

Algorithms

MITP - Summer school

Aug. 1st , 2025

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Outline - Part 3

- Part 0
 - Markov Chain Monte Carlo
 - Hybrid Monte Carlo algorithm
- Part 1
 - Linear solvers, Krylov subspace solvers
 - Preconditioners, smoothers and coarse grid
- Part 3
 - Details on multigrid preconditioning
 - Fermions in simulations

Recap: Krylov subspace solver

Iterative solver: define Krylov subspace

$$K_m = \text{span}(r, Ar, A^2r, \dots, A^{m-1}r)$$

with

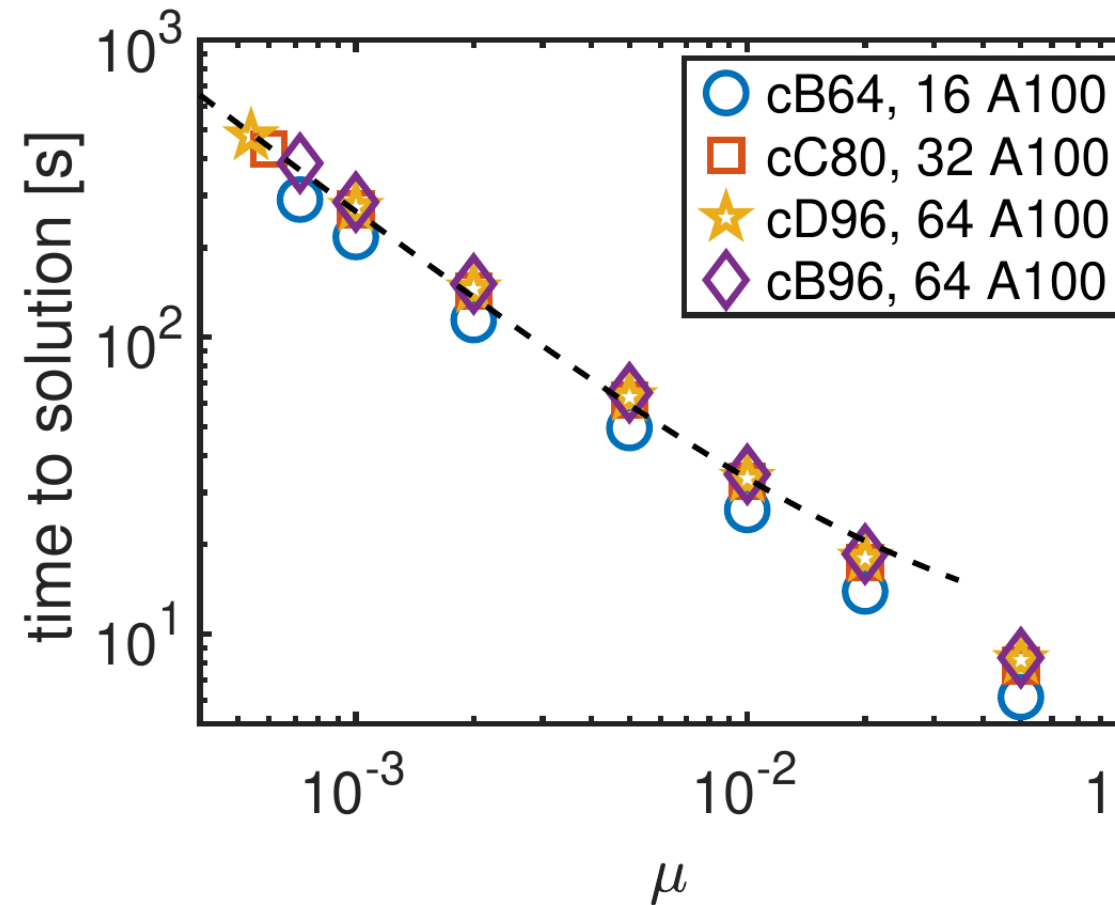
$$\tilde{x} \in x_0 + K_m \quad \text{and} \quad r \perp L$$

For **CG** solver follows

$$\text{cost} \approx V \frac{c_0}{\mu}$$

Iteration count proportional to condition number

- depends on the smallest mode
- iteration count increases drastically at physical point



Recap Multigrid

Idea: Preconditioning **IR** and **UV** modes

Error can be split:

$$e = e_{\text{low}} + e_{\text{high}}$$

- a good smoother eliminates e_{high} high effectively

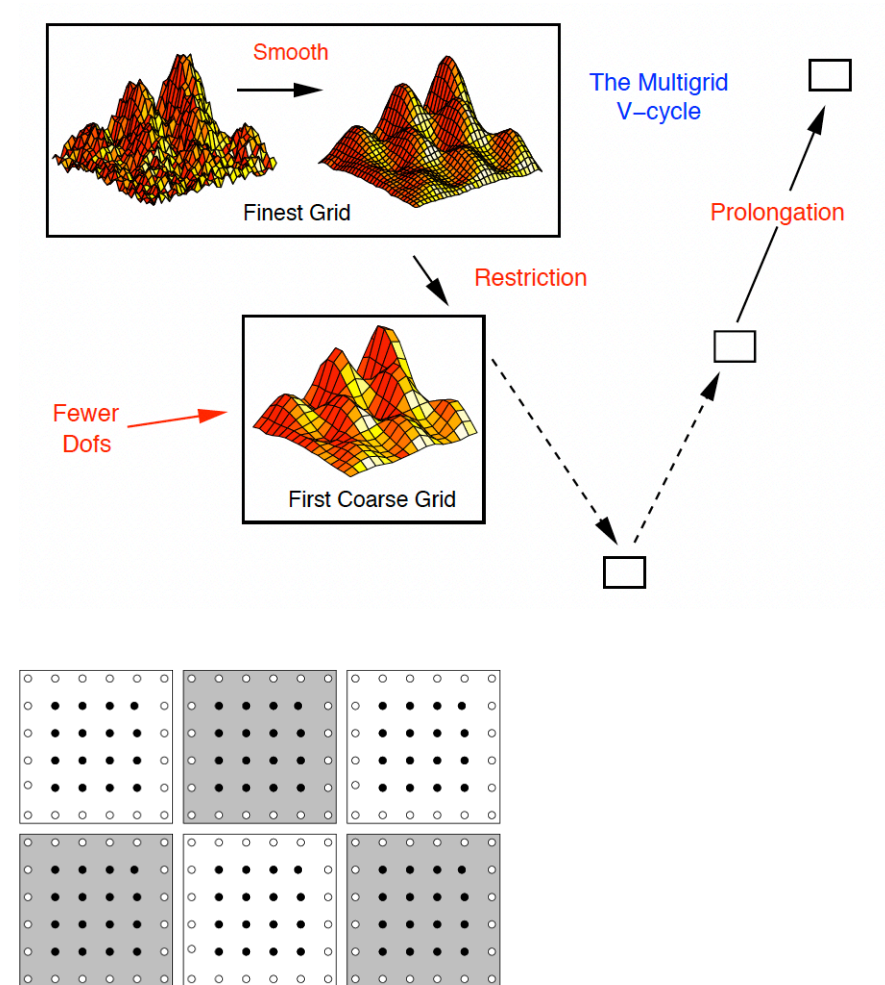
A good choice: SAP which apply block inverses in alternating procedure

$$x^{(k)} \leftarrow (1 - SA)x^{(k)} + Sb$$

where $S = A_r^{-1} + A_b^{-1} - A_b^{-1}A_{br}A_r^{-1}$

and the error scales

$$e_{\text{SAP}} = 1 - SA = (1 - A_b^{-1}A)(1 - A_r^{-1}A)$$



Algebraic multigrid: non-geometric

Two-level AMG

- Petrov-Galerin projection

$$A_c = RDP$$

with R restriction operator, P prolongation operator, A_c coarse grid operator

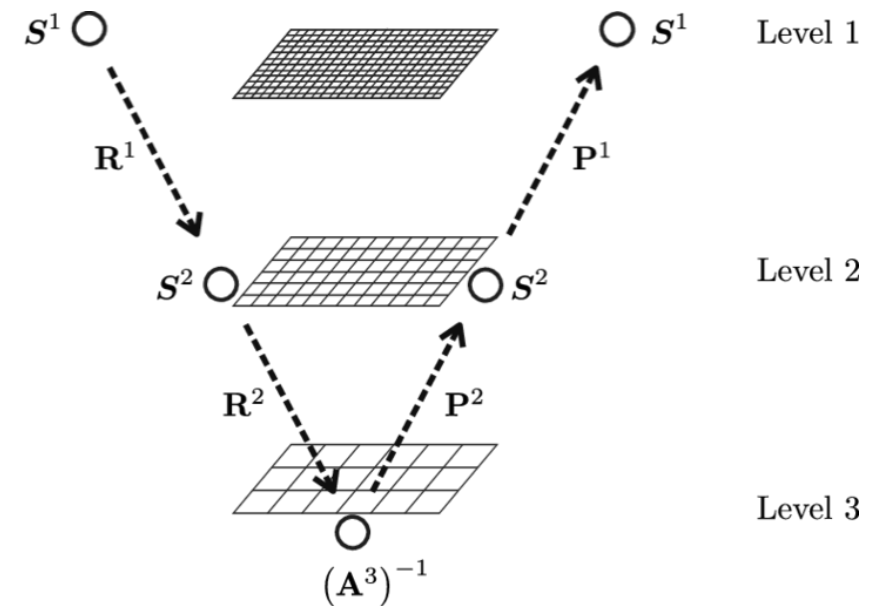
- Coarse-grid correction

$$x^{(k)} \leftarrow x^{(k)} + PA_c^{-1}R \cdot r^{(k)}$$

- Then for the error propagation follows

$$e^{(k)} = I - PD_c^{-1}RA$$

Task: Capture sufficient low modes within P



Aggregation

Construction of P . Lets order the subspaces:

$$L \times S \times C$$

with L spacial lattice, S spin space, C color space

Aggregation blocks:

$$A^{(i,\tau)} = L^{(i)} \times S^{(\tau)} \times C$$

with $(A^{i,\tau} : j = 1, \dots, n^{(L)}; \tau = 0, 1)$

The **prolongation operator** fullfills:

$$\gamma_5 P = P \gamma_5^c$$

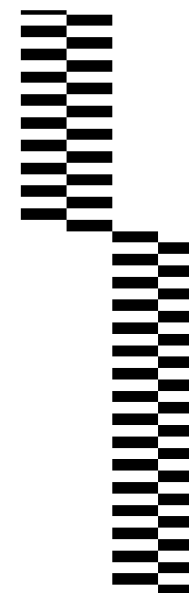
γ_5^c diagonal on the coarse grid. Setting $R = P^\dagger$, we get:

$$A_c = P^\dagger D P \quad \text{and it follows} \quad \gamma_5^c A_c = A_c^\dagger \gamma_5^c$$

Using N test vectors: Split them up into $N \times s$

$$(v_1 \mid \dots \mid v_N) = \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix} \longrightarrow P = \begin{pmatrix} \boxed{} & & & \\ & \boxed{} & & \\ & & \ddots & \\ & & & \boxed{} \end{pmatrix} \begin{matrix} \mathcal{A}_1 \\ \mathcal{A}_2 \\ \vdots \\ \mathcal{A}_s \end{matrix}$$

Test-vector aggregation
additional in spin
space:



Building the coarse grid space

Test vectors: use approximate eigenvectors in the construction of P

An ideal approach: Take eigenspace of small eigenvalues

- direct approach to expensive (although iterative procedures for eigenspace calculations exists)
- indirect approach **approximation via A^{-1} . Start with random vector w and apply A^{-1} k -times

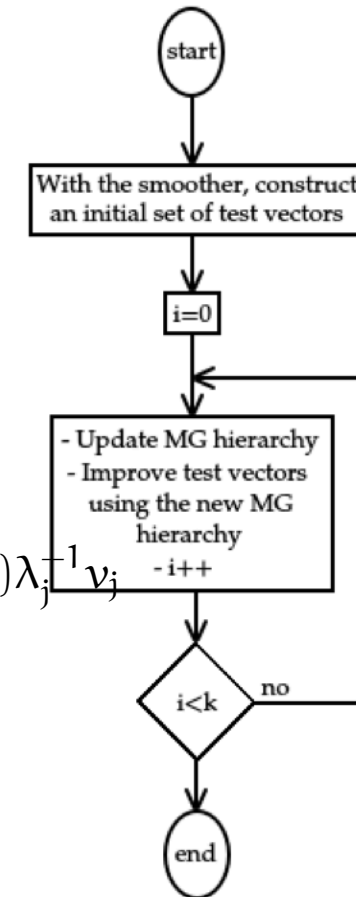
$$w^{(k)} \leftarrow (A^{-1})w^{(0)} \quad \text{with} \quad w^{(1)} = A^{-1}w^{(0)} = \sum_j (v_j, w^{(0)}) \lambda_j^{-1} v_j$$

for k large, $w^{(k)}$ good approx. of $v_{\text{smallest } \lambda}$ and $A = V\Lambda V^\dagger$ (if $A = A^\dagger$)

- application of k -times A^{-1} for each test vector too expensive

Idea: Use multigrid hierarchy to approx. A^{-1} , update multigrid hierarchy as test vectors improves

$$w^{(k+1)} \leftarrow A^{-1}(v^{(k)}) \quad v^{(k)}$$



[Luescher 2007]

Parameters of DDalphaAMG

	parameter		default
setup	number of iterations	n_{inv}	6
	number of test vectors	N	20
	size of lattice-blocks for aggregates on level 1		4^4
	size of lattice-blocks for aggregates on level $\ell > 1$		2^4
	coarse system relative residual tolerance (stopping criterion for the coarse system) ^(*)	ϵ	$5 \cdot 10^{-2}$
solver	restart length of FGMRES	n_{kv}	10
	relative residual tolerance (stopping criterion)	tol	10^{-10}
	number of post-smoothing steps ^(*)	ν	5
	size of lattice-blocks in SAP ^(*)		2^4
K-cycle	number of Minimal Residual (MR) iterations to solve the local systems in SAP ^(*)		3
	maximal length ^(*)		5
	maximal restarts ^(*)		2
	relative residual tolerance (stopping criterion) ^(*)		10^{-1}

(*) : same in solver and setup



[<https://wwwold.mathematik.tu-dortmund.de/lisix/events/UQ18/talks/Frommer-Dortmund-2018.pdf>]

Conclusion and outlook

Lattice libraries

Plenty of solver library exists like

QUDA [<https://github.com/lattice/quda>] : implements a multi-grid solver procedure for various operators on GPUs (Nvidia and AMD)

openQCD : implements a 2 lvl-MG procedure optimized for the Wilson-Dirac discretization (currently for CPUs)

DDalphaAMG : implements a multi-grid procedure for Wilson-Dirac discretization

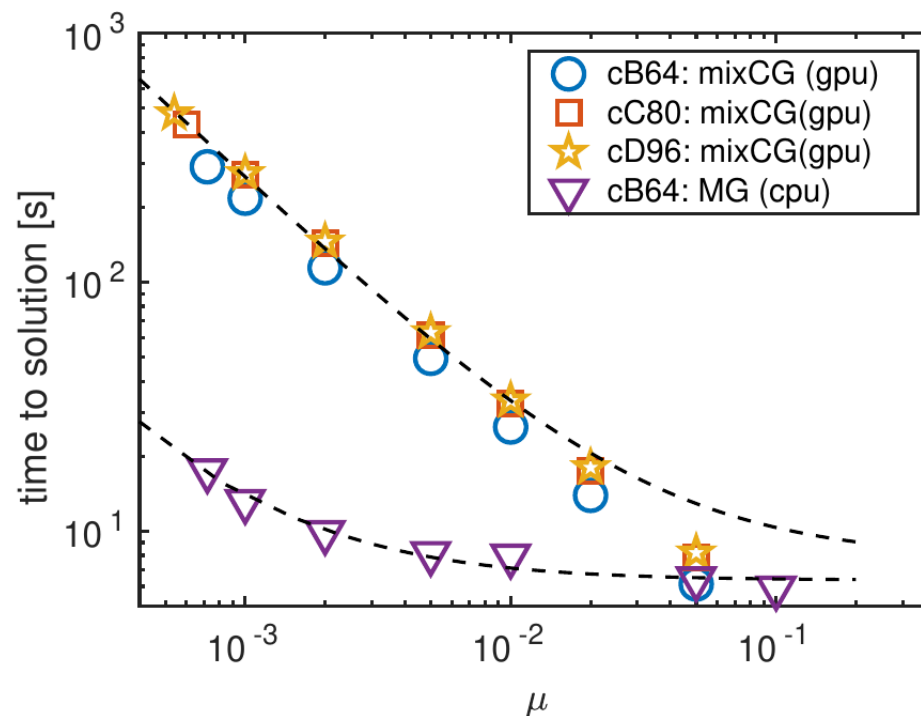
grid : implements also multi-grid procedure

multi-grid is computational limited by

- less scalable (coarse grid boundary surface large)
- memory bound

... more ..

Usually main computational challenge:



$$\text{cost} \approx V \left(C_0 + \frac{C_1}{\mu} \right) \quad \text{with} \quad C_0 \gg C_1$$

Goal: Evaluation of pathintegral

Recap: Motivation for MCMC

$$\langle O \rangle = \frac{1}{Z} \int D\phi e^{-S(\phi)} O(\phi) \quad D\phi = \prod_{i=1}^M d\phi_i \quad \text{e. g.} \quad \phi = U, \bar{\psi}, \psi$$

- Deterministic integration methods not feasible!

Current lattice QCD simulations can have $M = O(10^9)$

- Monte Carlo: evaluates integral by sampling the integrand at points selected via probability under the integration measure

Basic idea

1. Generate sequence of field configurations with probability

$$P(\phi^{(t)}) = \frac{1}{Z} e^{-S(\phi^{(t)})}$$

1. Evaluate

$$\bar{O} = \frac{1}{N} \sum_{t=1}^N O(\phi^{(t)})$$

Hybrid Monte Carlo

Ideal HMC algorithm

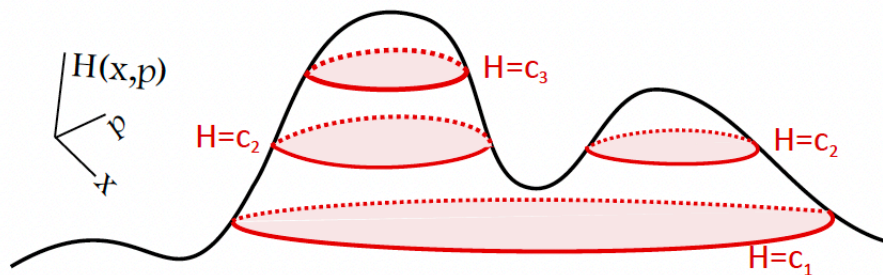
1. Start from a gauge-field $U(0)$
2. Sample a momentum field $P(0)$ from the Gaussian distribution

$$P_\pi = e^{(\pi, \pi)/2} / Z$$

3. Solve Hamilton equations for a time τ

$$(\pi(0), U(0)) \rightarrow (\pi(\tau), U(\tau))$$

4. Repeat 2. and 3. taking $U(0) = U(t)$



Fermions in simulations

Lattice QCD path-integral

$$\begin{aligned}\langle O \rangle &= \frac{1}{Z} \int D\mathbf{U} D\bar{\psi} D\psi e^{-S_g[\mathbf{U}]} e^{-\bar{\psi} D[\mathbf{U}] \psi} O[\mathbf{U}, \bar{\psi}, \psi] \\ &= \frac{1}{Z} \int D\mathbf{U} e^{-S_g[\mathbf{U}]} \det(D[\mathbf{U}]) O[\mathbf{U}]\end{aligned}$$

Fermionic observable via generating function:

$$O[\mathbf{U}, \bar{\psi}, \psi] \rightarrow O'[\mathbf{U}] = O \left[\mathbf{U}, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \bar{\eta}} \right] e^{\bar{\eta} D^{-1}[\mathbf{U}] \eta}$$

Determinant as observable:

$$\langle O \rangle = \frac{\langle \det(D[\mathbf{U}]) O'[\mathbf{U}] \rangle}{\langle \det D[\mathbf{U}] \rangle}$$

- Calculation of $\det(D[\mathbf{U}])$ requires $O(V^3)$ operations
- Overlap problem $\rightarrow$ large statistical fluctuations

Fermions in simulations

Lattice QCD path-integral

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Fermionic observable via generating function

$$O[\mathbf{U}, \bar{\psi}, \psi] \rightarrow O'[\mathbf{U}] = O \left[\mathbf{U}, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \bar{\eta}} \right] e^{\bar{\eta} D^{-1}[\mathbf{U}] \eta}$$

Determinant in Metropolis

$$P_A \propto e^{-S_g[\mathbf{U}'] - S_g[\mathbf{U}]} \frac{\det D[\mathbf{U}']}{\det D[\mathbf{U}]}$$

- for a single link update $\det(D[\mathbf{U} + \delta\mathbf{U}]D[\mathbf{U}]^{-1})$ for a full sweep follows proportional to V^2
- $\det D[\mathbf{U}]$ must be real and positiv

Fermions in simulations

Lattice QCD path-integral

$$\begin{aligned}\langle O \rangle &= \frac{1}{Z} \int D\mathbf{U} D\bar{\psi} D\psi e^{-S_g[\mathbf{U}]} e^{-\bar{\psi} D[\mathbf{U}] \psi} O[\mathbf{U}, \bar{\psi}, \psi] \\ &= \frac{1}{Z} \int D\mathbf{U} e^{-S_g[\mathbf{U}]} \det(D[\mathbf{U}]) O[\mathbf{U}]\end{aligned}$$

Fermionic observable

$$O[\mathbf{U}, \bar{\psi}, \psi] \rightarrow O'[\mathbf{U}] = O \left[\mathbf{U}, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \bar{\eta}} \right] e^{\bar{\eta} D^{-1}[\mathbf{U}] \eta}$$

Determinant as effective action

$$S^{\text{eff}} = -\text{tr} \ln(D[\mathbf{U}]) \quad \Rightarrow \quad F^{\text{eff}} = -\text{tr}(D[\mathbf{U}]^{-1} \partial D[\mathbf{U}])$$

- Difficult and impractical to make the algorithm efficient (and exact)
- $\det D[\mathbf{U}]$ must be real and positiv

Fermions in simulations

Pseudofermions [Weingarten, Petcher 81]

$$\det(D)^2 = \det(Q^2) \propto \int D\phi^\dagger D\phi e^{-\phi^\dagger Q^{-2} \phi} \quad [Q = \gamma_5 D = Q^\dagger]$$

- $\det Q^2$ is expressed in terms of a bosonic Gaussian integral with pseudo-fermions interacting non-locally

$$\det(Q)^* = \det(Q^\dagger) = \det Q \in \mathbb{R}$$

but for Wilson quarks not necessarily positive

- positive definite of the fermion kernel is required for the convergence of the integral
- using two degenerate quarks guarantee positive definite operator and allow for an easy pseudo-fermion generation
- more difficult for single quarks

HMC with pseudofermions

Heat-bath

$$P_\eta[\eta] \propto \int D\eta^\dagger D\eta e^{-\eta^\dagger \eta} \Rightarrow \phi = Q\eta \Rightarrow P_\phi[\phi]$$

- Generate pseudo-fermions from Gaussian fields between HMC steps
- Averaging results over many trajectories effectively samples the contribution from the pseudofermion integral

Hamiltonian

$$H = \frac{1}{2}(\pi, \pi) + S \quad S = S_g + S_{\text{pf}} \quad S_{\text{pf}} = (Q^{-1}\phi, Q^{-1}\phi)$$

with the Dynamics: $\partial_t U(x, \mu) = \pi(x, \mu)U(x, \mu) \quad \partial_t \pi(x, \mu) = -F(x, \mu) \quad \text{with} \quad F^a(x, \mu) =$

Idea: pseudofermions are held fixed during the Hamiltonian evolution (not additional momentas needed)

Fermionic forces

$$0 = \partial(M^{-1}M) = \partial M^{-1} \cdot M + M^{-1} \partial M \implies \partial M^{-1} = -M^{-1}(\partial M)M^{-1}$$

$$F_{\text{pf}}^a{}_{x,\mu} = \partial^a{}_{x,\mu}(\psi, \psi) = -2\text{Re}(\chi, (\partial^a{}_{x,\mu}Q)\psi) \quad \text{with} \quad \psi = Q^{-1}\phi \quad \text{and} \quad \chi = Q^{-1}\psi$$

Challenges of simulating fermions

Fermionic forces

- Single pseudofermion HMC is not efficient. **Namely:**

$$F_{\text{pf}} = (\phi, \partial Q^{-2} \phi) \quad \text{vs.} \quad F_{\text{F}}^{\text{eff}} = -2\partial(\text{tr} \ln(Q))$$

F_{pf} is a stochastic estimate of F^{eff} at the start of the trajectory $\langle F_{\text{pf}} \rangle = F_{\text{F}}^{\text{eff}}$

- F_{pf} has very large fluctuations

$$\|F_{\text{pf}}\| \gg \|F_{\text{F}}^{\text{eff}}\| \implies \text{var}(\|F_{\text{pf}}\|) \gg \text{var}(F_{\text{F}}^{\text{eff}})$$

- **Recall** the shadow Hamiltonian

$$\Delta H_{\text{OMF2}} = (c_1 \|F\|^2 + c_2 \pi^2 \partial^2 S) h^2 + O(h^4)$$

$$\text{large var}(\|F_{\text{pf}}\|) \Rightarrow \text{large var}(\Delta H) \Rightarrow \text{low } P_A \Rightarrow \text{small } h$$

- large forces also trigger instabilities more easily $\rightarrow$ limits the step size h

$\Rightarrow$ try/use similar preconditioners idea like for Krylov solvers (separation of IR and UV modes)

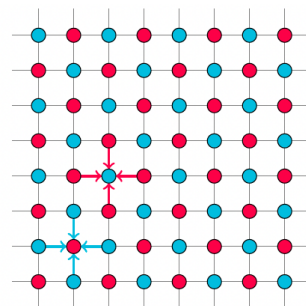
Even-odd reduction/preconditioning

If D only connects nearest-neighboring sites the fermionic problem can be effectively reduced to half of the lattice

Checkerboard decomposition

Even or odd point

Schur decomposition



$$D = \begin{bmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{bmatrix} \quad \det D = \det \hat{D} \det D_{oo} \quad \hat{D} = D_{ee} - D_{eo} D_{oo}^{-1} D_{oe}$$

Even-odd action

$$S_{\text{pf}} \rightarrow S_{\text{pfe}} + S_{\text{det}} = (\hat{Q}^{-1} \phi_e, \hat{Q}^{-1} \phi_e) - 2\text{tr} \ln(Q_{oo})$$

- S_{pfe} involves pseudo-fermions residing only on the even sites of the lattice, helps in speed and reducing fluctuations
- S_{det} and corresponding force can be evaluated exactly, i.e., without introducing pseudofermions
 - leads to a speed-up of ~ 2

Hasenbusch mass-preconditioning

Frequency splitting [*Hasenbusch 01, Hasenbusch, Jansen 03*]

$$\det(Q^2) = \det(Q^2 + \mu^2) \prod_{k=0}^{n-1} \det\left(\frac{Q^2 + \mu_k^2}{Q^2 + \mu_{k+1}^2}\right) \quad 0 = \mu_0 < \dots < \mu_n$$

Actions and forces

$$S_{\text{pf},n} = (\phi_n, (Q^2 + \mu_n^2)^{-1} \phi_n)$$

$$S_{\text{pf},k} = (\phi_k, (Q^2 + \mu_{k+1}^2)(Q^2 + \mu_k^2)^{-1} \phi_k) \quad k = 0, \dots, n-1$$

$$(F_{\text{pf},k})^a(x, \mu) = -2(\mu_{k+1}^2 - \mu_k^2) \text{Re}(\chi_k, (\partial_{x,\mu}^a Q) \psi_k)$$

- A proper tuning of μ can lead to a significant improvement
- smaller $\text{var}(\|F_{\text{pf}}\|) \Rightarrow$ smaller $\text{var}(\Delta H) \Rightarrow$ larger $P_A \Rightarrow$ larger h
- for QCD, at the physical point,

$$\mu_1 \sim m_q; \quad \mu_{k+1} \sim 10\mu_k$$

Typically $\|F_{\text{pf},k+1}\| \gg \|F_{\text{pf},k}\|$ while opposite for their cost, multiple time-step integration is useful

Single-quark determinante [Kennedy et al. 98, Clark, Kennedy 03]

$$\det(Q) \rightarrow \det(\sqrt{Q^2}) = \det(W) \det R^{-1} \quad W = |Q|R$$

where $R = r_b R^{n,\epsilon} (r_b^{-2} Q^2)$, $\epsilon = (r_a/r_b)^2$ and $\lambda(|Q|) \in [r_a, r_b]$

Rational approximation

$$R^{n,\epsilon}(x) = A \frac{(x + a_1) \cdots (x + a_{2n-1})}{(x + a_2) \cdots (x + a_{2n})} \approx \frac{1}{\sqrt{x}} \quad a_1 > \dots > a_{2n} > 0$$

- Zolotarev rational function of degree (n,n)
- Guarantees smallest possible $\delta = \max_{\epsilon \leq x \leq 1} |1 - \sqrt{x} R^{n,\epsilon}(x)|$

Frequency splitting (e.g. $n = 10$)

$$\det(R^{-1}) \propto \det(P^{-1}_{1,4}) \det(P^{-1}_{5,7}) \det(P^{-1}_{8,10})$$

$$\text{with} \quad P_{k,l} = \prod_{j=k}^l \frac{Q^2 + \nu_j^2}{Q^2 + \mu_j^2} = 1 + \sum_{j=k}^l \frac{\rho_j}{Q^2 + \mu_j^2} \quad \mu_1 > \dots > \mu_n$$

Actions and forces

$$S_{\text{pf}, k, l} = (\phi_{k, l}, P_{k, l} \phi_{k, l}) \quad (F_{\text{pf}, k, l})^a(x, \mu) = \partial^a_{x, \mu} S_{\text{pf}, k, l}$$

Remarks

- We have to ensure $\det(Q) > 0$ this is ensured by measure the spectral range $[r_a, r_b]$ of Q^2
If that fails, sign flip need to be included as a reweighting factor (on some CLS ensembles thats the case [*Mohler, Schaefer 19*])
- Choose a large enough n to have a good approximation of R
- For Wilson quarks the RHMC is typically used for heavy quarks, (charm and strange), for staggered it required for taking 4th root
- $\det(W)$ can be included in the accept-reject step or in the observable as a reweighting factor. It can be estimated stochastically

$$\langle O \rangle_{|Q|} = \frac{\langle OW \rangle_{R^{-1}}}{\langle W \rangle_{R^{-1}}} \quad W = \langle e^{-\eta^\dagger [(1+Z)^{-1/2} - 1] \eta} \rangle_P$$

Critical slowing down

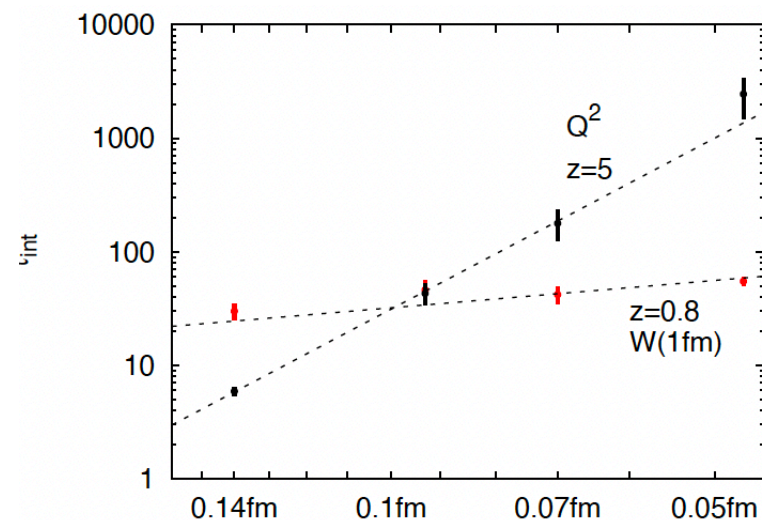
Approaching the continuum limit

$$\tau^{\text{int},0} \propto a^{-z}$$

where z depends on the algorithms

certain algorithms can be analyzed as QFTs :

- Simulation time is the $(D+1)$ th dimension
[Parisi, Wu 81, Zinn-Justin 86]
- HMC can not be analyzed this way:
empirically $z = 2$
- this might be true if topology issue is absent



[Schaefer, Virota, et al. 2010]

Approaching the continuum limit at constant physics, the cost to obtain a set of statistical independent configurations scales like

$$C \propto V a^{-4} \quad V^{1/8} a^{-1/2} \quad a^{-z} \propto V^{9/8} a^{-4.5-z}$$

where the first term comes from the solver, the second from the integrator and the third from the autocorrelation

- Open boundary conditions: $z=2$, Periodic boundary conditions $z=5$
 - note that topological charge need to diffuse into lattice in case of OBC, leads to $\tau^{\text{int}} \approx O(10^2)$ at $a \sim 0.05$ at physical point [McGlynn, Mawhinney, 2014]

On a GPU machine with nodes each with 4*Mt250 costs are roughly given:

- $O(1000)$ trajectories
- A physical volume of $L=7.3$ fm and $a=0.057$ fm
- $N_f=2+1+1$ twisted mass fermions at physical masses

$$C \approx 0.5 \text{ Mt node hours on Lumi-G}$$

Challenges are at the horizon and they waiting **to be solved** !!!

- topological freezing not sufficient solved (at least at physical pion masses)
- algorithmic challenges, e.g. chiral fermions like overlap fermions, very large lattices
- signal to noise and excited states
- and sampling with a sign

Looking forward to your contributions !!!

For HMC there are advance techniques:

- tuning of optimal solver methods, of kernels for GPU systems,...
- higher order integrators, force gradient integrators,...
- domain decomposition, multi-level sampling , master fields ...
- combination with flows ...

See for some current challenges (mentioned in some recent reviews) see:

- Peter Boyle [*Advances in algs for solvers and sim.* <https://arxiv.org/abs/2401.16620>]
- Gurtej Kanwar [*Flow-based sampling for LFT* <https://arxiv.org/abs/2401.01297>]
- J.F. [*Future trends in LQCD sim.* <https://cds.cern.ch/record/2928997>]
- J.F. [*Reviews on Algs for dyn. fermions.* <https://arxiv.org/abs/2402.11704>]

References

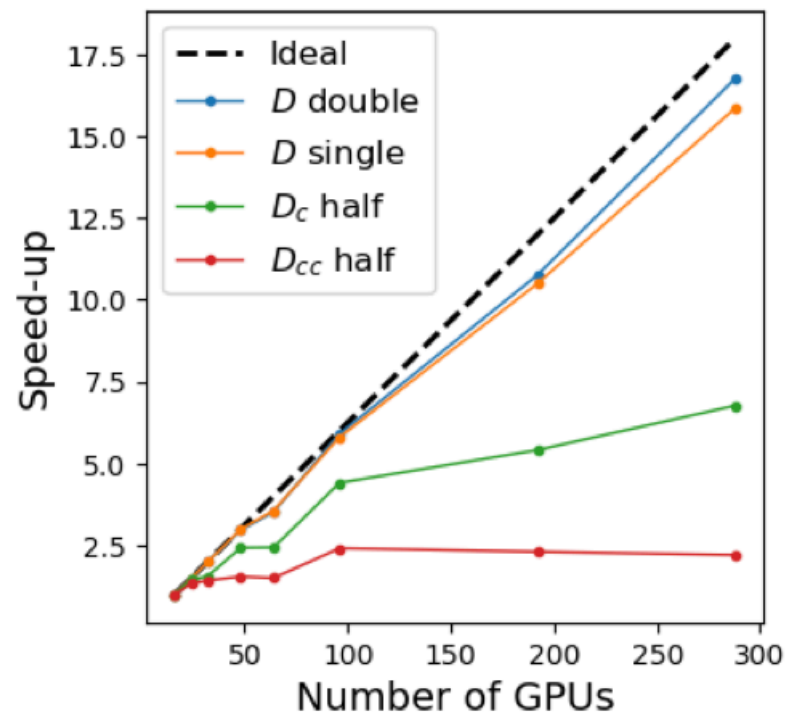
- Some part of the talk is based on Mattia Della Brida's Lattice Practice Contribution of 2021

Other references:

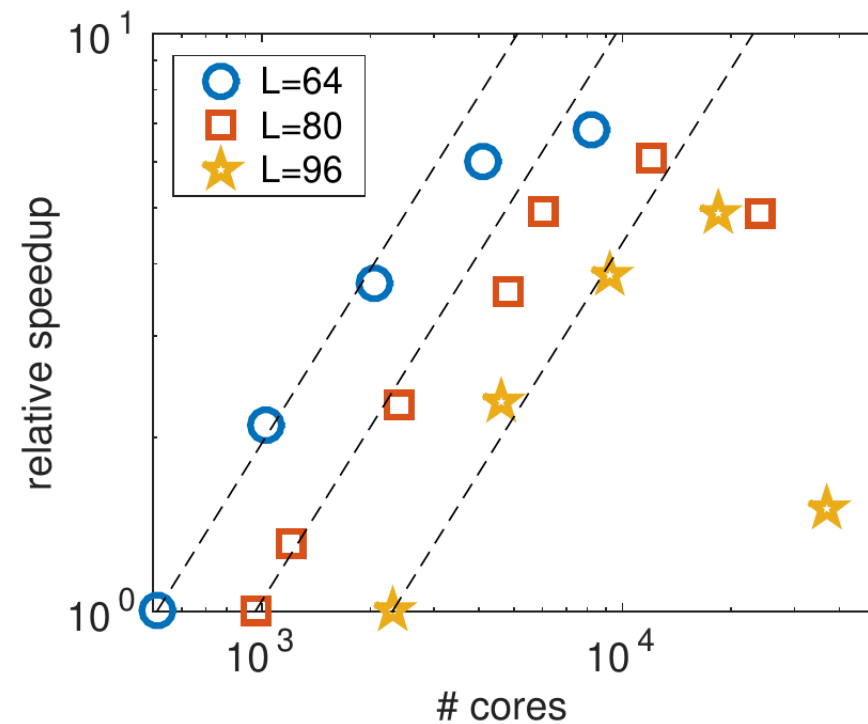
- M. Lüscher, Computational Strategies in Lattice QCD, in Les Houches Summer School: Session 93: Modern perspectives in lattice QCD: Quantum field theory and high performance computing, pp. 331–399, 2, 2010, 1002.4232.
- A. D. Kennedy, Algorithms for dynamical fermions, hep-lat/0607038.
- S. Schaefer, Simulations with the hybrid Monte Carlo algorithm: Implementation and data analysis, in Les Houches Summer School: Session 93: Modern perspectives in lattice QCD: Quantum field theory and high performance computing, pp. 401–422, 8, 2009.
- S. Schaefer, Simulation Algorithms, Lattice Practices 2018
- S. Schaefer, Status and challenges of simulations with dynamical fermions, PoS LATTICE2012 (2012) 001, [1211.5069].
- S. Duane, A. D. Kennedy, B. J. Pendleton and D. Roweth, Hybrid Monte Carlo, Phys. Lett. B 195 (1987) 216–222.
- A. Barp, F.-X. Briol, A. D. Kennedy and M. Girolami, Geometry and Dynamics for Markov Chain Monte Carlo, 1705.0289
- ALPHA collaboration, U. Wolff, Monte Carlo errors with less errors, ComputPhys. Commun. 156 (2004) 143–153, [hep-lat/0306017].
- ALPHA collaboration, S. Schaefer, R. Sommer and F. Virotta, Critical slowingdown and error analysis in lattice QCD simulations, Nucl. Phys. B 845 (2011) 93–119, [1009.5228].

Scaling of multi-grid

Scaling of operators within the multi-grid procedure (QUDA, Juwels Booster)

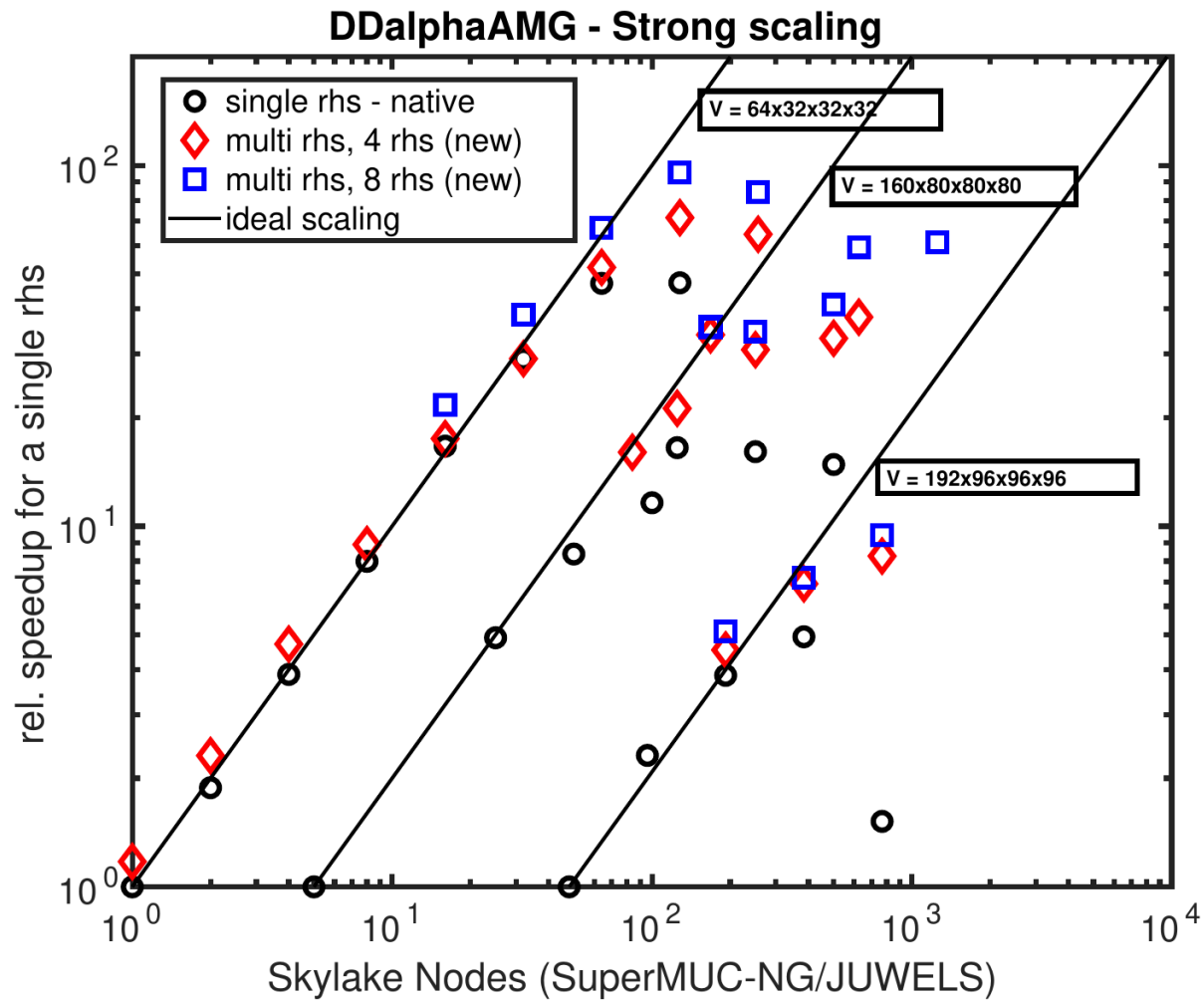


Scaling of the multi-grid solver (DDalphaAMG, SuperMUC-NG)



Remarks

Improve scaling via multi-rhs



Parameter example for ETMC cB48 - lattice for QUDA

```
./quda/test/invert_test \  
--compute-clover 1 --verbosity verbose --epsilon 0.0 --solve-type direct-pc --dslash-type twisted-  
--dim ${XDIM} ${YDIM} ${ZDIM} ${TDIM} --gridsize ${XGRID} ${YGRID} ${ZGRID} ${TGRID} \  
--load-gauge conf.1000 --prec double --prec-sloppy single --prec-precondition half \  
--prec-null half --recon 12 --recon-sloppy 8 --recon-precondition 8 \  
--kappa 0.1394265 --mu 0.00072 --clover-csw 1.69 \  
--mass-normalization mass --pipeline 24 --ngcrkrylov 24 \  
--niter 1000 --tol 1.0e-9 --inv-multigrid true --inv-type gcr --nsrc 120 \  
--mg-levels 3 --mg-mu-factor 2 1.0 \ # 3 level multigrid - fine (0) + intermediate (1) + coarsest  
--mg-setup-tol 0 5e-7 --mg-setup-tol 1 5e-7 --mg-setup-maxiter 0 1000 \  
--mg-setup-maxiter 1 1000 --mg-setup-inv 0 cg --mg-setup-inv 1 cg \  
--mg-setup-iters 0 1 --mg-pre-orth false --mg-post-orth true \  
--mg-block-size 0 4 4 4 4 --mg-block-size 1 2 2 2 2 \ # blocking from 0 → 1 and 1 → 2  
--mg-nu-pre 0 0 --mg-nu-pre 1 0 --mg-nu-post 0 4 --mg-nu-post 1 2 \  
--mg-verbosity 0 silent --mg-verbosity 1 silent --mg-verbosity 2 silent \  
--mg-verbosity 3 silent --mg-omega 0.85 --mg-smoother 0 ca-gcr --mg-smoother 1 ca-gcr \  
--mg-nvec 0 24 --mg-nvec 1 32 --mg-smoother-tol 0 0.22 --mg-smoother-tol 1 0.46 \  
--mg-schwarz-cycle 0 1 --mg-schwarz-cycle 1 1 --mg-coarse-solver 2 ca-gcr --mg-coarse-solver-ca-b  
--mg-coarse-solver-tol 1 0.22 --mg-coarse-solver-tol 2 0.46 --mg-coarse-solver-maxiter 2 50 \  
--mg-eig 2 true --mg-eig-type 2 trlm \ #exact deflation on coarse level  
--mg-eig-n-ev 2 1000 --mg-nvec 2 1000 \  
--mg-eig-require-convergence 2 false --mg-eig-n-kr 2 1500 \  
--mg-eig-tol 2 1e-4 --mg-eig-poly-deg 2 100 --mg-eig-amin 2 6e-2 \  
--mg-eig-amax 2 8.0 --mg-eig-max-restarts 2 8 \  
--mg-eig-use-dagger 2 false --mg-eig-use-normop 2 true \  
--mg-eig-preserve-deflation true
```