Rational domain-decomposed HMC

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Introduction

RDDHMC is a HMC algorithm combined DDHMC and RHMC

- Domain decomposition (Lüscher '03):
  - the Schur complement of Dirac operator with respect to the block decomposition
  - remarkable cost reduction by deflation accelerated DDHMC (Lüscher '07)
  - very good performance on (talk by A. Nobile on Fri.)
- RHMC (Clark, Joó, Kennedy '02):
  - widely used
  - odd flavour simulations
  - cost reduction by Nth root method and relaxing some residuals of shifted problem for partial fractions (Clark, Kennedy '07)

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Dividing $\det D$

$$\det D = \det D_1 \det D_2$$

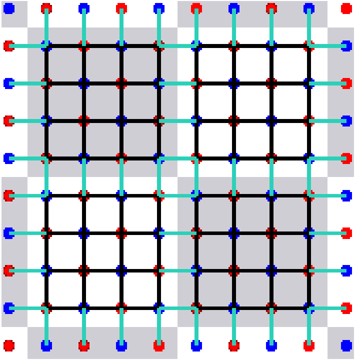
- considerable method
  even-odd prec., mass prec.(Hasenbusch '01), Nth-root method, etc.
- general strategy
  - dividing into inexpensive/large-force D_1 and expensive/small-force D_2 somehow
  - putting D_1 at finer time scale and D_2 at coarser time scale

$$\exp(\frac{\delta t}{2}T)\exp(\delta t V)\exp(\frac{\delta t}{2}T) \approx$$

$$[\exp(\frac{\delta t}{2n}T)\exp(\frac{\delta t}{n}V_1)\exp(\frac{\delta t}{2n}T)]^n \exp(\delta t V_2)[\exp(\frac{\delta t}{2n}T)\exp(\frac{\delta t}{n}V_1)\exp(\frac{\delta t}{2n}T)]^n$$

Dividing $\det D$ for RDDHMC

- Domain decomposition



$$\det D = \det \begin{pmatrix} D_{EE} & D_{EO} \\ D_{OE} & D_{OO} \end{pmatrix} = \det D_{EE} \det \hat{D}_{EE} \det D_{OO}$$

$$\hat{D}_{EE} = 1 - D_{EE}^{-1} D_{EO} D_{OO}^{-1} D_{OE}$$

- Even-Odd precondition

$$\det \tilde{D} \equiv \det D_{EE} \det D_{OO} = \det(1 - D_{eo}D_{oe})_{EE} \det(1 - D_{eo}D_{oe})_{OO}$$

- Clover fermion case
  before DD

$$\begin{aligned}\det D &= \det \begin{pmatrix} T_{ee} & D_{oe} \\ D_{oe} & T_{oo} \end{pmatrix} \\ &= \det \begin{pmatrix} 1 & T_{ee}^{-1} D_{eo} \\ T_{oo}^{-1} D_{oe} & 1 \end{pmatrix} \det T_{ee} \det T_{oo} \\ &= \det \begin{pmatrix} 1 & M_{eo} \\ M_{oe} & 1 \end{pmatrix} \det T_{ee} \det T_{oo}\end{aligned}$$

where

$$T = 1 - \frac{i\kappa c_{SW}}{2} \sigma_{\mu\nu} F_{\mu\nu}$$

- Rational approximation, partial fraction form

$$f(x) \approx \frac{p(x)}{q(x)}$$
$$\approx \alpha_0 + \sum_{i=1}^{m} \frac{\alpha_i}{x + \beta_i}$$

where:

- $p(x), q(x)$ Chebyshev polynomial
- x is $\tilde{D}^\dagger \tilde{D}$ or $\hat{D}^\dagger \hat{D}$
- α_i and β_i are determined as approximation error is small in given range

we get

$$(\det D)^n = [\det(\tilde{D}^\dagger \tilde{D})^{\frac{n}{2m_1}}]^{m_1} [\det(\hat{D}^\dagger_{EE} \hat{D}_{EE})^{\frac{n}{2m_2}}]^{m_2} ,$$

where:

- $\tilde{D}$ is block diagonal matirx that diagonal element is $(1 - D_{eo} D_{oe})_b$
- $\hat{D}_{EE} = 1 - D_{EE}^{-1} D_{EO} D_{OO}^{-1} D_{OE}$
- $\tilde{D}$, $\hat{D}_{EE} \in \mathbb{C}^{6V \times 6V}$

$$S_F = \sum_{i=1}^{m_1} \phi_i^\dagger \left[\tilde{\alpha}_0 + \sum_{j=1}^{l_1} \frac{\tilde{\alpha}_j}{\tilde{D}^\dagger \tilde{D} + \tilde{\beta}_j} \right] \phi_i + \sum_{i=m_1+1}^{m_1+m_2} \phi_i^\dagger \left[\hat{\alpha}_0 + \sum_{j=1}^{l_2} \frac{\hat{\alpha}_j}{\hat{D}^\dagger_{EE} \hat{D}_{EE} + \hat{\beta}_j} \right] \phi_i$$

Feature

some of DDHMC and RHMC feature

- D must be local
- data layout for operator $(1 - D_{eo}D_{oe})_b$
- communication overhead can be minimized
- suited for (non)active link method
- Nth-root method and relaxing some residuals of shifted problem for partial fractions
- need to calculate minimum/maximum eigenvalue of $\tilde{D}^\dagger\tilde{D}$ and $\hat{D}^\dagger_{EE}\hat{D}_{EE}$ (when action is calculated, re-scaling of approximation range may be needed)

Test on 8^4

Action: Wilson glue + 2 flaovur Wilson fermions, $\beta = 5.00$, $\kappa_c = 0.187(1)$

EO:

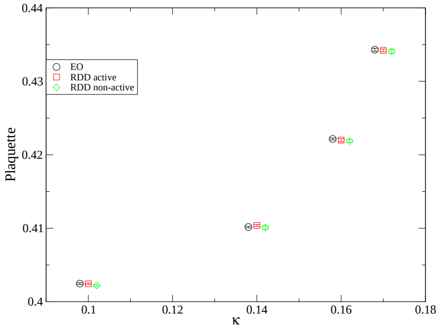
tol = 10^{-10}(MC), 10^{-8}(MD) $(|Ax - b|/|b|)$

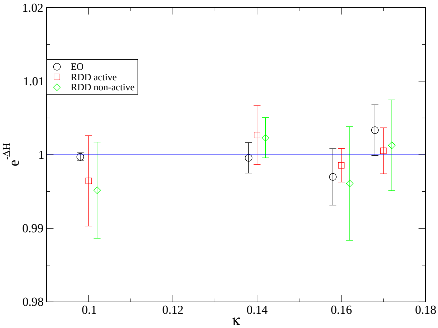
RDD:

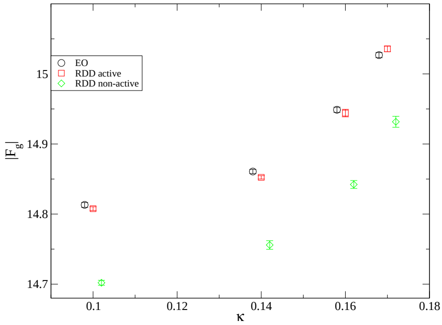
$V_{Block} = 4^4$, $m_1 = m_2 = 2$, $l_1 = l_2 = 25$(MC), 20(MD)

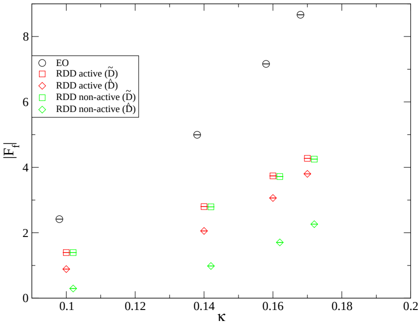
Solver: multi-shift-CG, gmres(15) for $D^{-1}_{EE/OO}$

tol = 10^{-10}(MC), 10^{-6}(MD) $(|Ax - b|/|b|)$






EO
RDD active
RDD non-active
$|F_g|$
κ
15
14.9
14.8
14.7
0.1
0.12
0.14
0.16
0.18

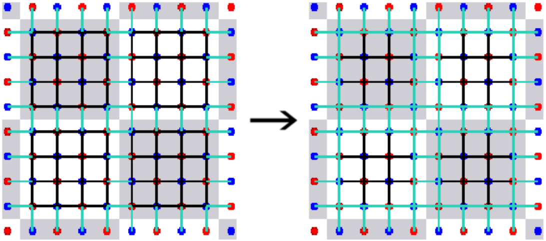

EO
RDD active ($\tilde{D}$)
RDD active ($\hat{D}$)
RDD non-active ($\tilde{D}$)
RDD non-active ($\hat{D}$)
$|F_f|$
κ
8
6
4
2
0
0.1
0.12
0.14
0.16
0.18
0.2

Fat non-active link method

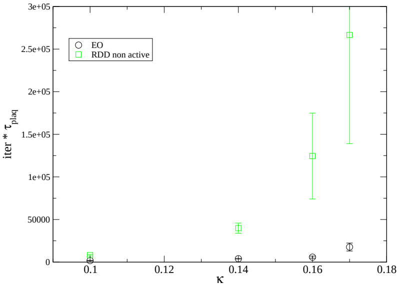
When non-active links are fat links, all links which are used to make fat link are non-active

SLiNC femion:

- 1 level stout link for hopping term, thin link for clover term
- staples around non active links becomes non active
- efficiency weakening



Cost check before expensive simulations



in RDDHMC

$$(\hat{D}_{EE}^{\dagger}\hat{D}_{EE} + \beta_i I)x_i = b$$

is solved

$\hat{D}_{EE} = 1 - D_{EE}^{-1} D_{EO} D_{OO}^{-1} D_{OE}$

(80% - 90% time)

$D_{EE/OO}^{-1}$:

- deflation
  to solve $(\hat{D}_{EE}^{\dagger}\hat{D}_{EE} + \beta_i I)x_i = b$ is multi-R.H.S problem for $D_{EE/OO}$
  (was not helpful for tested cases)
- SSOR + BiCGStab (or GCRO-DR if BiCGStab stagnates)
  (PACS-CS)
- DFL+SAP + preconditionable solver
  require domains in domain, maybe fitted on QPACE

Conclusion

RDDHMC

- seems to work
- efficiency?
  - machine performance should be as good as DDHMC
  - algorithmic performance
    may be improved
- non-active link method with SLiNC fermions (efficiency?)
  (possible for any local fat link Dirac op. with all link active)