Domain decomposition efforts in Chroma

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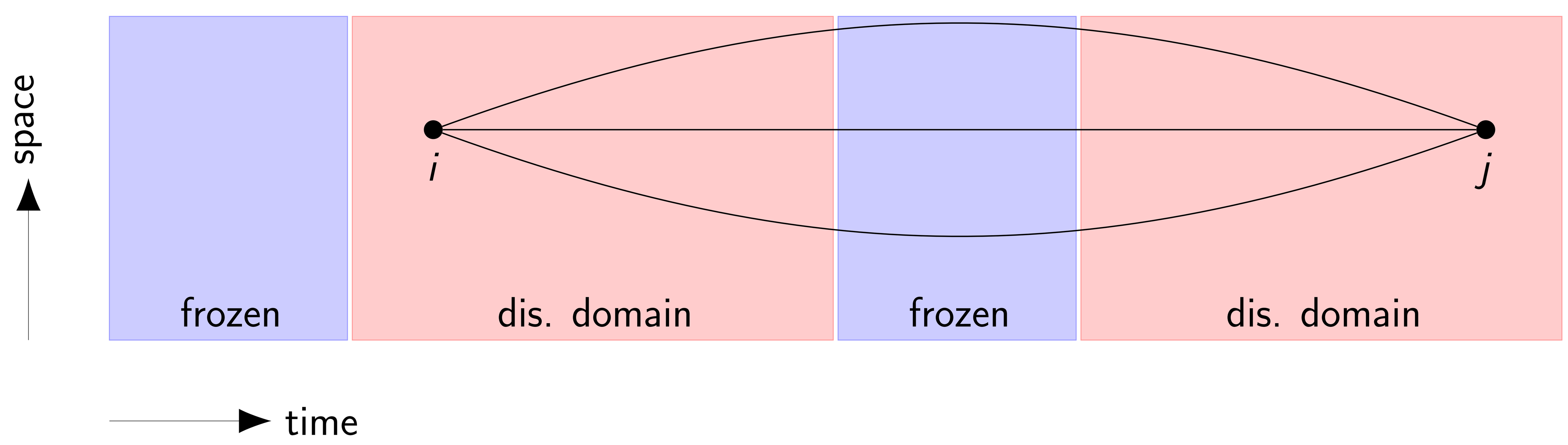
Motivation for domain decomposition

- Finer lattice spacing pushes existing algorithms in a voracious increase in computational cost and accuracy
- Benefits of Domain decomposition for solvers on Dslash:
  - Limit the maximum volume that a linear solver deals with, limiting the accumulation of rounding errors
  - Trade inter-node communications for more intra-node communications
  - Approximate long-distance effects in an efficient way
  - Exploit the sparsity of the right-hand-sides
- Multilevel integration:
  - Decompose the correlation functions into factors that depend only on fields localized into subdomains that can be independently integrated
  - Challenging in the presence of fermions as the action is not local
- First approach for multilevel integration with distillation
  - Work with approximations of the fermionic determinant and propagator that depends on gauge fields within specific lattice subdomains
  - Use *reweighting* for correcting the action and approximate the statistical bias of the approximate correlation functions
  - The efficiency of the technique depends on having cheap and accurate first-level approximations

Multilevel integration example



- Divide the domain and image of a matrix D into two non-overlapping domains F (frozen sites) and R (disconnected domains)
- We are interested in D^{-1} restricted to R:

$$\begin{bmatrix} D_F & D_{FR} \\ D_{RF} & D_R \end{bmatrix}^{-1} = \begin{bmatrix} \cdots & \cdots \\ \cdots & D^{-1}(R,R) \end{bmatrix}$$

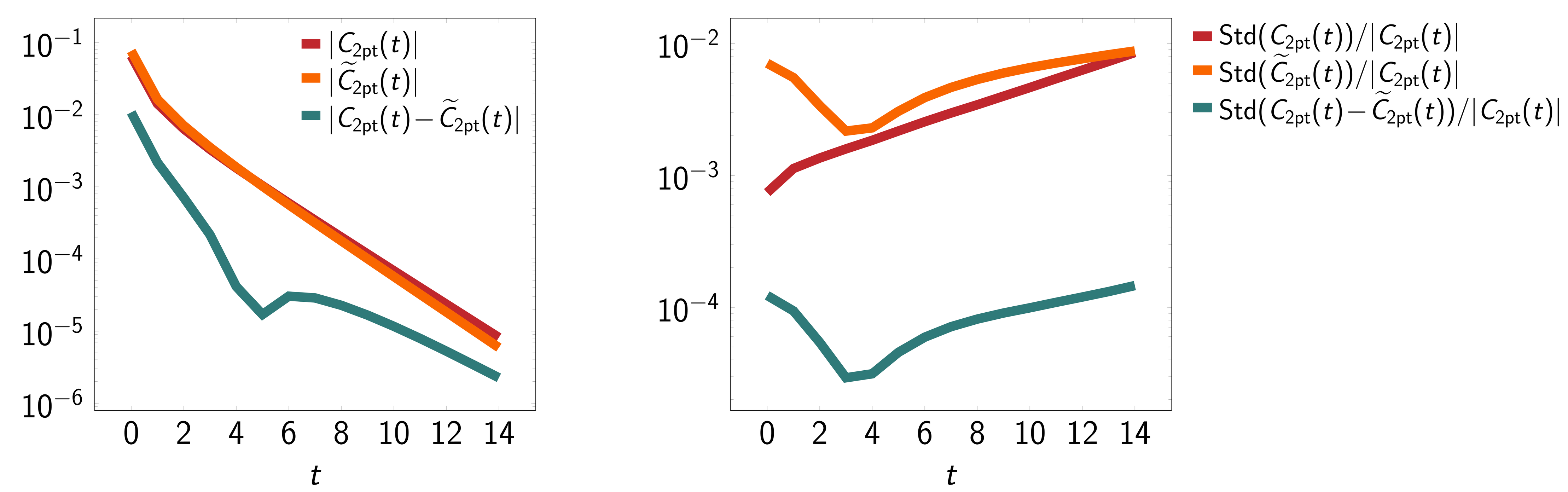
$$D^{-1}(R,R) = D_R^{-1} + D_R^{-1} D_{RF} (D_F - D_{FR} D_R^{-1} D_{RF})^{-1} D_{FR} D_R^{-1}$$

$$\text{(by Neumann series)} = D_R^{-1} + D_R^{-1} D_{RF} D_F^{-1} \left(\sum_{n=0}^{\infty} \left(D_{FR} D_R^{-1} D_{RF} D_F^{-1} \right)^n \right) D_{FR} D_R^{-1}$$

- We truncate the summation at $n = 0$ for generating cheaper perambulators:

$$V^\dagger D^{-1}(R,R) V \approx V^\dagger (D_R^{-1} + D_R^{-1} D_{RF} D_F^{-1} D_{FR} D_R^{-1}) V$$

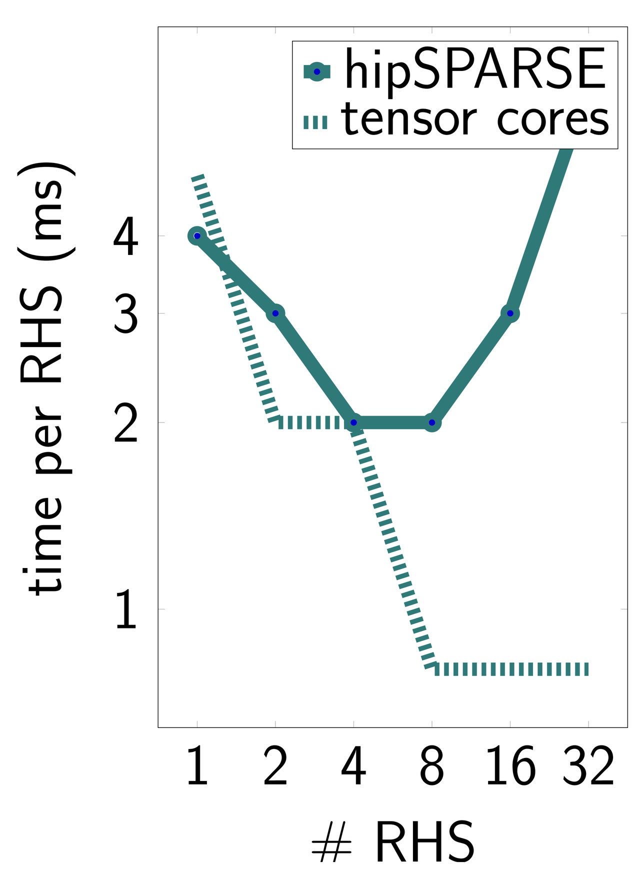
- Comparison of a nucleon 2 point correlation function on a $32^3 \times 64$ lattice ensemble with the full perambulator, $C_{2pt}(t) = \langle \mathcal{N}(t) \overline{\mathcal{N}}(0) \rangle$, and with the cheap perambulator, $\widetilde{C}_{2pt}(t)$. Each frozen and domain region has 2 and 30 units, respectively:



Implementation details

- `superbblas` is a CPU/GPU library that supports:
  - dense and block sparse format tensors
  - arbitrary distribution of tensors among computing nodes
  - current tensor operations: AXPY, contraction, factorization (Cholesky, LU)
  - AXPY tensor operations can be restricted to slices or masks
  - superbblas uses an extension of BSR for representing the Dslash and its coarse projection for multigrid

Ex. of Dslash timings on a Frontier node for a $32^3 \times 64$ lattice



- `mgproton` is a solver collection within Chroma, which includes:
  - slicing, coloring, and cloning of sparse operators
  - linear solvers: FGMRES, GCR...
  - preconditioners: Multigrid, Even-odd Schur complement, block Jacobi, SVD deflation
  - based on `superbblas`

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