Stochastic locality and master-field simulations of very large lattices
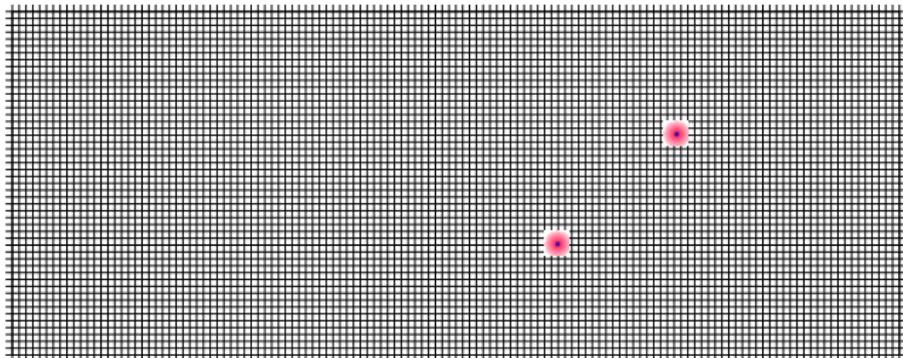
Martin Lüscher, Theoretical Physics Department, CERN

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Master-field simulations

Example

- Consider QCD on a 256^4 lattice with periodic bc
  $$a = 0.05 \, \text{fm} \quad \Rightarrow \quad L = 12.8 \, \text{fm}$$

- Generate 1 representative gauge field

- The translation averages

  $$\langle\!\langle \mathcal{O}(x) \rangle\!\rangle = \frac{1}{V} \sum_z \mathcal{O}(x + z)$$

  of local observables then satisfy

  $$\langle\!\langle \mathcal{O}(x) \rangle\!\rangle = \langle \mathcal{O}(x) \rangle + \text{O}(V^{-1/2})$$

Note: $1 \times 256^4 = 256 \times 64^4 \quad \Rightarrow \quad$ does not require astronomical resources!

Outline

- Statistical error estimation

- Some illustrative calculations

- Generation of master fields
  - ◇ Simulation algorithm
  - ◇ Global operations & decisions
  - ◇ SMD w/o accept-reject step

- Calculation of hadron propagators

Statistical error estimation

The translation average

$$\langle\!\langle \mathcal{O}(x) \rangle\!\rangle$$

is a stochastic variable with mean $\langle \mathcal{O}(x) \rangle$ and variance

$$\left\langle \{\langle\!\langle \mathcal{O}(x) \rangle\!\rangle - \langle \mathcal{O}(x) \rangle\}^2 \right\rangle = \frac{1}{V} \sum_y \langle \mathcal{O}(y)\mathcal{O}(0) \rangle_{\mathrm{c}}$$

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$$= \frac{1}{V} \Big\{ \sum_{|y| \leq R} \langle \mathcal{O}(y)\mathcal{O}(0) \rangle_{\mathrm{c}} + \mathrm{O}(\mathrm{e}^{-mR}) \Big\}$$

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Double sum over y and z done with computational effort $\propto V \ln V$ using the FFT

Statistical error estimation (cont.)

The variance of the average

$$\overline{\mathcal{O}}(x) = \frac{1}{n} \sum_{k=1}^{n} \mathcal{O}(x)|_{U=U_k}$$

over several fields $U_1, \ldots, U_n$ is similarly given by

$$\frac{1}{V} \Big\{ \sum_{|y| \leq R} \langle\!\langle \overline{\mathcal{O}}(y) \overline{\mathcal{O}}(0) \rangle\!\rangle_{\mathrm{c}} + \ldots \Big\}$$

provided the autocorrelation functions of $\mathcal{O}(x)$

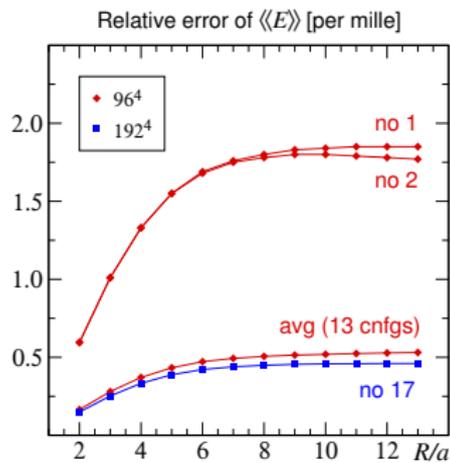★ are translation invariant and

★ decay rapidly in space

Sample calculations

SU(3) gauge theory

96^4 and 192^4 lattice with $a = 0.1$ fm

E = YM action density at gradient-flow
    time $t \simeq t_0$

Using 64 nodes @ CESGA (1536 cores, 8 TB)

Relative error of $\langle\langle E \rangle\rangle$ [per mille]

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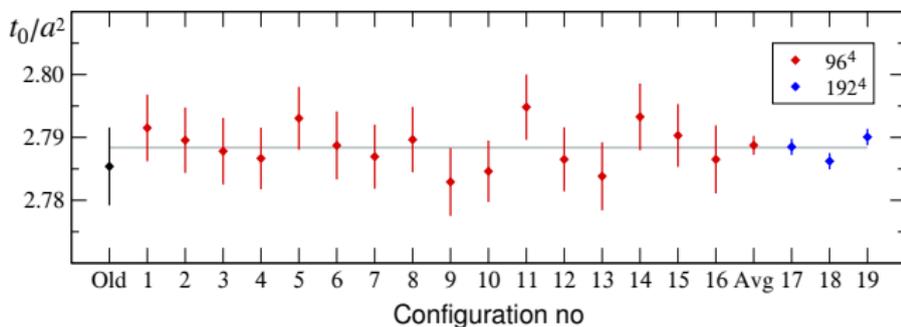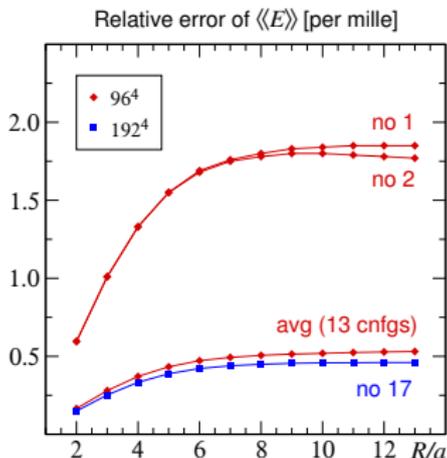   time $t \simeq t_0$

Using 64 nodes @ CESGA (1536 cores, 8 TB)

Relative error of $\langle\!\langle E \rangle\!\rangle$ [per mille]

- 96^4
- 192^4

no 1
no 2

avg (13 cnfgs)
no 17

2.0
1.5
1.0
0.5

2   4   6   8   10   12 R/a

t_0/a^2

2.80
2.79
2.78

- 96^4
- 192^4

Old 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 Avg 17 18 19
Configuration no

Sample calculations (cont.)

The topological susceptibility

$$\chi_t = \sum_{|y| \leq R} \langle\!\langle q(y)q(0) \rangle\!\rangle_{\mathrm{c}} + \mathrm{O}(\mathrm{e}^{-mR}) + \mathrm{O}(V^{-1/2})$$
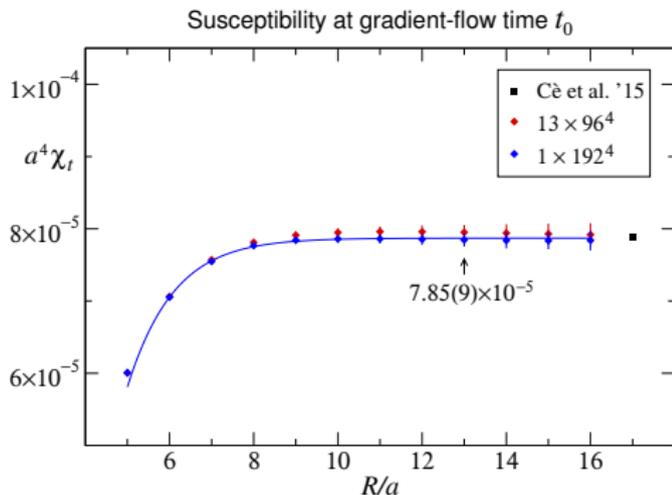
may be calculated with 1 master field

- Fixed-topology effects are $\propto V^{-1}$ and thus subleading!

  Brower et al. '03, Aoki et al. '07

- The observable here is

  $$\mathcal{O}(x) = \sum_{|y| \leq R} q(x+y)q(x)$$

Susceptibility at gradient-flow time t_0

Legend:
- Cè et al. '15
- 13×96^4
- 1×192^4

$a^4 \chi_t$ (y-axis), R/a (x-axis)

$7.85(9) \times 10^{-5}$

Sample calculations (cont.)

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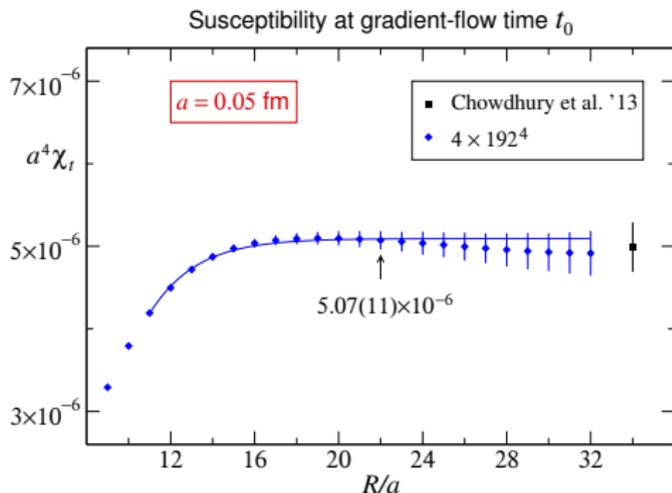
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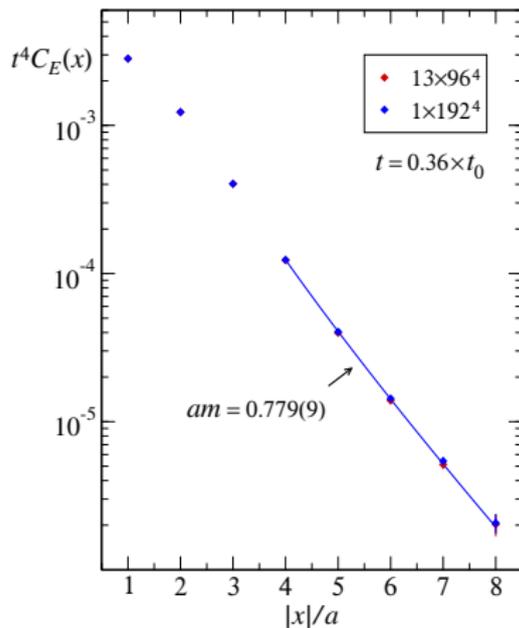
$a = 0.05$ fm

- Chowdhury et al. '13
- 4×192^4

$5.07(11) \times 10^{-6}$

$a^4\chi_t$

R/a

Sample calculations (cont.)

Correlation functions such as

$$C_E(x) = \langle E(x)E(0)\rangle_{\mathrm{c}}$$

$$\underset{|x|\to\infty}{\propto} |x|^{-3/2}\mathrm{e}^{-m|x|}$$

can be calculated too provided $|x| \ll L$

The projection to $\vec{P} = 0$ however tends
to increase the noise

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Generation of master fields

Any correct simulation algorithm may in principle be used

In the thermalization phase

- Use space-time reflections to build configurations
  from smaller lattices

- May study autocorrelations on these lattices

Generation of master fields (cont.)

Global operations & decisions must be reconsidered on very large lattices

Solver stopping criterion

$$\|D\psi - \eta\|_2 \leq \rho \, \|\eta\|_2, \qquad \|\eta\|_2 \propto \sqrt{V} \quad \text{(in the HMC algorithm)}$$

Will have to

- Replace $\| \cdot \|_2$ by $\| \cdot \|_\infty$

- Use SAP, local deflation, multigrid, ...

Generation of master fields (cont.)

HMC accept-reject step

$$\Delta H \propto \epsilon^p \sqrt{V}, \qquad \text{loss of significance} \propto V$$

$\Rightarrow$ numerical precision must increase with V

Other options include

- Localizing the algorithm
  Cè, Giusti & Schaefer '16f → plenary talk by Leonardo Giusti

- Using the SMD algorithm w/o accept-reject step

Generation of master fields (cont.)

Stochastic molecular dynamics (SMD) Horowitz '85ff, Jansen & Liu '95

Random rotation: $\quad \pi \to c_1 \pi + c_2 v, \qquad c_1 = \mathrm{e}^{-\gamma \epsilon}, \quad c_1^2 + c_2^2 = 1$

$\qquad\qquad\qquad\quad \phi \to c_1 \phi + c_2 \chi$

MD evolution: $\qquad (\pi, U)_t \to (\pi, U)_{t+\epsilon}$

Generation of master fields (cont.)

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Theorem:

The SMD process converges to a unique stationary state if $\epsilon < \bar{\epsilon}$,
where $\bar{\epsilon}$ depends on the gauge action and the MD integrator

Proof based on
Yet another look at Harris' ergodic theorem for Markov chains (Hairer & Mattingly '08)

Generation of master fields (cont.)

Example

Wilson gauge action

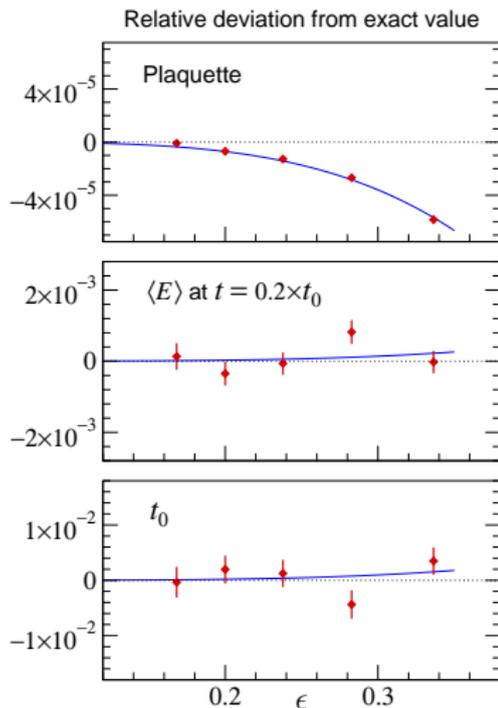4th order OMF integrator (1 step)

$\Rightarrow \quad \bar{\epsilon} = 0.06 \times g_0^2$

Expect systematic errors $\propto \epsilon^4$

64^4 lattice, $a = 0.05$ fm

Run length $= 1.8 \times 10^4$ [MD time]

$\Rightarrow$ *Viable algorithm for large lattices*

Relative deviation from exact value

Calculation of hadron propagators

No of source points $\propto V$

However

- Useful range of distances is a few fm

- Since
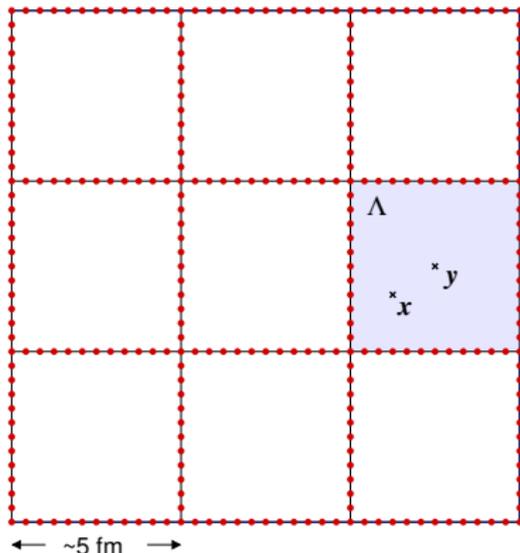
    $$|S(x,y)| \propto \exp\{-\tfrac{1}{2}m_\pi |x-y|\}$$

    may solve Dirac equation in subvolume

- Random-field representation

    $\text{action} = (D^\dagger \phi, D^\dagger \phi)$

    $$S(x,y) = S_\Lambda(x,y) + \big\langle D^\dagger \underbrace{\chi(x)}_{\sim\, e^{-\frac{1}{2}m_\pi d(x)}} \otimes \chi(y)^\dagger \big\rangle_\phi$$

Λ

$^\times y$

$^\times x$

$\longleftarrow$ ~5 fm $\longrightarrow$

Conclusions

Master-field simulations of physically large lattices

★ Extend the scope of numerical LQCD

★ Provide a solution to the topology-freezing problem

Further algorithm R&D is desirable

★ Revisit global operations & decisions

★ Implement multilevel strategies   →   parallel talk by Marco Cè

Technical challenges

★ Memory requirement ($5 \ldots 100$ TB on 256^4 lattices)

★ Parallel I/O, storage   →   parallel talk by Marcus Hardt