Hierarchical HMC
Computational aspects

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Dirac operators for hierarchical HMC

Dirac operator sample with two slots:

$$D = \left[\begin{array}{c|cc} D_F & D_{F0} & D_{F1} \\ \hline D_{0F} & D_i & \\ D_{1F} & & D_j \end{array}\right] = \left[\begin{array}{c|c} D_F & D_{FR} \\ \hline D_{RF} & D_R \end{array}\right]$$

- D_F, D_{0F}, D_{1F} are fixed for all Dirac operators
- There #patches possibilities for D_i and D_j
- All combinations of D_i and D_j make $\#\text{patches}^2$ distinctive Dirac operators

Fermionic determinant

$$\det\left(\left[\begin{array}{c|cc} D_F & D_{F0} & D_{F1} \\ \hline D_{0F} & D_i & \\ D_{1F} & & D_j \end{array}\right]\right) = \det\left(\left[\begin{array}{c|c} D_F & D_{FR} \\ \hline D_{RF} & D_R \end{array}\right]\right)$$

Lets decompose the determinant:

$$\begin{aligned}
\det(D) &= \det(D_F)\det(D_R - D_{RF}D_F^{-1}D_{FR}) \qquad \text{(Schur complement)} \\
&= \det(D_F)\det(D_R)\det(I - D_R^{-1}D_{RF}D_F^{-1}D_{FR}) \\
&= \det(D_F)\det(D_R)\det((I - D_R^{-1}D_{RF}D_F^{-1}D_{FR})^{-1})^{-1} \\
&= \det(D_F)\det(D_R)\sum_{n=0}^{\infty}\det(D_R^{-1}D_{RF}D_F^{-1}D_{FR})^n \qquad \text{(Neumann series)} \\
&= \det(D_F)\det(D_i)\det(D_j)\sum_{n=0}^{\infty}\left(\det(D_i)^{-1}\det(D_j)^{-1}\det(D_{RF}D_F^{-1}D_{FR})\right)^n
\end{aligned}$$

Propagator

$$\begin{bmatrix} D_F & D_{F0} & D_{F1} \\ \hline D_{0F} & D_i & \\ D_{1F} & & D_j \end{bmatrix}^{-1} = \left[\begin{array}{c|c} D_F & D_{FR} \\ \hline D_{RF} & D_R \end{array}\right]^{-1} = \left[\begin{array}{c|c} \cdots & \cdots \\ \hline \cdots & D^{-1}(R,R) \end{array}\right]$$

where, by Gaussian elimination (Schur complement),

$$\begin{aligned} D^{-1}(R,R) &= D_R^{-1} + D_R^{-1} D_{RF} (D_F - D_{FR} D_R^{-1} D_{RF})^{-1} D_{FR} D_R^{-1} \\ \text{(by Neumann series)} &= D_R^{-1} + D_R^{-1} D_{RF} D_F^{-1} \left(\sum_{n=0}^{\infty} \left(D_{FR} D_R^{-1} D_{RF} D_F^{-1} \right)^n \right) D_{FR} D_R^{-1} \\ \text{(truncation)} &\approx \underbrace{D_R^{-1}}_{\#\text{patches invs.}} + \underbrace{D_R^{-1} D_{RF} D_F^{-1} D_{FR} D_R^{-1}}_{4 \text{ x } \#\text{patches invs.}} \end{aligned}$$

Cost of applying $\#\text{patches}^{\#\text{slots}}$ approx. $D^{-1}(t,t')$ is O(#patches) inversions and O($\#\text{patches}^{\#\text{slots}}$) in contractions/IO

Distillation costs

For a collection gauge fields generated from a number of #patches and #slots:

- Distillation basis, mesons and baryon elementals:
  - cost and IO is O(#patches)

- Propagators and generalized propagators:
  - O(#patches x #slots) inversions
  - O($\#\text{patches}^{\#\text{slots}}$) contractions & IO

- Disconnected components, tr D^{-1}:
  - Deflation can be affordable if basis restricted to time slices
  - No problem with probing and frequency splitting
  - O(#patches x #slots) inversions
  - O($\#\text{patches}^{\#\text{slots}}$) contractions & IO

NOTE: Props, genprops, and disconnected components will require corrections

Ready to test

superbblas: CPU/GPU library for operating sparse and dense tensors

- support for copying tensor slices and arbitrary patterns
- dense and block sparse format
- arbitrary distribution among computing nodes
- current operations: tensor AXPY, contraction, and factorization (Cholesky, LU)

mgproton: iterative linear solvers and LQCD multigrid

- coloring and cloning of sparse operators
- linear solvers with communication avoiding optimizations
- general porpoise preconditioners: block Jacobi, SVD deflation, Schur complement

Jingle bells, jingle bells,
jingle all the pathway,
how much fun is to renormalize
in a Minkowski space. Hey!

– R. Feynman