Some challenges

from a "mainstream" perspective,
i.e. $d = 4$, $T = \mu = 0$ SU($N_c = 3$), $N_f \in \{2+1, 1+1+1, 2+1+1, 1+1+1+1\}$.

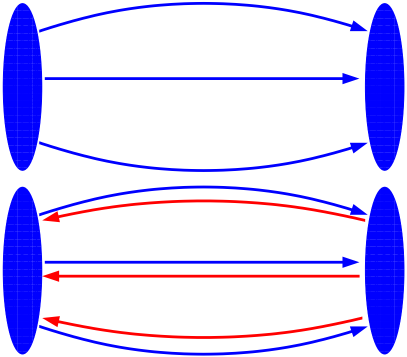
- Critical slowing down with $a \to 0$
  How serious is it? How much should we bother?
- Volumes $V = N_t N^3 \propto (L/a)^4 \propto (L/M_\pi)^4$ become large towards small a, M_π.
  Also $\exists$ "master field" simulations.
  Rounding issues, decrease of HMC step sizes, some algorithms scale with V^2 (eigenvectors and similar objects) or with V/a^2 scaling (smearing etc.): how to beat this?
- Noise/signal issues
  Baryons, disconnected quark/gluon loops on large volumes etc.: multiscale schemes? Are there solutions that give many quantities at once?
- Efficient algorithms to compute $n > 3$-point functions.
  Applications: nuclear physics, $K \to \pi\pi$, quasi/pseudo-PDFs, QCD+QED etc.
- Bad communication and memory over peak FLOPs ratios on modern architectures.

One example for bad noise/signal

HW Hamber, E Marinari, G Parisi, C Rebbi, NPB225 (83) 475 (Appendix B)

GP Lepage, http://inspirehep.net/record/287173

$$C_N(t) \sim \quad \sim \exp\left(-m_N t\right)$$



$$[\Delta C_N(t)]^2 \sim \quad \sim \exp\left(-3 m_\pi t\right)$$

$$\frac{\Delta C_N(t)}{C_N(t)} \sim \exp\left[\left(m_N - \frac{3}{2} m_\pi\right) t\right]$$

One random transparency: low mode averaging

T DeGrand, S Schäfer CPC 159 (04) 185; L Giusti et al, JHEP 0404 (04) 013.

$$\langle C_{\mathrm{LMA}}(t)\rangle = \langle C_{\mathrm{low}}(t)\rangle + \langle C^{\mathrm{pa}}(t) - C^{\mathrm{pa}}_{\mathrm{low}}(t)\rangle\,.$$

C_{low}: contribution from low eigenmodes of $\mathrm{Q} = \gamma_5 M$ ($\mathrm{Q} = \mathrm{Q}^\dagger$), all-to-all, averaged over the lattice volume.
C^{pa}: standard point-to-all 2-point function.
$C^{\mathrm{pa}}_{\mathrm{low}}$: low mode contribution (point-to-all), needs to be subtracted since this is already included into C^{pa}.

Exploits the translational invariance of expectation values: $\langle C_{\mathrm{low}}\rangle = \langle C^{\mathrm{pa}}_{\mathrm{low}}\rangle$.
This does not affect the expectation value but may reduce the error, due to the self-averaging of the low-mode contribution.

This works very well for positive parity baryons and negative parity mesons:
GB, L Castagnini, S Collins, PoS (LATTICE2010) 096.

Works best at small quark masses. Problem: cost of eigenvectors $\propto V^2 \propto 1/M_\pi^8$.

Wishlist (homework)

- Good ideas.
- Efficient communication-avoiding implementations with small memory footprint.
- Integrators that allow for less time spent on evaluations of fermionic force.
- Fast (incl. set-up) solver for HMC (or other MC).
- Fast solver for multi-right-hand-sides (possibly with expensive set-up).
- Efficient way of computing (approximate) eigenvectors of $\gamma_5 M$ (within above solver?).

NB: start from discretized Dirac operator $M = U\Sigma V^\dagger$ with U and V unitary.
Singular values Σ (diagonal) are uniquely determined, U and V are not.
Eigenvectors of $\mathrm{Q} = \gamma_5 M$ are eigenvectors of $\mathrm{Q}^2 = M^\dagger M$.
Eigenvectors $|u^i\rangle$ of Q are right singular vectors of M (i.e. columns of V):

$$\gamma_5 M|u^i\rangle = |u^i\rangle q_i$$

$$M\underbrace{(|u_1\rangle,\ldots,|u_{12V}\rangle)}_{V} = \underbrace{\gamma_5(\mathrm{sign}(q_1)|u_1\rangle,\ldots,\mathrm{sign}(q_{12V})|u_{12V}\rangle)}_{U}\underbrace{\mathrm{diag}(|q_1|,\ldots,|q_{12V}|)}_{\Sigma}$$