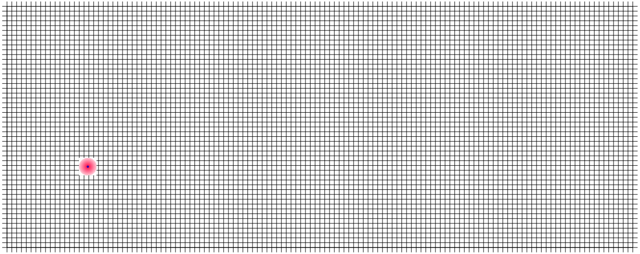
Stochastic locality and master-field simulations of very large lattices

Martin Lüscher, Theoretical Physics Department, CERN



35^{th} International Symposium on Lattice Field Theory

Granada, June 19-24, 2017

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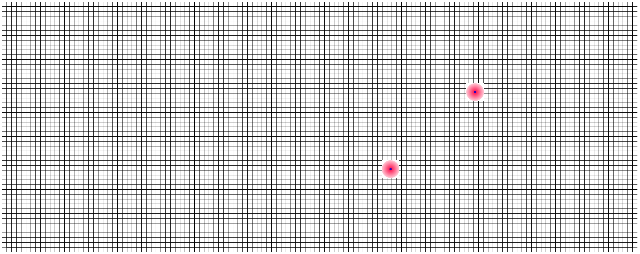

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Master-field simulations

Example

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

- 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

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

Note: $1 \times 256^4 = 256 \times 64^4$ $\Rightarrow$ 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

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

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

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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

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

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

- ⋆ are translation invariant and
- ⋆ decay rapidly in space

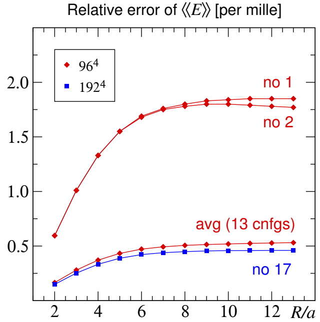
Sample calculations

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)



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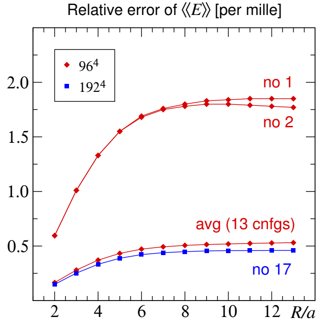
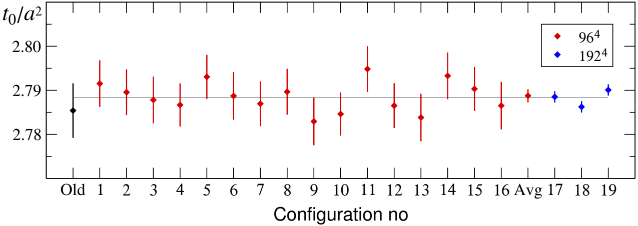




Sample calculations (cont.)

The topological susceptibility

$$\chi_t = \sum_{|y|\leq R} \langle\langle q(y)q(0)\rangle\rangle_c + \mathrm{O}(\mathrm{e}^{-mR}) + \mathrm{O}(V^{-1/2})$$

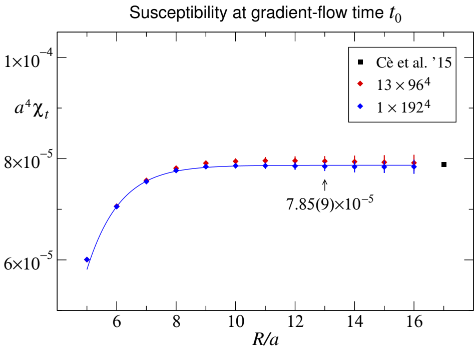
may be calculated with 1 master field

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

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

- The observable here is

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



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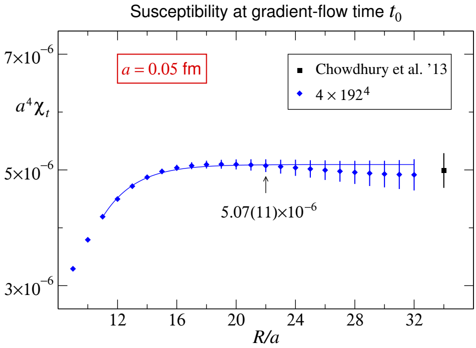


Sample calculations (cont.)

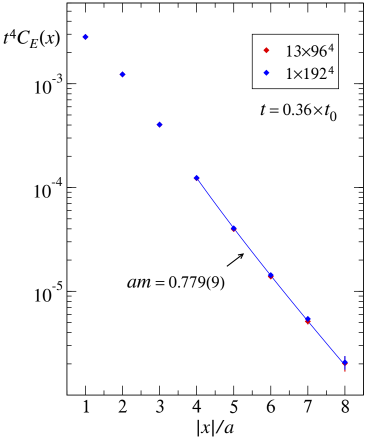
Correlation functions such as

$$C_E(x) = \langle E(x)E(0)\rangle_c$$

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

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

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



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

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

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

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

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

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

4^{th} order OMF integrator $(1$ step$)$

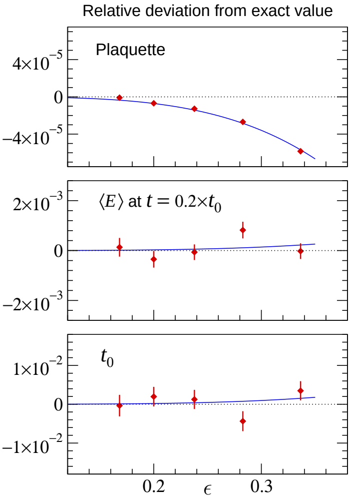
$\Rightarrow \quad \bar{\epsilon} = 0.06 \times g_0^2$

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*



Calculation of hadron propagators

No of source points $\propto V$

However

- Useful range of distances is a few fm
- Since

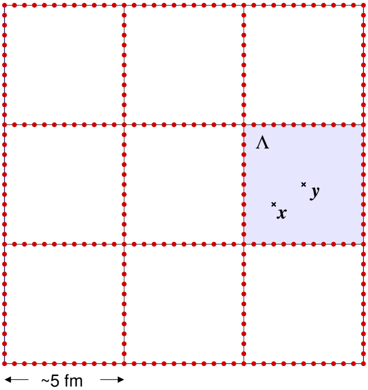
  $$|S(x,y)| \propto \exp\{-\tfrac{1}{2}m_\pi |x-y|\}$$

  may solve Dirac equation in subvolume

- Random-field representation

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

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



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 $\rightarrow$ parallel talk by Marco Cè

Technical challenges

- ⋆ Memory requirement ($5 \ldots 100$ TB on 256^4 lattices)
- ⋆ Parallel I/O, storage $\rightarrow$ parallel talk by Marcus Hardt