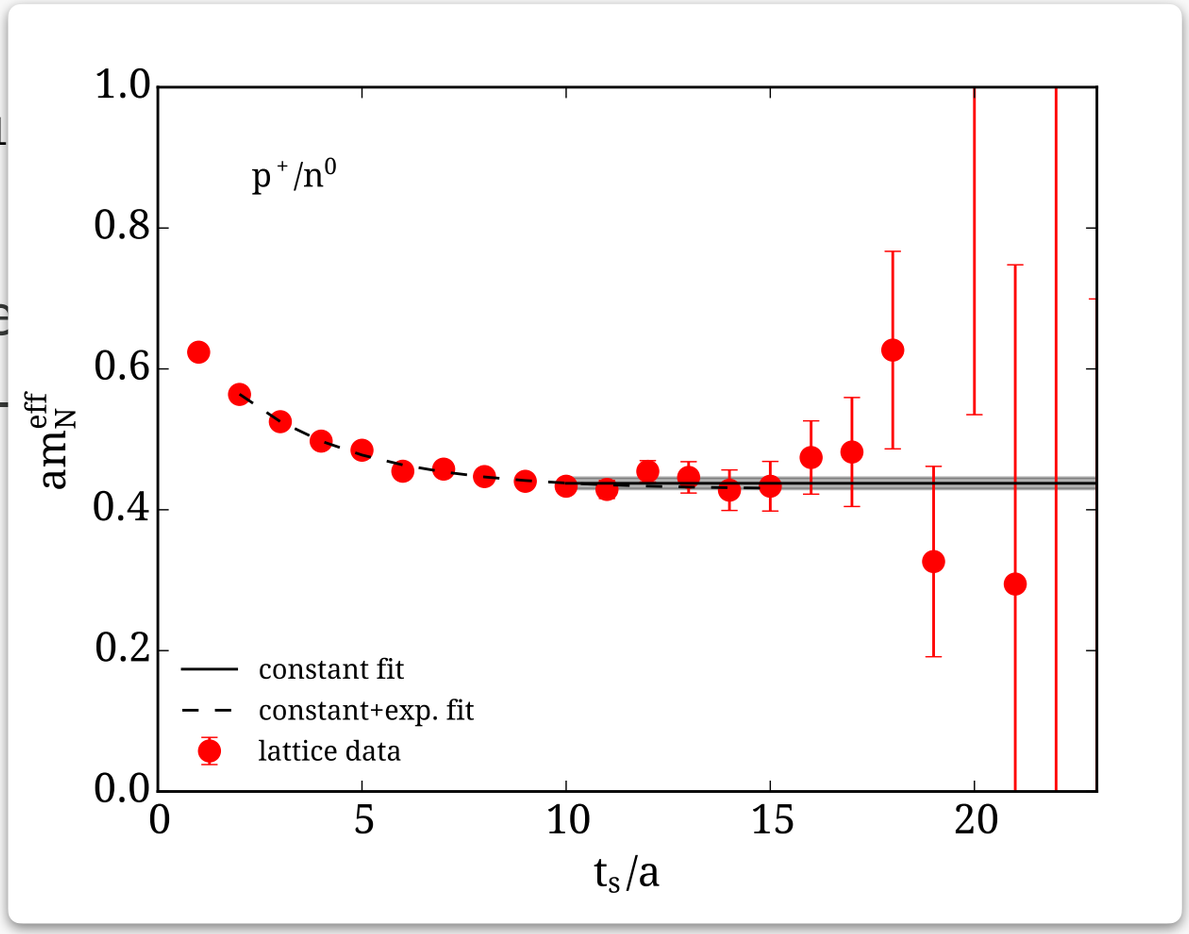

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  - **Analysis:** 10,000 matrix-inversions per configuration (typical requirements for hadron structure): **~10 Mi GPU-hours**

Iterative solvers

Sparse matrix inversion via iterative solvers

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  - Build y from Mb, M^2b, M^3b, ...
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  - **Examples**: Conjugate Gradient (CG), Generalised Minimum Residual (GMRES), Stabilised Bi-Conjugate Gradient (BiCGStab), etc.

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$\rho = \|\mathrm{r}\|$
while $\rho > \rho_{min}$ **do**
    $\mathrm{p}' = A\mathrm{p}$
    $\alpha = \rho/(\mathrm{p}^\dagger\mathrm{p}')$
    $\mathrm{x} \leftarrow \mathrm{x} + \alpha\mathrm{p}$
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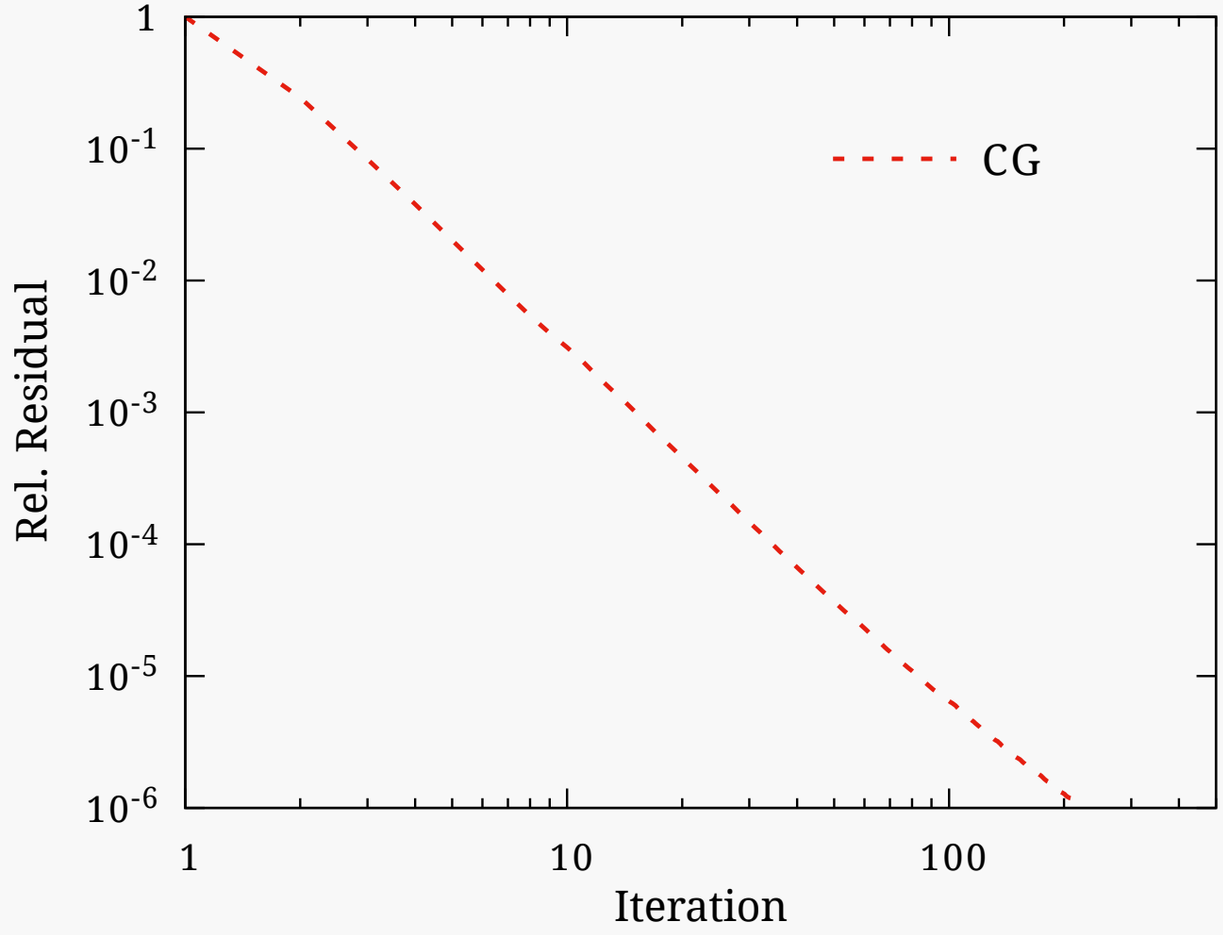

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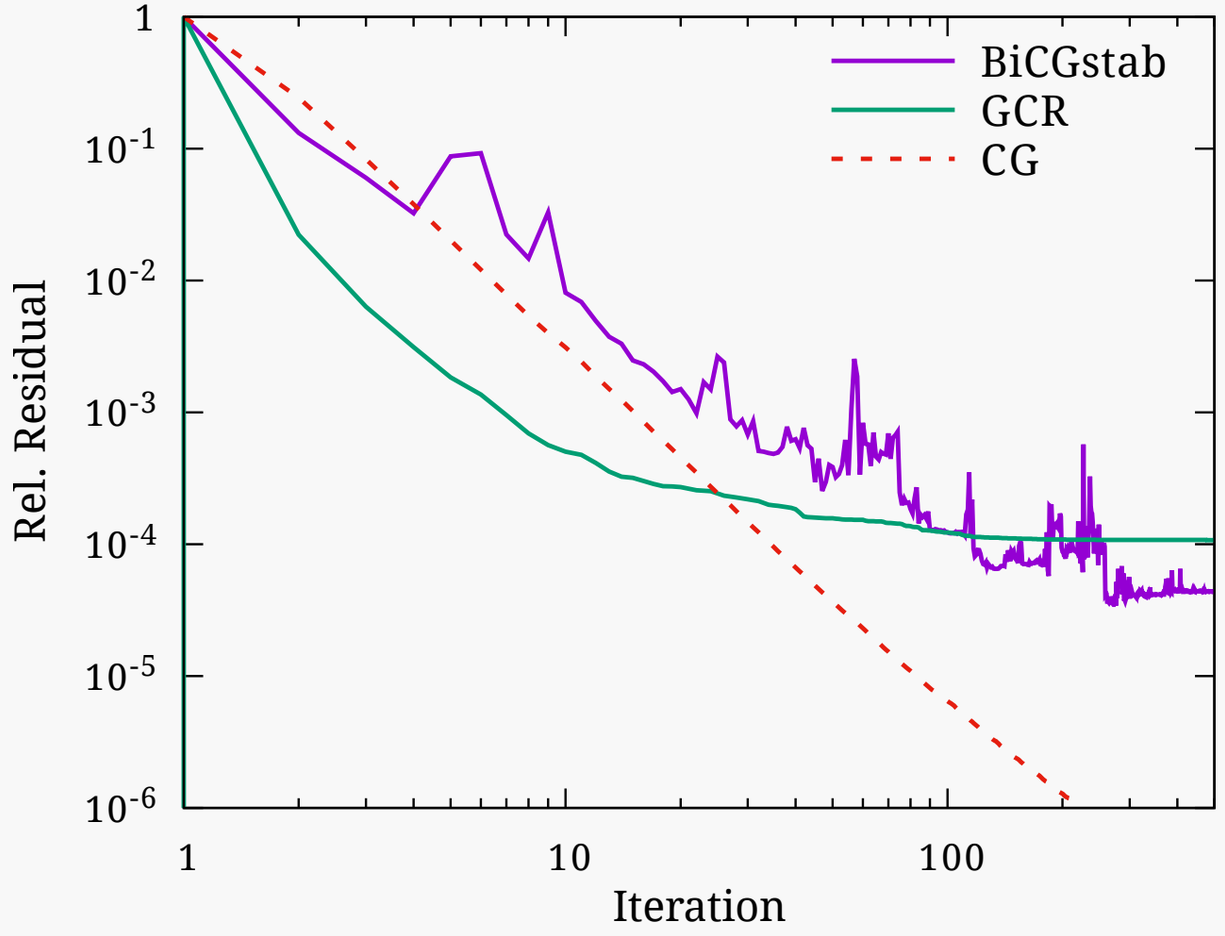

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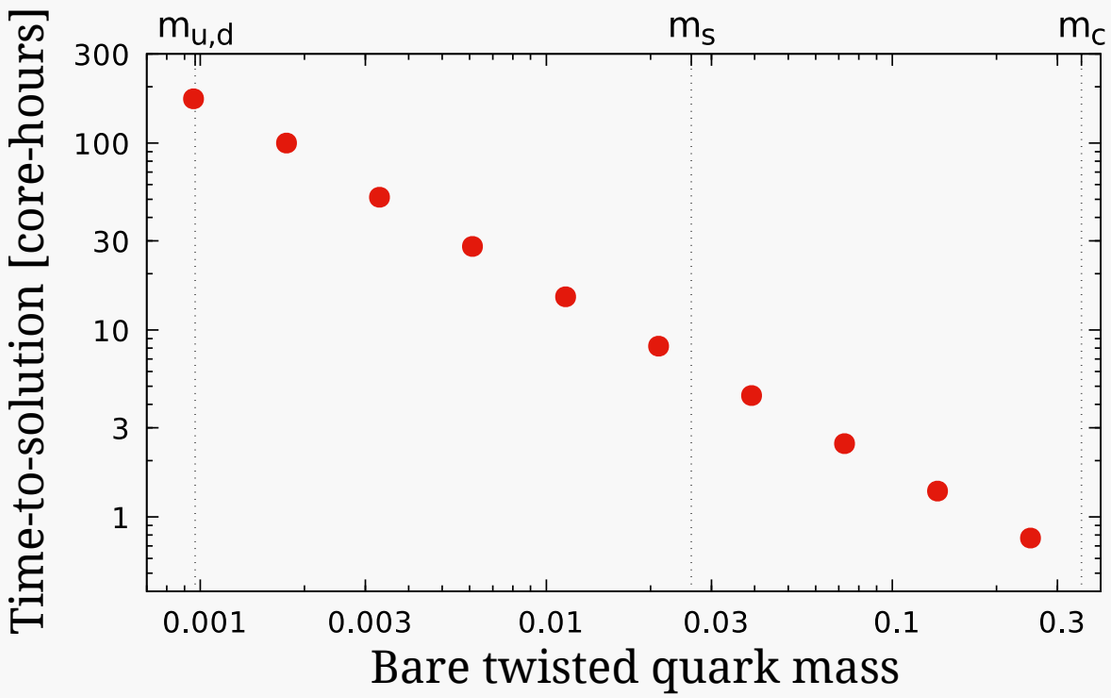

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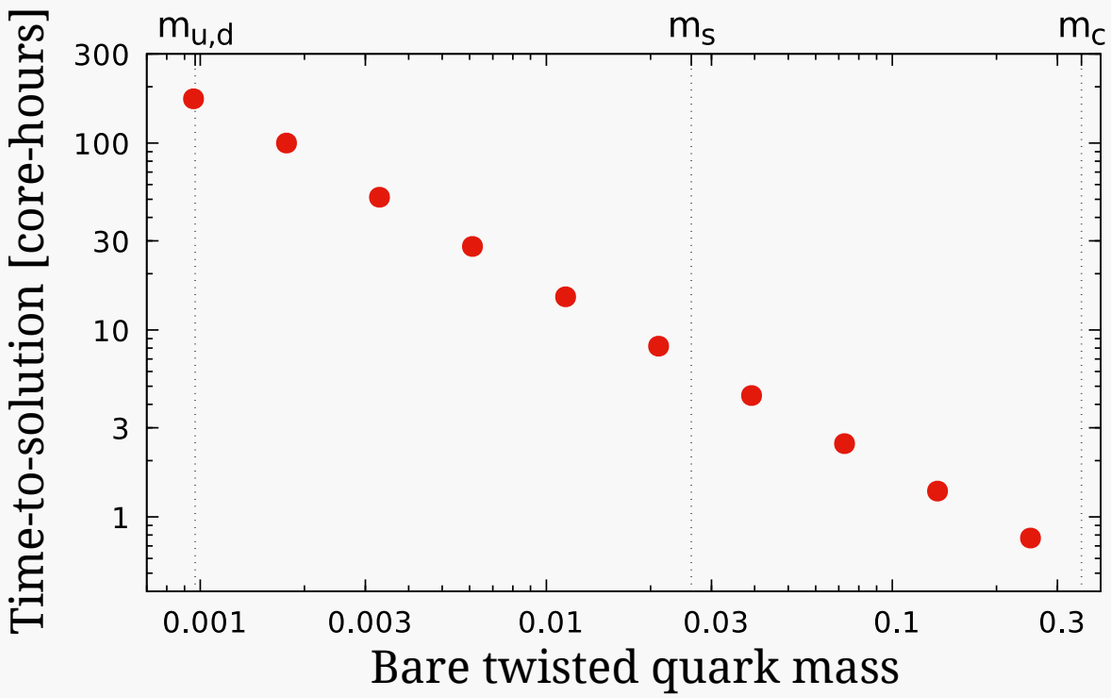
  - λ_{min} proportional to fermion mass
    → **critical slowing down**



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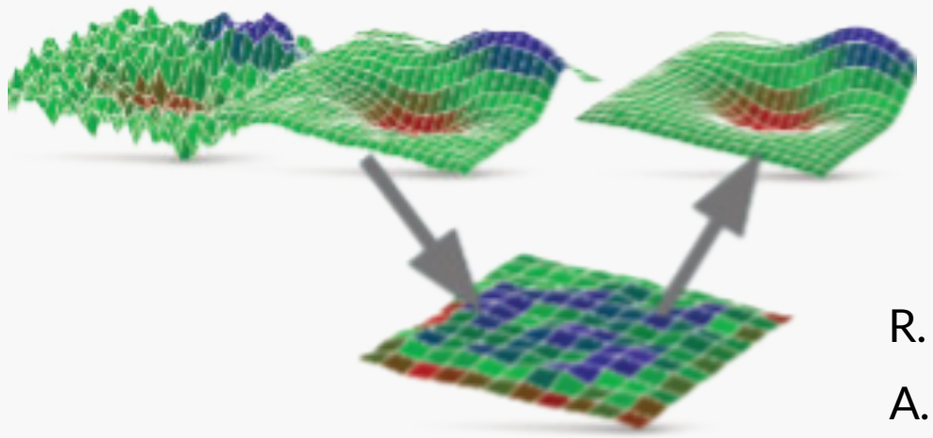
- **Multigrid methods**
  - Precondition a Krylov subspace solver using a *coarse grid operator*



  - $\mathrm{M_c}=\mathrm{RMP}$: Coarse grid operator
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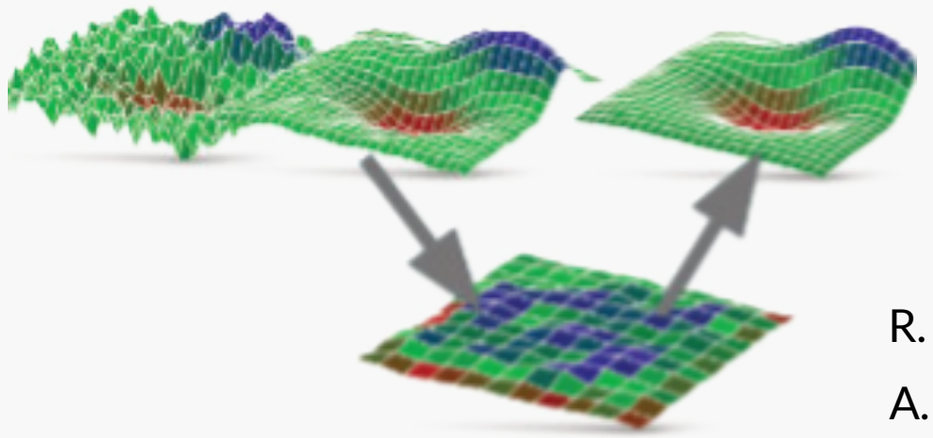

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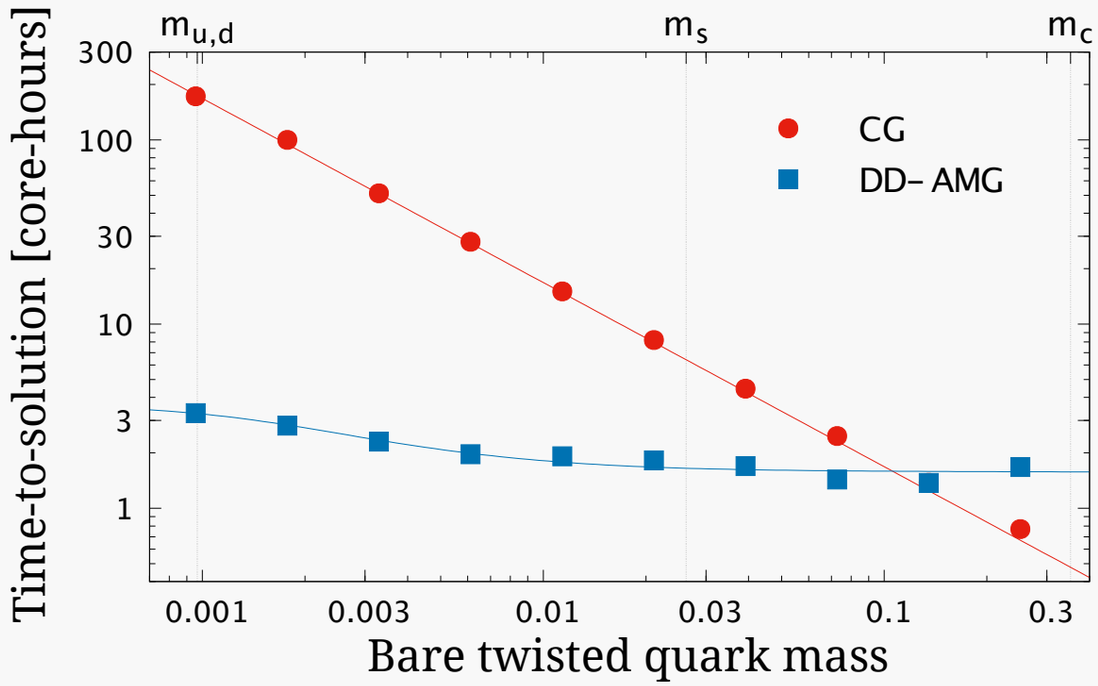
  - Allows simulations directly at physical quark masses
  - ×100 improvement in time-to-solution
  - Requires set-up: building-up R and P. Minor for $m \rightarrow m_{u,d}$

- **Right:** for twisted mass fermions



C. Alexandrou *et al.* Phys. Rev. D 94 (2016) 11, 114509

Markov chain Monte Carlo

Monte Carlo integration

- Path integral formulation

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U]\mathcal{D}[\bar{\phi}]\mathcal{D}[\phi]\mathcal{O}e^{-S_G[U]-\bar{\phi}(M^+M)^{-1}\phi}$$

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    - $\int \mathcal{D}(U)p(U)T(U,U') = p(U')$, i.e. the transition probability is symmetric: **Balance**

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Metropolis sampling

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- Since the configurations U are distributed according to the desired $p(U)$:

$$\langle \mathcal{O} \rangle = \frac{1}{N_{stat}} \sum_{i=1}^{N_{stat}} \mathcal{O}(U^i)$$

and statistical errors scale like $\frac{1}{\sqrt{N_{stat}}}$

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Metropolis sampling in Markov chain Monte Carlo

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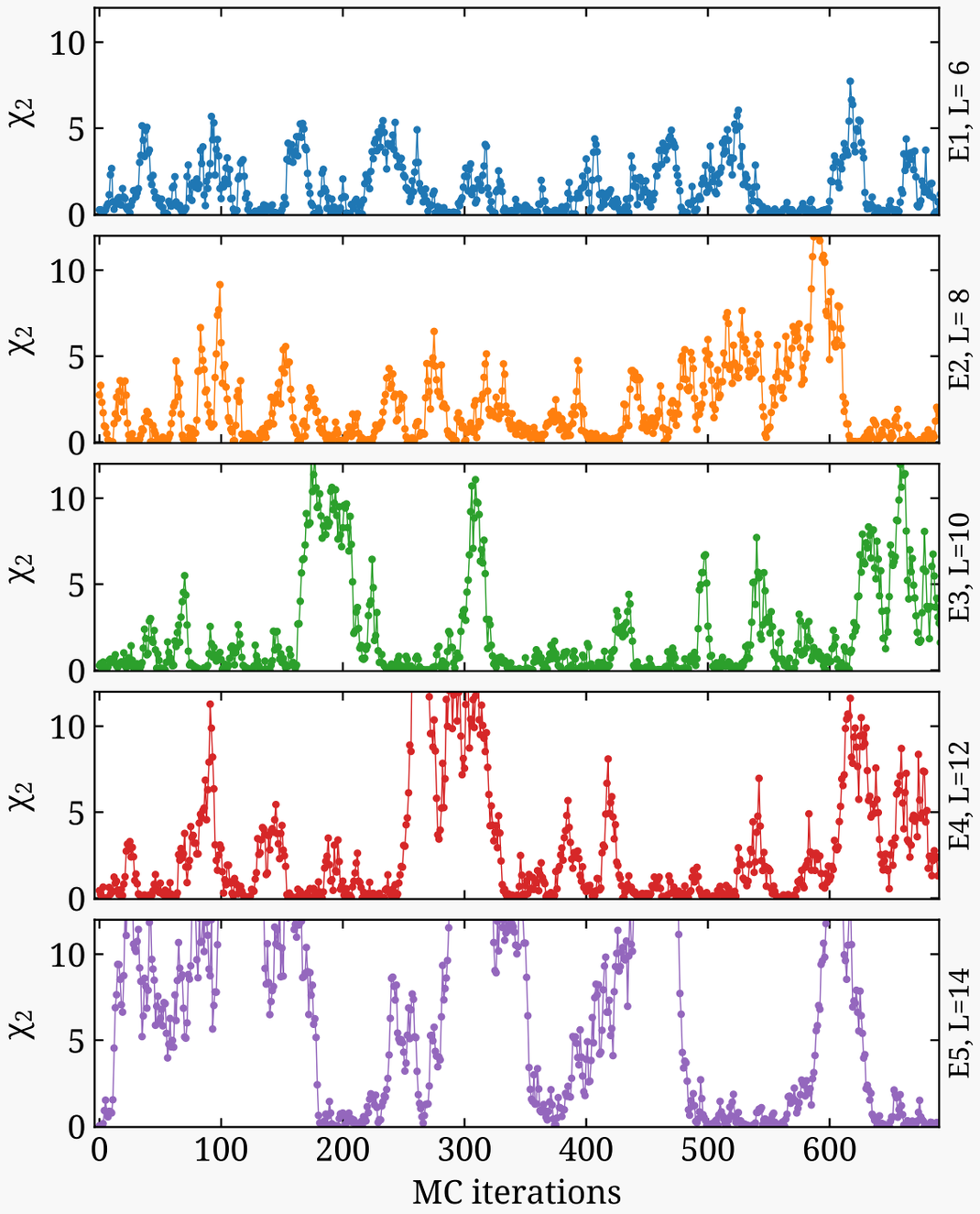
Largely depend on the choice of $p'(U)$, and how closely it approximates $p(U)$

Markov chain Monte Carlo

Example of critical slowing down



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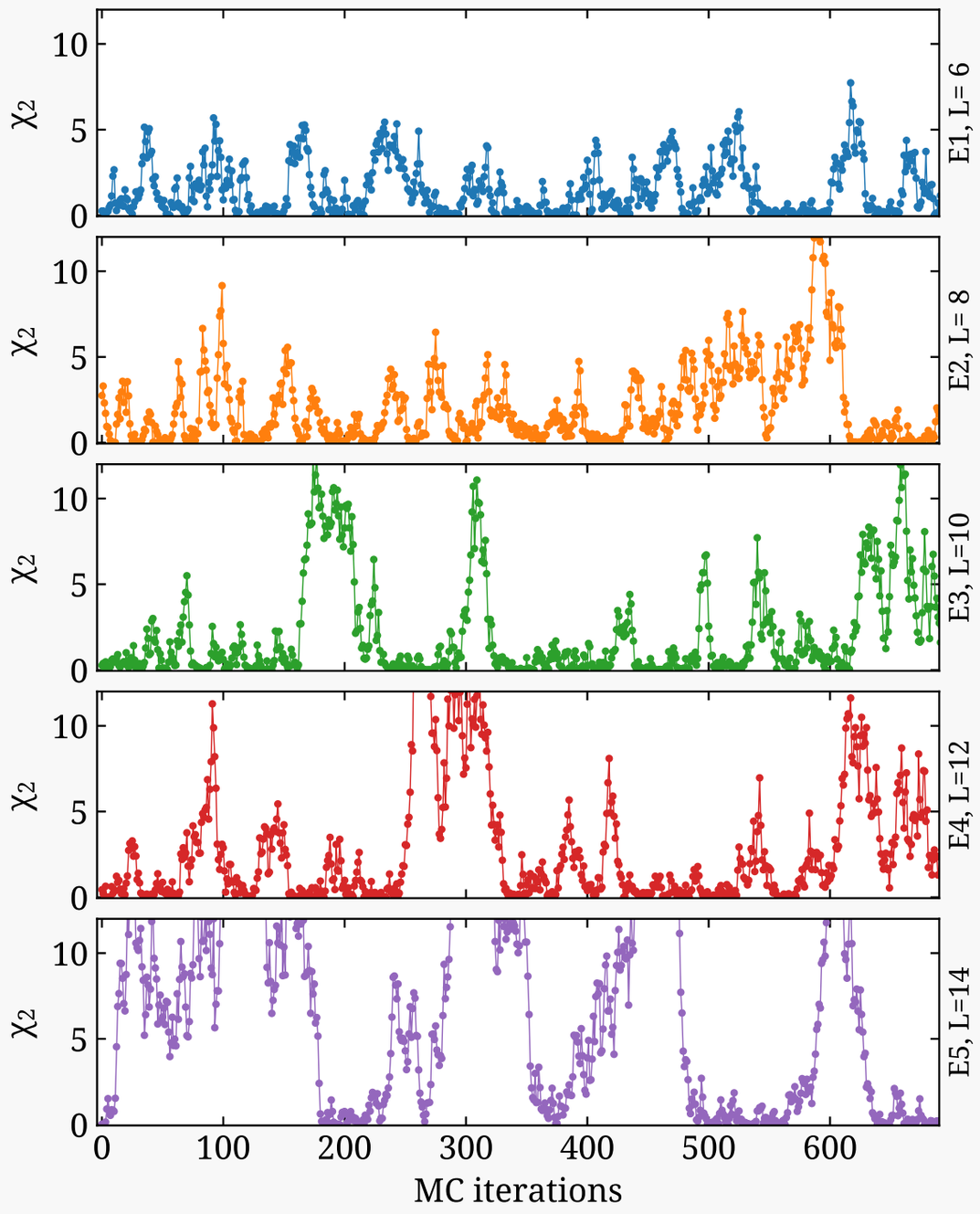

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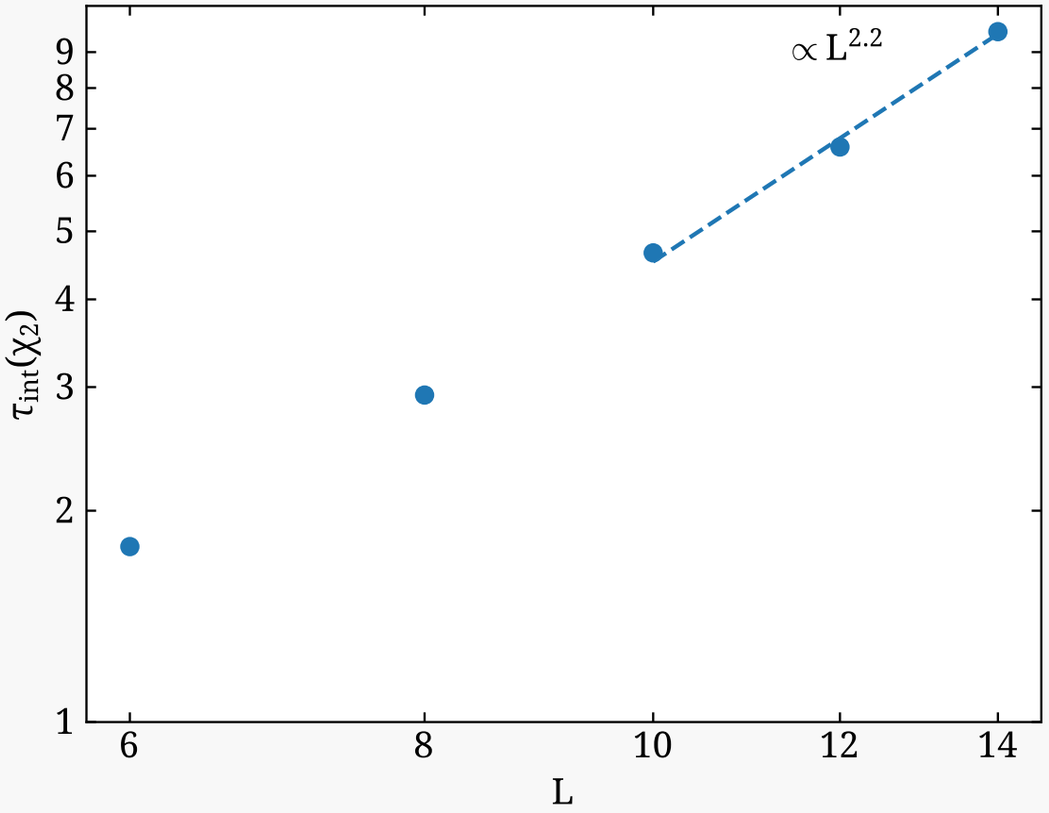

Hybrid Monte Carlo

- *Hybrid Monte Carlo (HMC):* algorithm for updating U motivated by molecular dynamics

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U, \bar{\phi}, \phi] \mathcal{O} e^{-S} = \frac{1}{Z} \int \mathcal{D}[U, \bar{\phi}, \phi, \bar{\pi}, \pi] \mathcal{O} e^{-\frac{\pi^2}{2} - S}$$

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E.g. Leap-frog integration

$$\begin{aligned}
\pi(\delta\tau/2) &= \pi(0) - \frac{\delta\tau}{2} \frac{\partial}{\partial U} S|_{U(\tau=0)} \\
U(\delta\tau) &= U(0) + \delta\tau \pi(\delta\tau/2) \\
\pi(3\delta\tau/2) &= \pi(\delta\tau/2) - \delta\tau \frac{\partial}{\partial U} S|_{U(\tau=\delta\tau)} \\
&\vdots \\
\pi(T) &= \pi(T - \delta\tau/2) - \frac{\delta\tau}{2} \frac{\partial}{\partial U} S|_{U(\tau=T-\delta\tau)}
\end{aligned}$$

S. Duane, Kennedy, Pendleton, Roweth, Phys. Lett. B195, 216 (1987)

Hybrid Monte Carlo

- An example of a *global updating* algorithm
- Introduction of fictitious time τ and time-step $\delta\tau = T/N$
- Calculation of "forces" requires inversion for each time-step:

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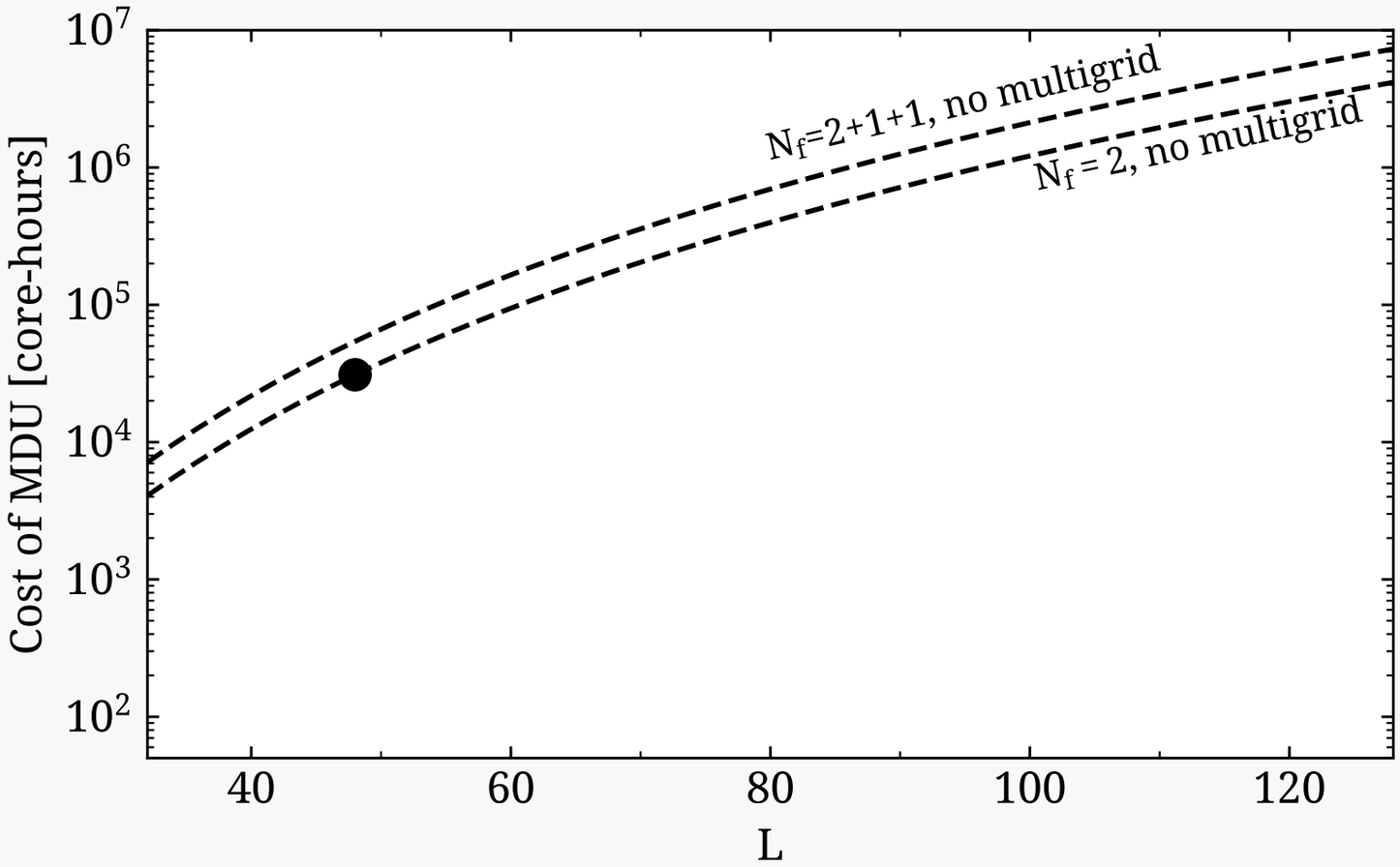
- In practice:
  - Multiple time-step integration (e.g.: `hep-lat/0506011`)
  - Higher order integration schemes (e.g.: `arXiv:1210.6600 [hep-lat]`)
  - Hasenbusch mass preconditioning (`hep-lat/0211042`)

Lattice QCD — Large-scale simulations

A combination of

- Multi-grid solver improvements
- Integration schemes
- Computers becoming faster



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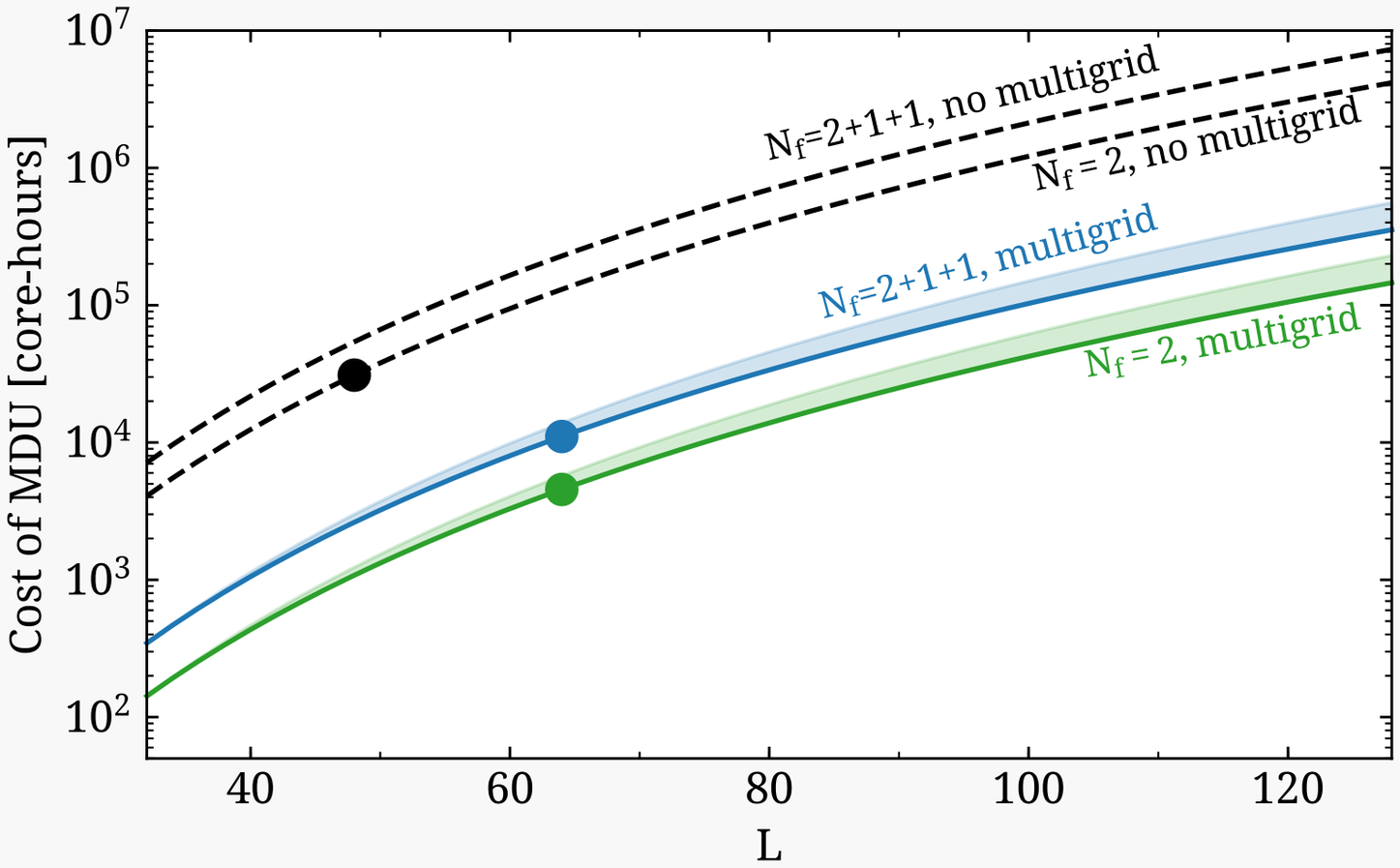

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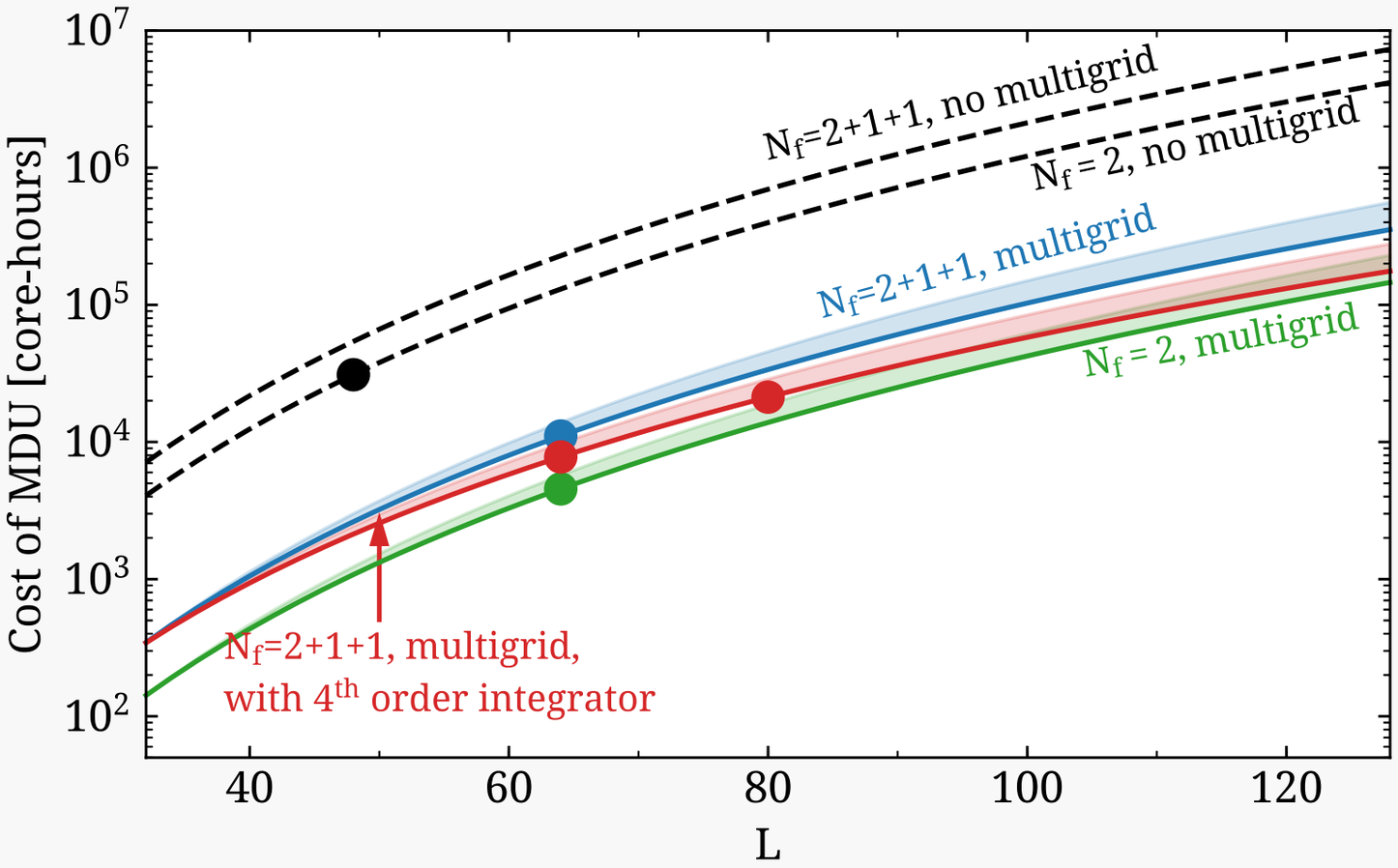

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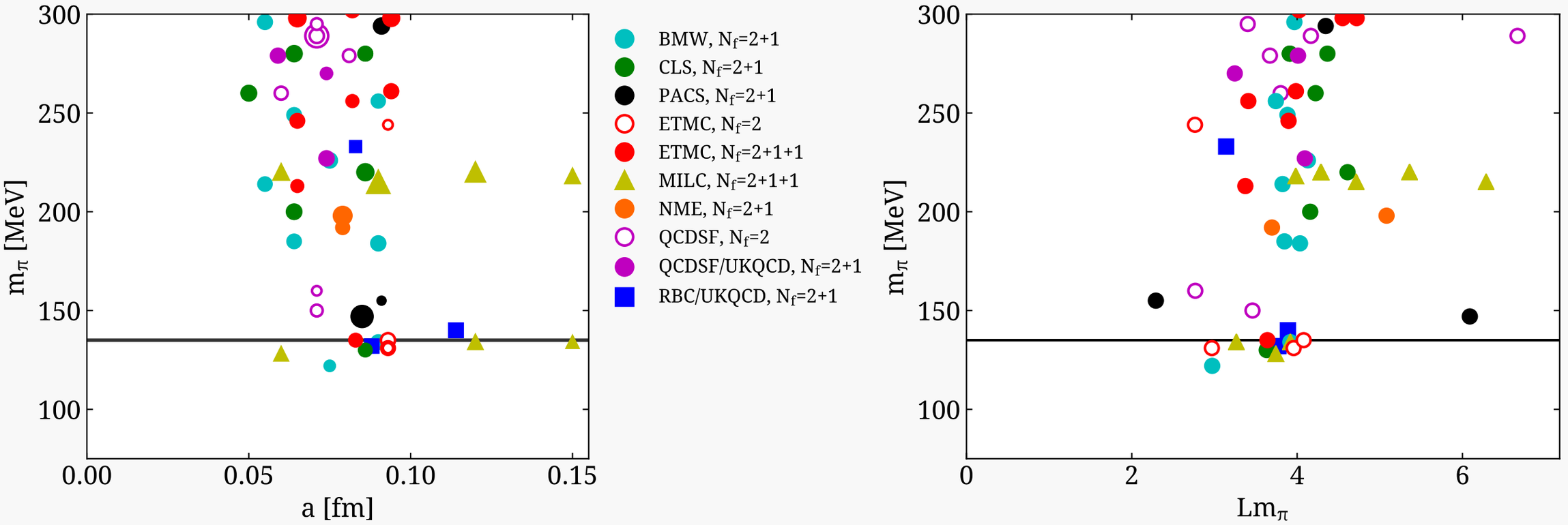
- 2018: Added 4th-order integration scheme

Simulation landscape



Selected lattice simulation points from various collaborations

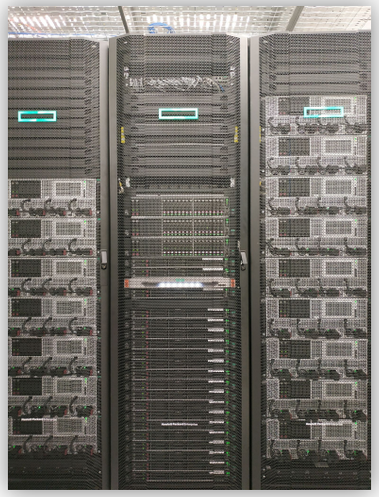
- Multiple collaborations simulating at physical pion mass
- Size of points indicates $m_\pi L$

Acknowledgements

Computer time used to produce some of the data shown

Marconi100, CINECA
PRACE Tier-0 project

SuperMUC-NG, LRZ
Gauss Large Scale project



Cyclone, CyI
Local project

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