

Temporal Preconditioning for Wilson-like Fermions

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Preconditioning in Lattice QCD

- In lattice QCD we solve large sparse linear systems involving the fermion matrix M
- During configuration generation we solve

$$M^\dagger M \phi = \chi$$

- for the pseudofermionic action $\phi^\dagger (M^\dagger M)^{-1} \phi$
- for the computation of the Molecular Dynamics (MD) force:

$$\phi^\dagger (M^\dagger M)^{-1} \left[\frac{\partial M^\dagger}{\partial U} M + M^\dagger \frac{\partial M}{\partial U} \right] (M^\dagger M)^{-1} \phi$$

- For post analysis (propagators, noisy estimators) we solve:

$$M \phi = \chi$$

Preconditioning in Lattice QCD

- Preconditioning is essential to reduce cost of solves AND
- Preconditioning also changes the simulation 'action' AND
- Preconditioning changes the MD fermion forces
 - Forces change because the action changes
 - Roughly:

$$F \propto \kappa (M^\dagger M)^\nu$$

- can take larger MD steps avoiding the integrator instabilities
- put fermionic term on a slower timescale
- cf. Mike Clark's talk.

Example: Schur Style Even-Odd Preconditioning

- colour lattice sites as even and odd (red-black)
- Write M as $\begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix}$
- Perform a Schur Decomposition:

$$\begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix} = \overbrace{\begin{pmatrix} 1 & 0 \\ M_{oe}M_{ee}^{-1} & 1 \end{pmatrix}}^L \begin{pmatrix} M_{ee} & 0 \\ 0 & \tilde{M} \end{pmatrix} \overbrace{\begin{pmatrix} 1 & M_{ee}^{-1}M_{eo} \\ 0 & 1 \end{pmatrix}}^U$$

where

$$\tilde{M} = M_{oo} - M_{oe}M_{ee}^{-1}M_{eo}$$

- Note that: $\det L = \det U = 1$
- Inverses of L and U are trivial (flip sign of off diag. piece)
- M_{ee}^{-1} should be straightforward to apply.

Example: Propagators Computations

- Rewrite propagator system

$$\begin{aligned}
 M \phi &= \chi \\
 \Rightarrow L \begin{pmatrix} M_{ee} & 0 \\ 0 & \tilde{M} \end{pmatrix} U \phi &= \chi \\
 \Rightarrow \begin{pmatrix} M_{ee} & 0 \\ 0 & \tilde{M} \end{pmatrix} \phi' &= \chi'
 \end{aligned}$$

with $\phi' = U\phi$ and $\chi' = L^{-1}\chi$.

- The hard work solving $\tilde{M}\phi'_o = \chi'_o$ (since M^{-1} is easy)
- At the end $\phi = U^{-1}\phi'$

Example: Schur Even-Odd Preconditioning and HMC

- Want to simulate $\det(M^\dagger M)$.
- From the Schur Decomposition:

$$\det(M^\dagger M) = \det(M_{ee}^\dagger M_{ee}) \det(\tilde{M}^\dagger \tilde{M})$$

- Can rewrite our action as:

$$\exp\{-\phi^\dagger (M^\dagger M) \phi\} \Rightarrow \exp\left\{\log \det(M_{ee}^\dagger M_{ee}) - \phi'^\dagger (\tilde{M}^\dagger \tilde{M})^{-1} \phi'\right\}$$

- Now try to take advantage of knowledge of M_{ee} :
 - M_{ee} is independent of gauge fields \Rightarrow drop altogether (Wilson Fermions, Domain Wall Fermions)
 - Compute $\log \det(M_{ee}^\dagger M_{ee})$ directly (Clover Fermions)
- **Key Point: Preconditioning modifies simulation action**

Example: Schur Even-Odd Preconditioning and HMC

- Two new force terms in MD
 - From $\exp \left\{ \log \det \left(M_{ee}^\dagger M_{ee} \right) \right\}$
 - From $\exp \left\{ -\phi'^\dagger \left(\tilde{M}^\dagger \tilde{M} \right)^{-1} \phi' \right\}$
- New pseudofermionic force involves \tilde{M} rather than M .
- \tilde{M} has better condition than M
 - we get smaller forces
 - further from integrator step size instabilities
 - Can take bigger steps in MD at same overall cost
 - Larger step-size integrators become useful
 - Fewer inversions for fixed MD trajectory length.
 - All the benefits Mike discussed

Previously Successful Preconditionings

- Even Odd (previous example), Lexicographic SSOR
- Domain Decomposition Combined with HMC (Lüscher)
- Hasenbusch Mass Preconditioning (Hasenbusch et. al)
 - Simulate

$$\frac{\det(M_1^\dagger M_1)}{\det(M_2^\dagger M_2)} \det(M_2^\dagger M_2)$$

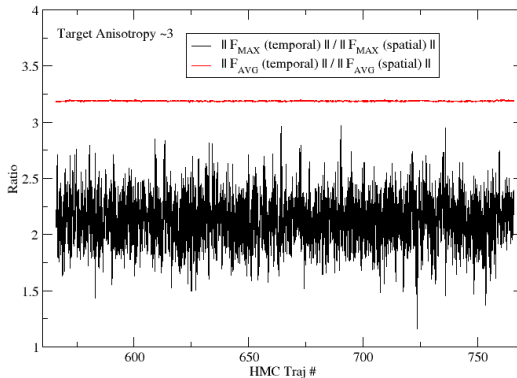
- Choose $M_2 = M_1 + \delta$
 - M_2 is better conditioned, Ratio is close to $1 + O(\delta)$
- Nth-rootery / Multipseudofermions (Clark et. al):

$$\det(M^\dagger M) = \left[\det(M^\dagger M)^{\frac{1}{N}} \right]^N \Rightarrow \prod_{i=1}^N e^{\left\{ -\phi_i^\dagger (M^\dagger M)^{-\frac{1}{N}} \phi_i \right\}}$$

- Now have N terms each with condition number $\kappa^{\frac{1}{N}}$.
- Win if $N \kappa^{\frac{1}{N}} < \kappa$

Anisotropic Lattices

- Ideal world
 - Want fine lattice spacing (close to continuum)
- Real World:
 - Fine lattice too costly, do as coarse as possible
- Compromise: Make just one dimension (time) fine
 - 2 lattice spacings: a_s (spatial) and a_t (temporal)
 - Typical choice: $a_t \ll a_s$
 - Important physics applications (eg: spectroscopy)
- Ramifications:
 - Lowest modes of fermion matrix result from fine a_t
 - Largest forces from a_t



Ratios of spatial and Temporal forces in Anisotropic RHMC for $\xi \approx 3$

Motivation for Temporal Preconditioning

- Basic Idea

- Write $M = M_s + M_t = M_t \left(M_t^{-1} M_s + 1 \right)$
- The preconditioned matrix is $\tilde{M} = 1 + M_t^{-1} M_s$
- Deal separately with $\det(M_t)$ in HMC

- Expect

- To still have even-odd preconditioning spatial dimensions
- To gain an improvement in condition number \approx anisotropy
- To gain a reduction in temporal pseudofermion force in HMC

The Wilson Fermion Operator

- Unpreconditioned Wilson Fermion Operator ($r = 1$):

$$M = D_s + D_t$$

$$D_s = - \sum_{k=1}^3 P_-^k U_k(x) \delta_{x+\hat{k},y} + P_+^k U_k^\dagger(x - \hat{k}) \delta_{x-\hat{k},y}$$

$$D_t = \hat{m} - P_- \tilde{U}_t(x) \delta_{x+\hat{t},y} - P_+ \tilde{U}_t^\dagger(x - \hat{t}) \delta_{x-\hat{t},y}$$

with

$$P_\pm^k = (1/2)(1 \pm \gamma_k) \quad k = 1, 2, 3$$

$$P_\pm = (1/2)(1 \pm \gamma_4)$$

$$\tilde{U}(x) = \frac{\nu}{\xi_0} U(x), \quad U \in SU(3)$$

$$\hat{m} = 1 + (N_d - 1) \frac{\nu}{\xi_0} + M$$

Central Temporal Preconditioning

- Define Matrices:

$$T(\vec{x})_{t,t'} = \hat{m} - \tilde{U}_t(\vec{x}, t)\delta_{t+1,t'} \text{ with periodic boundaries in time}$$

$$C_L^{-1} = P_+ + P_- T$$

$$C_R^{-1} = P_- + P_+ T^\dagger$$

- Then we have (playing Projector games): $C_L^{-1} C_R^{-1} = D_t$
- Precondition as:

$$\tilde{M} = C_L M C_R = C_L D_S C_R + 1$$

- We retain a kind of γ_5 hermiticity:

$$\gamma_5 C_L^{-1} \gamma_5 = (C_R^{-1})^\dagger \quad \gamma_5 C_R^{-1} \gamma_5 = (C_L^{-1})^\dagger, \quad \gamma_5 \tilde{M} \gamma_5 = \tilde{M}^\dagger$$

Inverting the Preconditioning Matrices

The Sherman Morrison Woodbury Formula

- Consider C_L only (C_R proceeds similarly)

$$C_L^{-1} = P_+ + P_- T \Rightarrow C_L = P_+ + P_- T^{-1}$$

with

$$T = \begin{pmatrix} \hat{m} & -U_t(\vec{x}, 0) & 0 & \dots & & \\ 0 & \hat{m} & -U_t(\vec{x}, 1) & 0 & \dots & \\ \vdots & 0 & \ddots & \ddots & & \\ 0 & \dots & 0 & \hat{m} & -U_t(\vec{x}, N_t - 2) & \\ -U_t(\vec{x}, N_t - 1) & 0 & \dots & 0 & \hat{m} & \end{pmatrix}$$

- Write T as $T = T_0 + V W^T$ with

$$T_0 = \begin{pmatrix} \hat{m} & -U_t(\vec{x}, 0) & 0 & \dots & & \\ 0 & \hat{m} & -U_t(\vec{x}, 1) & 0 & \dots & \\ \vdots & 0 & \ddots & \ddots & & \\ 0 & \dots & 0 & \hat{m} & -U_t(\vec{x}, N_t - 2) & \\ 0 & 0 & \dots & 0 & \hat{m} & \end{pmatrix}$$

$$V = \begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \\ -U_t(\vec{x}, N_t - 1) \end{pmatrix} \quad W = \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \\ 0 \end{pmatrix}$$

- Sherman Morrison Woodbury Formula:

$$T^{-1} = T_0^{-1} - P(1 + W^T P)^{-1} W^T T_0^{-1} \quad \text{with } P = T_0^{-1} V$$

- T_0^{-1} easy to apply with back substitution

- We can compute $P = T_0^{-1} V$ by solving $TP = V$

$$P_{N_t-1} = -\frac{1}{\hat{m}} U_t(N_t - 1)$$

$$P_{N_t-2} = -\frac{1}{\hat{m}^2} U_t(N_t - 2)U_t(N_t - 1)$$

$$P_i = -\frac{1}{\hat{m}^{N_t-i}} \prod_{j=N_t-i}^{N_t-1} U_t(j)$$

$$P_0 = -\frac{1}{\hat{m}^{N_t}} \prod_{j=0}^{N_t-1} U_t(j)$$

- We define

$$Q = (1 + W^T P)^{-1} = (1 + P_0)^{-1}$$

and

$$T^{-1} = (1 - PQW^T)T_0^{-1}$$

Comments

- Computing P takes N_t $SU(3)$ multiplications per *spatial coordinate* \vec{x} (or 1 $SU(3)$ multiplication per site)
- P_0 is essentially just the Polyakov Loop
- Computing Q takes 1 3×3 complex matrix inversion per *spatial coordinate*. We use LU decomposition.
- Life is made easy if all temporal sites for a spatial coordinate x are kept 'local' to a processor

HMC Considerations

The determinant to simulate

- Determinant of interest is:

$$\det(M^\dagger M) = \det\left[\left(C_R^{-1}\right)^\dagger C_R^{-1}\right] \times \det\left[\left(C_L^{-1}\right)^\dagger C_L^{-1}\right] \times \det\left[\tilde{M}^\dagger \tilde{M}\right]$$

- Using the γ_5 hermiticity of C_L^{-1} and C_R^{-1} :

$$\begin{aligned} \det(M^\dagger M) &= \left[\det\left(C_R^{-1}\right)\right]^2 \times \left[\det\left(C_L^{-1}\right)\right]^2 \times \det\left(\tilde{M}^\dagger \tilde{M}\right) \\ &= e^{2 \log \det\left(C_R^{-1}\right)} e^{2 \log \det\left(C_L^{-1}\right)} \int d\phi^\dagger d\phi e^{-\phi^\dagger \left(\tilde{M}^\dagger \tilde{M}\right)^{-1} \phi} \end{aligned}$$

HMC Considerations

$\det(C_L^{-1})$ and $\det(C_R^{-1})$

- In Dirac Basis:

$$P_+ = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad P_- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and so

$$\det(C_L^{-1}) = \det(P_+ + P_- T) = \det(T)^2$$

$$\det(C_R^{-1}) = \det(P_- + P_+ T^\dagger) = \det(T^\dagger)^2$$

HMC Considerations

$\det(T)$

- Finally:

$$\begin{aligned} T &= T_0 + VW^T \\ &= T_0 \left(1 + T_0^{-1} VW^T \right) \\ &= T_0 \left(1 + PW^T \right) \end{aligned}$$

and

$$1 + PW^T = \begin{pmatrix} 1 + P_0 & 0 & \dots & 0 \\ P_1 & 1 & 0 & \dots \\ \vdots & 0 & \ddots & 0 \\ P_{N_t-1} & 0 & \dots & 1 \end{pmatrix}$$

so

$$\det(T) = \det(T_0) \det(1 + P_0)$$

- Recall that T_0 is upper diagonal with

$$\text{diag}(T_0) = \text{diag}(\hat{m}l_3, \hat{m}l_3, \dots)$$

so

$$\det(T_0) = \hat{m}^{3N_t}$$

- We also have

$$1 + P_0 = 1 - \frac{1}{\hat{m}^{N_t}} \prod_{j=0}^{N_t-1} U_t(j)$$

So

$$\det(T(\vec{x})) = \hat{m}^{3N_t} \det \left[1 - \frac{1}{\hat{m}^{N_t}} \prod_{j=0}^{N_t-1} U_t(\vec{x}, j) \right]$$

Clover Fermions

Improved Wilson Fermions

- Clover Fermions: Wilson Fermions + and Improvement (“Clover”) Term

$$M = D_S + D_t + A \quad \text{where} \quad A(x) = -\frac{C_{SW}\sigma_{\mu\nu}}{4} F_{\mu\nu}(x)$$

- The clover term A is local and Hermitian
- Precondition with same C_L and C_R as before

$$M = C_L^{-1} C_R^{-1} + D_S + A$$

$$\tilde{M} = C_L M C_R = [1 + C_L (D_S + A) C_R]$$

Even–Odd Preconditioning in Space

Preliminaries

- Want even–odd preconditioning in space together with temporal preconditioning.
- Label sites as even or odd based on *spatial* coordinate \vec{x} :

$$-1^{x+y+z} = \begin{cases} +1 & \Rightarrow \text{even} \\ -1 & \Rightarrow \text{odd} \end{cases}$$

- D_t , C_L , C_R and T do not couple neighbours in \vec{x}
 - hence they are *diagonal* in even-odd space
- A is also diagonal in even-odd space
- D_S couples nearest neighbours in \vec{x}

The Operator in Even–Odd Space

- We write the clover operator as:

$$\tilde{M} = 1 + C_L(D_s + A)C_R = \begin{pmatrix} \tilde{M}_{ee} & \tilde{M}_{eo} \\ \tilde{M}_{oe} & \tilde{M}_{oo} \end{pmatrix} = \begin{pmatrix} 1 + C_L^e A^{ee} C_R^e & C_L^e D_s^{eo} C_R^o \\ C_L^o D_s^{oe} C_R^e & 1 + C_L^o A^{oo} C_R^o \end{pmatrix}$$

- Wilson operator simplifies since $A = 0$.
- We consider 2 spatial preconditionings
 - Schur decomposition based
 - Incomplete LU decomposition

Schur Decomposition

- We perform the Schur Decomposition:

$$\tilde{M} = L D U$$

$$L = \begin{pmatrix} 1 & & 0 \\ C_L^o D_s^{oe} C_R^e (1 + C_L^e A^{ee} C_R^e)^{-1} & 1 & \\ 0 & & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} 1 & (1 + C_L^e A^{ee} C_R^e)^{-1} C_L^e D_s^{eo} C_R^o \\ 0 & 1 & \\ & & \end{pmatrix}$$

$$D = \begin{pmatrix} 1 + C_L^e A^{ee} C_R^e & & 0 \\ 0 & 1 + C_L^o A^{oo} C_R^o - C_L^o D_s^{oe} C_R^e (1 + C_L^e A^{ee} C_R^e)^{-1} C_L^e D_s^{eo} C_R^o & \\ & & \end{pmatrix}$$

- Note the term:

$$1 + C_L A C_R = C_L (D_t + A) C_R$$

- We rewrite with $C_L(D_t + A)C_R$

$$L = \begin{pmatrix} 1 & 0 \\ C_L^o D_s^{oe} (D_t + A)_{ee}^{-1} C_L^{-1} & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} 1 & (C_R^e)^{-1} (D_t + A)_{ee}^{-1} D_s^{eo} C_R^o \\ 0 & 1 \end{pmatrix}$$

$$\mathcal{D} = \begin{pmatrix} C_L^e (D_t + A)_{ee} C_R^e & 0 \\ 0 & C_L^o (D_t + A)_{oo} C_R^o - C_L^o D_s^{oe} (D_t + A)_{ee}^{-1} D_s^{eo} C_R^o \end{pmatrix}$$

- The matrix $D_t + A$ is:

$$\begin{pmatrix} \hat{m} + A(0) & -U(0)P_- & 0 & \dots & -U^\dagger(N_t - 1)P_+ \\ -U^\dagger(0)P_+ & \hat{m} + A(1) & -U(1)P_- & 0 & \dots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & & -U^\dagger(N_t - 3)P_+ & \hat{m} + A(N_t - 2) & -U(N_t - 2)P_- \\ -U(N_t - 1)P_- & 0 & \vdots & -U^\dagger(N_t - 2)P_+ & \hat{m} + A(N_t - 1) \end{pmatrix}$$

- Now the P_\pm enter giving the matrix *spin structure*
- Dimension is increased by a factor of $N_s = 4$
- The matrix is Tridiagonal + Corner pieces.
 - Can still play the Woodbury Game

• Write

$$D_t + A = T + VW^T, \quad V = \begin{pmatrix} -U^\dagger(N_t - 1)P_+ \\ 0 \\ 0 \\ \vdots \\ 0 \\ -U(N_t - 1)P_- \end{pmatrix} \quad W = \begin{pmatrix} P_- \\ 0 \\ 0 \\ \vdots \\ 0 \\ P_+ \end{pmatrix}$$

and

$$T = \begin{pmatrix} \hat{m} + A(0) & -U(0)P_- & 0 & \dots & 0 \\ -U^\dagger(0)P_+ & \hat{m} + A(1) & -U(1)P_- & 0 & \dots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & \\ 0 & 0 & -U^\dagger(N_t - 3)P_+ & \hat{m} + A(N_t - 2) & -U(N_t - 2)P_- \\ 0 & 0 & \vdots & -U^\dagger(N_t - 2)P_+ & \hat{m} + A(N_t - 1) \end{pmatrix}$$

- At this point, things get a little messy for Clover
 - Inversion of T doable in principle
 - T^{-1} by LDU decomposition builds up continued fractions of $P_+ A^{-1} P_-$.
 - A has spin structure – doesn't commute with P_{\pm} .
 - Projectors destroy 6×6 block structure of A
 - Need minimally inversion of 12×12 matrices.
 - Iterative inversion is undesirable (multiplicative cost?)
- For Wilson Fermions the Schur method is straightforward
 - $(D_t + A)^{-1} \Rightarrow D_t^{-1} = C_L C_R$
 - We can already compute these easily.

Incomplete LU Decomposition

The other way to do even-odd preconditioning

- Recall our Clover Operator:

$$M = D_t + D_s + A = C_L^{-1} C_R^{-1} + D_s + A$$

- A property of C_L^{-1} and C_R^{-1} :

$$C_L^{-1} + C_R^{-1} = P_+ + P_- T + P_- + P_+ T^\dagger = C_L^{-1} C_R^{-1} + 1$$

so

$$M = C_L^{-1} + C_R^{-1} + D_s + A - 1$$

- From the previous page

$$M = C_L^{-1} + C_R^{-1} + D_s + A - 1$$

- Define

$$\mathcal{L}^{-1} = \begin{pmatrix} (C_R^e)^{-1} & 0 \\ D_s^{oe} & (C_R^o)^{-1} \end{pmatrix}$$

$$U^{-1} = \begin{pmatrix} (C_L^e)^{-1} & D_s^{eo} \\ 0 & (C_L^o)^{-1} \end{pmatrix}$$

- We can write an Incomplete LU decomposition of M as:

$$M = \mathcal{L}^{-1} + U^{-1} + (A - 1)$$

- Precondition as

$$\tilde{M} = \mathcal{L}MU = U + \mathcal{L} + \mathcal{L}(A - 1)U$$

- Precondition as

$$\tilde{M} = \mathcal{L}M\mathcal{U} = \mathcal{U} + \mathcal{L} + \mathcal{L}(A - 1)\mathcal{U}$$

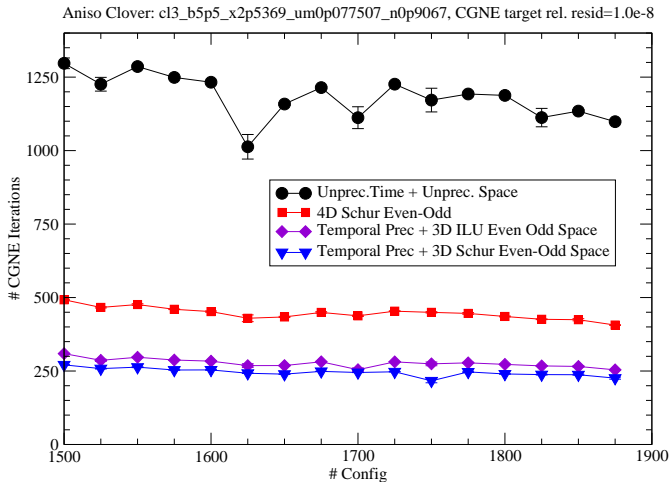
- Can immediately write down \mathcal{L} and \mathcal{U} :

$$\mathcal{U} = \begin{pmatrix} C_L^e & -C_L^e D_s^{eo} C_L^o \\ 0 & C_L^o \end{pmatrix} \quad \mathcal{L} = \begin{pmatrix} C_R^e & 0 \\ -C_R^o D_s^{oe} C_R^e & C_R^o \end{pmatrix}$$

- This preconditioning is very clean.
 - Same C_L and C_R as the spatially unpreconditioned case (just applied to different subsets of sites)
 - No spin structure in the T and T^\dagger .
 - I don't even need to compute A^{-1} .

- 16 Configurations from Anisotropic Clover Tuning Run
 - 3 Flavours of Degenerate Clover Quarks (for m_s tuning)
 - $\beta = 5.5$, $m = -0.077507$, $c_{SW}^R = 0.90671$, $c_{SW}^T = 0.62002$,
 $\xi_0 = 2.5369$, $\nu = 0.90671$
 - 2 Levels of Stout Smearing in the Linear Operator,
 $\rho = 0.22$. Time dimension not smeared
 - Volume= $16^3 \times 64$, Target Anisotropy: $\xi \approx 3$
 - Trajectories 1500-1875 generated by Rational Hybrid Monte Carlo
 - 3 Timescales: Fermions, Spatial Gauge, Temporal Gauge
 - Integrators: 2nd Order Omelyan, 2nd Order Leapfrog, 2nd Order Leapfrog
 - Relative step sizes: $\frac{1}{7}$, $\frac{1}{3}$, $\frac{1}{2}$
- Computed Propagators(CGNE), Condition Numbers for various Operators

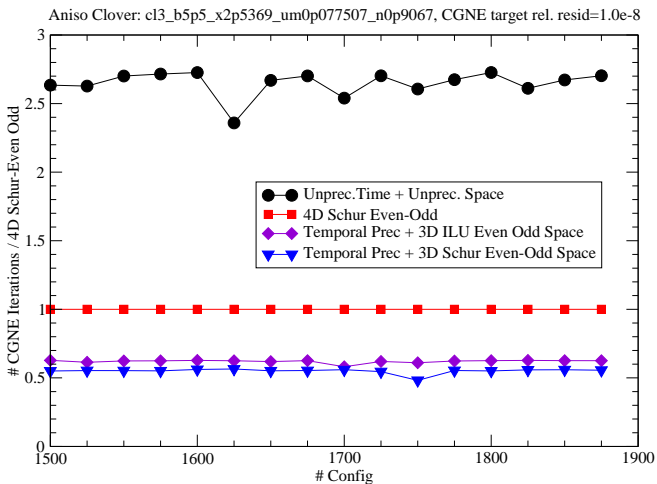
- Configurations were generated on Cray XT3/4 Facilities at
 - NCCS, Oak Ridge National Lab
 - Pittsburgh Supercomputing Center
- Inversions and condition numbers were computed on the USQCD 6n Intel-Infiniband Cluster at JLab
- The temporal preconditioning algorithms were coded with the Chroma software package



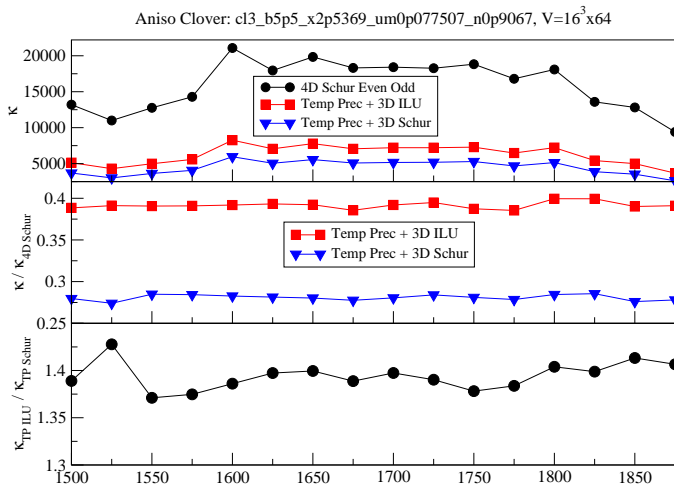
Raw Iteration Counts For Unpreconditioned, 4D Schur, Temp. Prec. + 3D ILU, Temp.

Prec. + 3D Schur





Iteration Counts Normalized to 4D Schur-Even Odd (the “standard”)



Condition Number Data

Summary

- We presented the motivation for and details of Temporal Preconditioning
- Compared to the standard 4D Even-Odd Preconditioning
 - Gain just under a factor of 2 in CGNE iteration counts
 - Temp Prec. Condition Numbers are about 60-73% lower
 - Schur Style 3D Spatial Preconditioning seems slightly better than ILU (but much more complicated)
- Future Work:
 - Determine and implement MD Force terms
 - Incorporate into current Chroma HMC Structure
 - Consider BiCGStabX where (X is 2, L, etc)
 - Optimized Level 3 software... (???)

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