Worldvolume Hybrid Monte Carlo method for lattice gauge theories

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Lattice 2026

July 28, 2026 @ Univ of Maryland

[Ref]

M. Fukuma
"Worldvolume Hybrid Monte Carlo algorithm for group manifolds"
[arXiv:2506.12002]

M. Fukuma
"Worldvolume Hybrid Monte Carlo algorithm for LGTs" (in prep)

Sign problem (1/2)

Sign problem :
major obstacle to first-principles computations of various problems

Examples

- finite-density QCD
- Quantum Monte Carlo in condensed-matter physics
  (strongly correlated electron systems, frustrated spin systems)
- finite θ term (topological term)
- real-time dynamics of quantum many-body systems

Sign problem (1/2)

Sign problem :
major obstacle to first-principles computations of various problems

Examples

WV-HMC for the doped Hubbard model
[MF-Namekawa, 2507.23748, 2508.02659]

- finite-density QCD **LGT**
- Quantum Monte Carlo in condensed-matter physics
  (strongly correlated electron systems, frustrated spin systems)
- finite θ term (topological term) **LGT**
- real-time dynamics of quantum many-body systems

Today's talk

Formulation of Worldvolume HMC for pure LGTs
(with a new GPU-oriented codebase built from scratch)

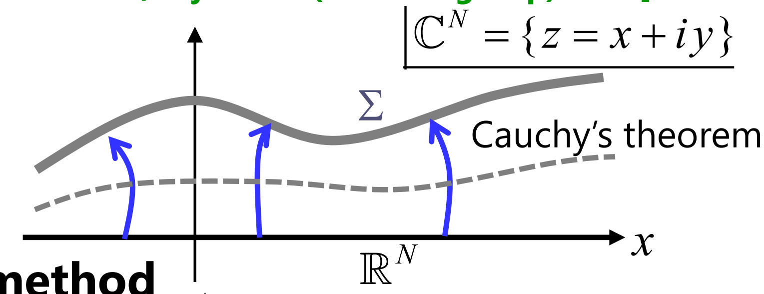
Sign problem (2/2)

■ **Lefschetz thimble method** [Witten 2010, Cristoforetti et al. 2012, Fujii et al. (Komaba group) 2013]

Generalized thimble method [Alexandru et al. 2015]

Deform the integ surface $\mathbb{R}^N$ into $\Sigma (\in \mathbb{C}^N)$

on which the oscillatory behavior is mild

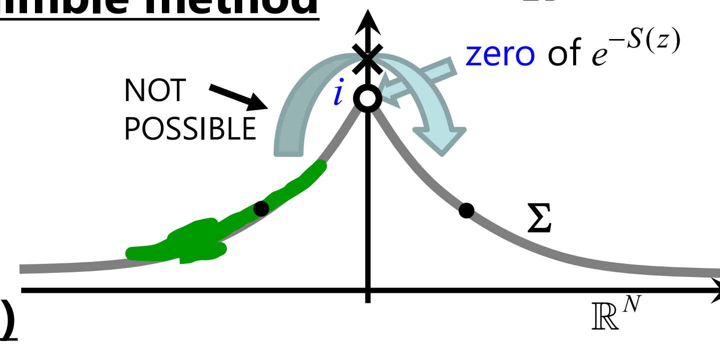


■ **Ergodicity problem in the Lefschetz thimble method**

Example : $e^{-S(z)} = e^{-(1/2)z^2}(z - i)$

zero of the Boltzmann weight

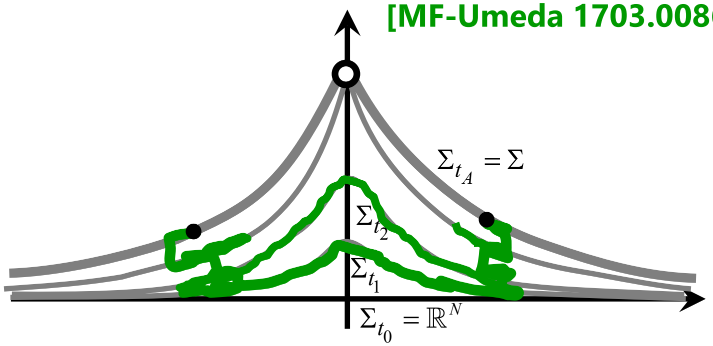
$\Leftrightarrow$ infinitely high potential barrier



■ **Solution : prepare detours (tempering)**

Tempered Lefschetz thimble method

[MF-Umeda 1703.00861]

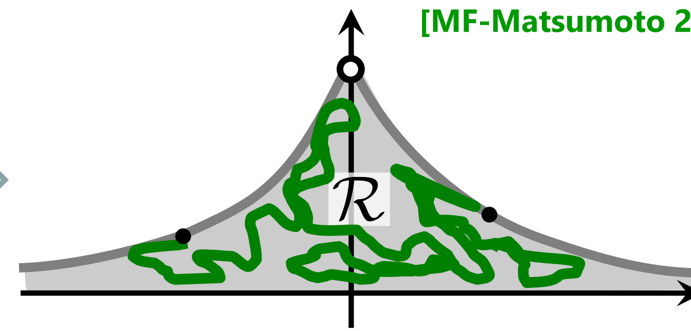


- Treat flow time as an extra dyn variable
- First algorithm that solves the sign and ergodicity problems simultaneously

WV-HMC

Worldvolume Hybrid Monte Carlo method

[MF-Matsumoto 2012.08468]



- Performs HMC on the worldvolume that is a continuous union of replicas
- Reduces comput cost significantly

Picard-Lefschetz theory for group manifolds

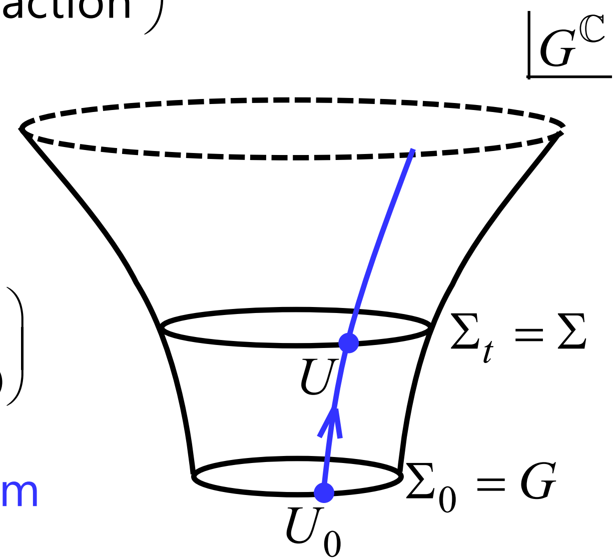
[MF 2506.12002]

$G=\{U_0\}$: <u>compact Lie group</u> ($N\equiv\dim G$: #dof)

We want to evaluate:

$$\boxed{\langle\mathcal{O}\rangle\equiv\frac{\int_G (dU_0)\, e^{-S(U_0)}\mathcal{O}(U_0)}{\int_G (dU_0)\, e^{-S(U_0)}}}\qquad\begin{pmatrix}U_0\in G : \text{dynamical variable}\\ S(U_0)\in\mathbb{C} : \text{complex action}\end{pmatrix}$$

Haar measure



$G^{\mathbb{C}}$: <u>complexification of G</u>

$$\begin{pmatrix}\mathfrak{g}=\bigoplus_a \mathbb{R}T_a \quad\Rightarrow\quad \mathfrak{g}^{\mathbb{C}}=\bigoplus_a \mathbb{C}T_a\\ G^{\mathbb{C}}\equiv\{e^Z e^{Z'}\cdots e^{Z''}\,|\,Z,Z',\ldots,Z''\in\mathfrak{g}^{\mathbb{C}}\}\end{pmatrix}\qquad\begin{pmatrix}G=SU(n)\\ \Rightarrow G^{\mathbb{C}}=SL(n,\mathbb{C})\end{pmatrix}$$

Cauchy's theorem

Haar measure

holomorphic N-form

$$\boxed{\langle\mathcal{O}\rangle=\frac{\int_G (dU_0)\, e^{-S(U_0)}\mathcal{O}(U_0)}{\int_G (dU_0)\, e^{-S(U_0)}}=\frac{\int_\Sigma (dU)_\Sigma\, e^{-S(U)}\mathcal{O}(U)}{\int_\Sigma (dU)_\Sigma\, e^{-S(U)}}}\qquad\begin{pmatrix}\theta=dUU^{-1}=T_a\theta^a\ \text{(Maurer-Cartan)}\\ \Rightarrow\ (dU)_\Sigma\equiv\theta^1\wedge\cdots\wedge\theta^N\end{pmatrix}$$

anti-holomorphic gradient flow

$$\boxed{\dot U=DS(U)^\dagger U\ \text{ with } U|_{t=0}=U_0}\qquad\left(\delta S(U)=\mathrm{tr}\left[\left(\delta UU^{-1}\right)DS(U)\right]\ \left(DS(U)\in\mathfrak{g}^{\mathbb{C}}\right)\right)$$

Path integral over the worldvolume

same as [MF-Matsumoto 2012.08468] [MF 2506.12002]

$$\langle \mathcal{O} \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)} \mathcal{O}(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}}$$

⇦ t-independent

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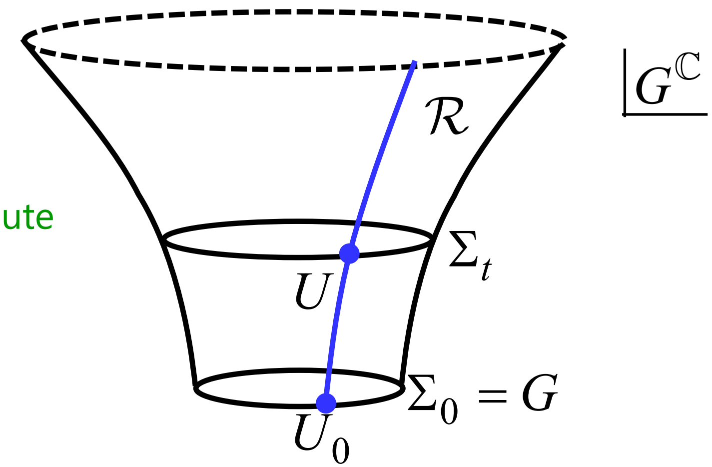
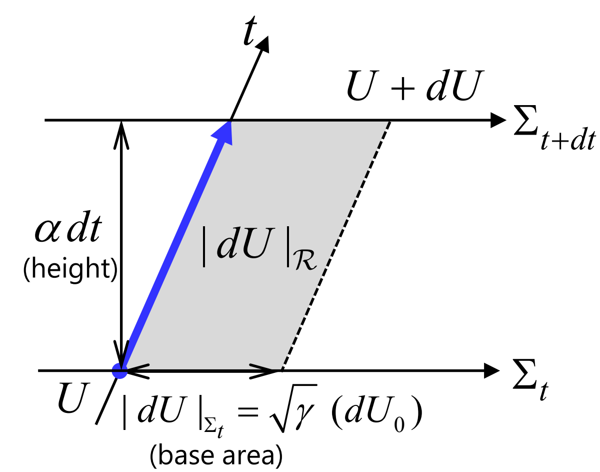


$$= \frac{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)} \mathcal{O}(U)}{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}}$$

$W(t)$: chosen s.t. configs distribute almost uniformly over t

$$= \frac{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)} \mathcal{F}(U) \mathcal{O}(U)}{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)} \mathcal{F}(U)}$$

$$\left(\begin{aligned} &V(U) = \mathrm{Re}\, S(U) + W(t(U)) \\ &\mathcal{F}(U) = \frac{dt\,(dU)_{\Sigma_t}}{|dU|_{\mathcal{R}}} e^{-i\,\mathrm{Im}\, S(U)} = \alpha^{-1} \frac{\det E}{\sqrt{\gamma}} e^{-i\,\mathrm{Im}\, S(U)} \end{aligned} \right)$$



$$\left(ds_\Sigma^2 = \mathrm{Re}\,\mathrm{tr}\,\theta_{\Sigma_t}^\dagger \theta_{\Sigma_t} = \gamma_{ab} \theta_0^a \theta_0^b \right)$$

introduce momentum (velocity) π

$$= \frac{\int_{T\mathcal{R}} d\Omega\, e^{-H(U,\pi)} \mathcal{F}(U) \mathcal{O}(U)}{\int_{T\mathcal{R}} d\Omega\, e^{-H(U,\pi)} \mathcal{F}(U)} \qquad \left(H(U,\pi) = \frac{1}{2} \mathrm{tr}\, \pi^\dagger \pi + V(U) \right)$$

Phase space : **tangent bundle of $\mathcal{R}$**

$$T\mathcal{R} \equiv \{ (U,\pi) \,|\, U \in \mathcal{R},\ \pi \in T_U \mathcal{R} \}$$

symplectic form $\omega = d\langle \pi, dU U^{-1} \rangle \Rightarrow$ symplectic volume form $d\Omega = \frac{1}{(N+1)!} \omega^{N+1}$

Molecular dynamics over $T\mathfrak{R}$

[MF 2506.12002]

Algorithm

(i) inital momentum

① $\tilde{\pi} = (\tilde{\pi}^i) \in T_U G^{\mathbb{C}} \leftarrow e^{-\mathrm{tr}\,\tilde{\pi}^\dagger \tilde{\pi}/2}$

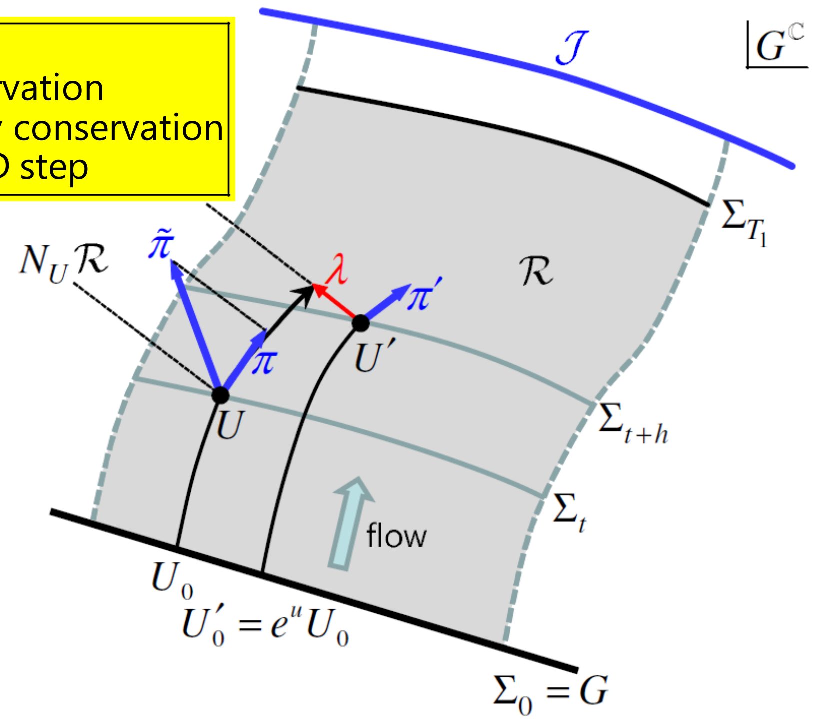
② $\tilde{\pi} \to \pi \in T_U \mathcal{R}$

- exact reversibility
- exact volume preservation
- approximate energy conservation to $O(\Delta s^2)$ at one MD step

(ii) constrained MD (RATTLE)

$$\begin{cases} \pi_{1/2} = \pi - \Delta s [DV(U)]^\dagger - \lambda \\ U' = e^{\epsilon(\pi_{1/2} - \pi_{1/2}^\dagger)} e^{\epsilon \pi_{1/2}^\dagger} U \\ \pi' = e^{\epsilon(\pi_{1/2} - \pi_{1/2}^\dagger)} \pi_{1/2} e^{-\epsilon(\pi_{1/2} - \pi_{1/2}^\dagger)} - \Delta s [DV(U')]^\dagger - \lambda' \end{cases}$$

where $\begin{cases} \lambda \in N_U \mathcal{R} \ \ \text{s.t.} \ \ U' \in \mathcal{R} \\ \lambda' \in N_{U'} \mathcal{R} \ \ \text{s.t.} \ \ \pi' \in T_{U'} \mathcal{R} \end{cases}$



(iii) Metropolis test

after repeating MD,

we update config from U to U' with prob $\min\left(1, e^{-H(U',\pi') + H(U,\pi)}\right)$

(iv) measurement

we estimate observables from the subsample

in a subregion $\widetilde{\mathcal{R}} = \left\{ U \in \mathcal{R} \,\middle|\, \tilde{T}_0 \le t(U) \le \tilde{T}_1 \right\}$

Molecular dynamics over $T\mathcal{R}$

[MF 2506.12002]

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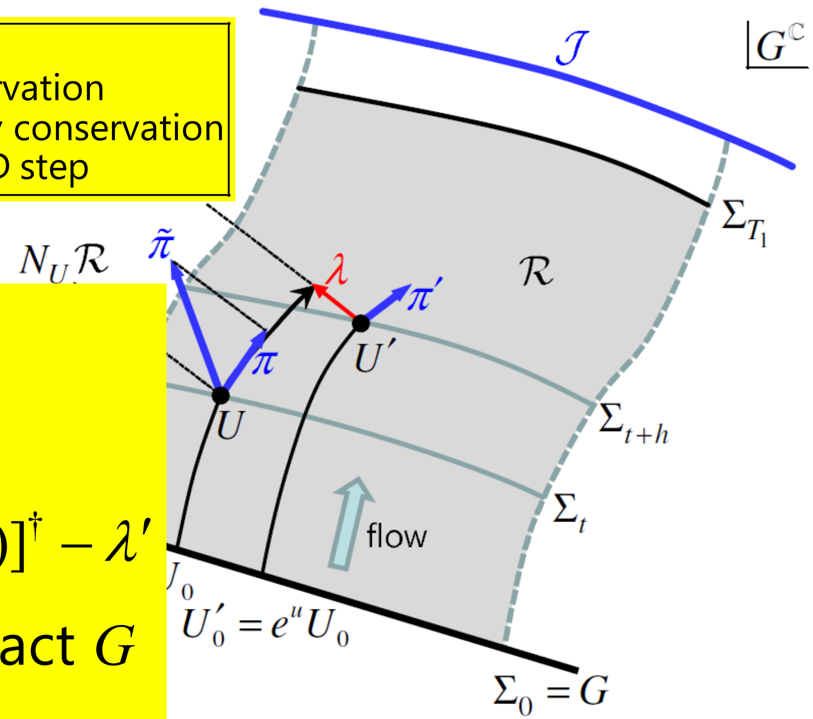
agrees with the standard MD for compact G (where $\pi_{1/2}^\dagger = -\pi_{1/2}$ and $\lambda = \lambda' = 0$)



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Group-manifold structure in lattice gauge theory

[MF (in prep)]

Gauge group

$$\begin{cases} \bar{G} \text{ : compact group } \left(\text{e.g. } \bar{G} = SU(n)\right) \\ \bar{\mathfrak{g}} = \bigoplus_a \mathbb{R} T_a \quad \text{with} \begin{cases} T_a^\dagger = -T_a \\ \mathrm{tr}\, T_a T_b = -\delta_{ab}, \\ [T_a,\ T_b] = C_{ab}{}^c\, T_c \end{cases} \end{cases}$$

Configuration space in LGT : **product group**

$$\begin{cases} G = \prod_{x,\mu} \underset{}{\overset{\bar{G}}{\overset{\shortparallel}{G_{x,\mu}}}} \ni\ U_0 = \left((U_0)_{x,\mu}\right) \\ \mathfrak{g} = \bigoplus_{x,\mu} \underset{\underset{\bar{\mathfrak{g}}}{\shortparallel}}{\mathfrak{g}_{x,\mu}} = \bigoplus_{x,\mu} \bigoplus_a \mathbb{R}(T_{x,\mu})_a \quad \text{with} \begin{cases} \mathrm{tr}\,(T_{x,\mu})_a (T_{y,\nu})_b = -\delta_{xy}\delta_{\mu\nu}\delta_{ab} \\ [(T_{x,\mu})_a,\ (T_{y,\nu})_b] = \delta_{xy}\delta_{\mu\nu} C_{ab}{}^c (T_{x,\mu})_c \end{cases} \end{cases}$$

Partition function

$$Z = \int_G (dU_0)\, e^{-S(U_0)} \quad \left((dU_0) \equiv \prod_{x,\mu} (d(U_0)_{x,\mu}) \right)$$

Gauge invariance

$$\begin{cases} S(U_0^g) = S(U_0) \\ (dU_0^g) = (dU_0) \end{cases} \quad \text{for} \quad (U_0^g)_{x,\mu} = g_x^{-1} (U_0)_{x,\mu}\, g_{x+\mu} \quad \left(g_x \in \bar{G}\right)$$

Gauge transforamtion group $\left\{ g_x \in \bar{G} \,\middle|\, x \right\}$: "redundancy"

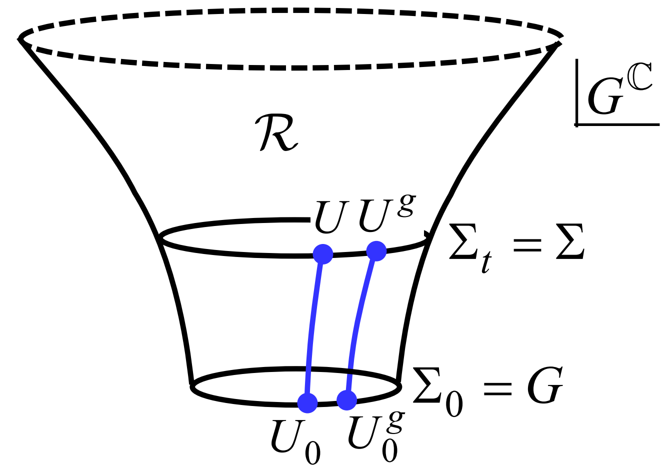
Gauge invariance in WV-HMC

[MF (in prep)]

Anti-holomorphic gradient flow

$$\boxed{\dot{U}_{x,\mu} = DS_{x,\mu}(U)^\dagger\, U_{x,\mu} \ \text{ with } U|_{t=0} = U_0}$$

$$\left(\delta S(U) = \sum_{x,\mu} \mathrm{tr}\left[\left(\delta U_{x,\mu} U_{x,\mu}^{-1}\right) DS_{x,\mu}(U)\right]\right)$$



Gauge invariance for flowed configurations **[MF]**

$$\begin{cases} t(U^g) = t(U) \\ S(U^g) = S(U) \\ (dU^g)_{\Sigma_t} = (dU)_{\Sigma_t} \\ |dU^g|_{\mathcal{R}} = |dU|_{\mathcal{R}} \end{cases} \quad \text{for } U^g_{x,\mu} = g_x^{-1} U_{x,\mu}\, g_{x+\mu} \quad \left(g_x \in \overline{G}\right)$$

NOT $\overline{G}^{\mathbb{C}}$ same redundancy!

Reweighted average on worldvolume $\mathcal{R}$:

$$\langle g(U)\rangle_{\mathcal{R}} \equiv \frac{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)} g(U)}{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)}} \quad \left(\langle \mathcal{O}\rangle = \frac{\langle \mathcal{F}(U)\mathcal{O}(U)\rangle_{\mathcal{R}}}{\langle \mathcal{F}(U)\rangle_{\mathcal{R}}}\right) \quad \left(\begin{array}{l} V(U) = \mathrm{Re}\, S(U) + W(t(U)) \\ \mathcal{F}(U) = \dfrac{dt\,(dU)_{\Sigma_t}}{|dU|_{\mathcal{R}}} e^{-i\,\mathrm{Im}\, S(U)} \end{array}\right)$$

has the same gauge invariance as the original PI!

Application to <u>pure</u> lattice gauge theory

[MF (in prep)]

$$\boxed{S(U) \equiv S_W(U) + S_\theta(U)}$$

Wilson

$$\boxed{S_W(U) \equiv \beta \sum_x e_x} \qquad \left(e_x \equiv -\frac{1}{2n} \sum_{\mu<\nu} \mathrm{tr}\left(U_{x,\mu,\nu} + U_{x,\mu,\nu}^{-1} \right) \right) \quad (\beta \in \mathbb{C})$$

θ term (clover)

$$\boxed{S_\theta(U) \equiv -i\theta \sum_x q_x} \qquad \left(\begin{aligned} q_x &\equiv \frac{1}{32\pi^2} \sum_{\mu,\nu,\rho,\sigma} \epsilon_{\mu\nu\rho\sigma}\, \mathrm{tr}\, F_{x,\mu,\nu} F_{x,\rho,\sigma} \\ F_{x,\mu,\nu} &\equiv \frac{1}{8}\left(U_{x,\mu,\nu} + U_{x,\nu,-\mu} + U_{x,-\mu,-\nu} + U_{x,-\nu,\mu} - (\mu \leftrightarrow \nu) \right) \end{aligned} \right)$$

(only for 4D)

Anti-holomorphic gradient flow

$$\boxed{\dot{U}_{x,\mu} = DS_{x,\mu}(U)^\dagger\, U_{x,\mu} \ \text{ with } U|_{t=0} = U_0} \qquad \left(\delta S(U) = \sum_{x,\mu} \mathrm{tr}\left[\left(\delta U_{x,\mu} U_{x,\mu}^{-1} \right) DS_{x,\mu}(U) \right] \right)$$

local

⇓

Hessian of S : sparse

$$\begin{cases} \text{configuration : } \dot{U} = (DS)^\dagger\, U \\ \text{tangent vector : } \dot{v} = D_v DS + [(DS)^\dagger, v] \\ \text{normal vector : } \dot{n} = -DD_n S - [DS, n] \end{cases}$$

⇓

Expected computational cost : $\boxed{O\left(N [\log N]^{0-2} \right)}$ (N : #DOF $\propto$ volume)

[MF 2311.10663]

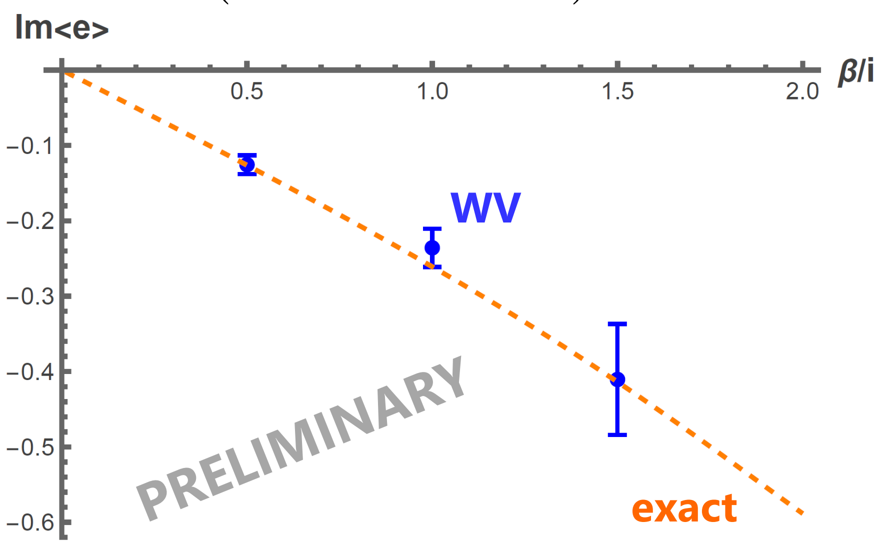
Check of algorithm

[MF (in prep)]

$SU(2)$ Wilson action with $\beta \in i\mathbb{R} \left(\Rightarrow \mathrm{Re}\langle e \rangle = 0 \right)$

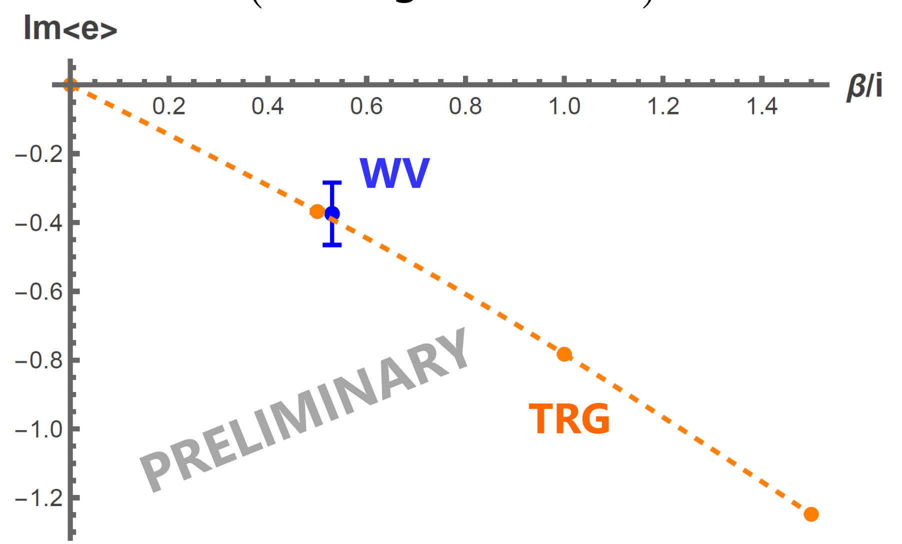
2D : 2x2 (Nconf=200)

(CPU : grid={2,2})



3D : 2x2x2 (Nconf=100)

(CPU : grid={2,2,2})



compared with exact values

$$< e >_{\text{exact}} = -\frac{\partial}{\partial \beta} \ln \sum_{n=1}^{\infty} [(2/\beta) I_n(\beta)]^{\text{vol}}$$

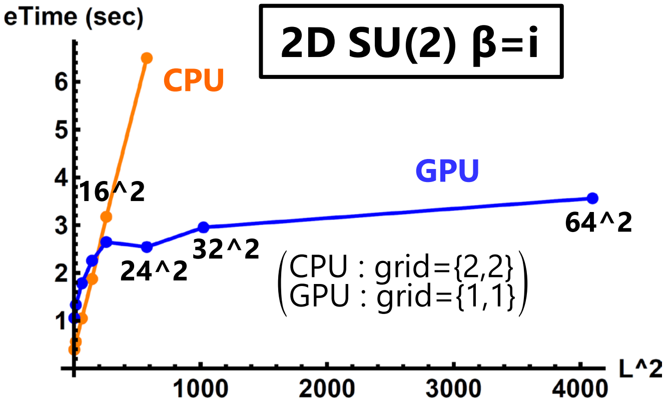
compared with Tensor RG results

[MF-Kuwahara (in prep)]

Kuwahara's talk
16:30, Friday, July 31
Algorithms and AI

Computational cost scaling

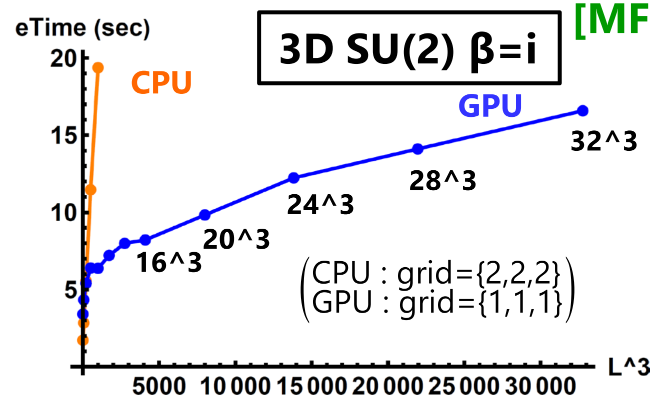
2D SU(2) β=i



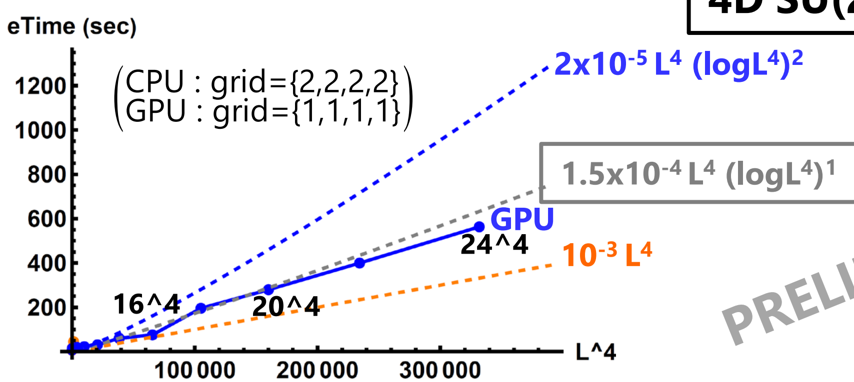
PRELIMINARY

3D SU(2) β=i

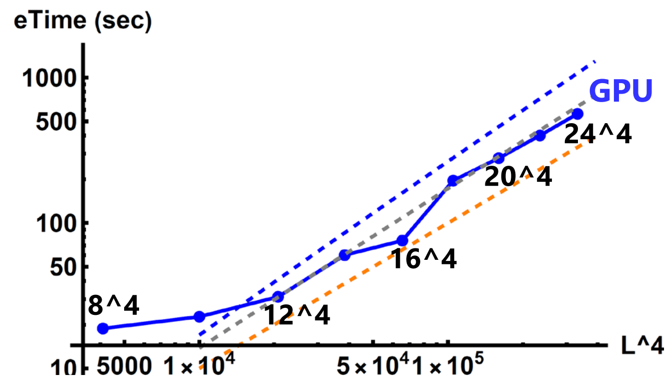
[MF (in prep)]



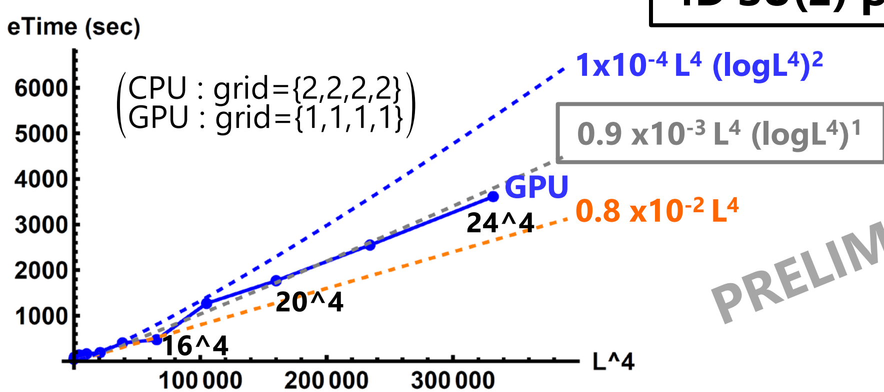
4D SU(2) β=2i



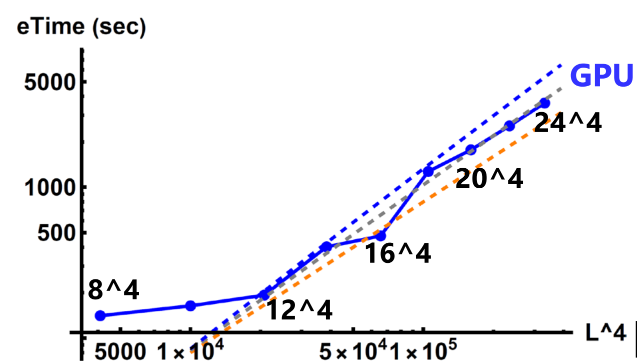
PRELIMINARY



4D SU(2) β=2, θ=π



PRELIMINARY



Summary and outlook

■ **Summary** : Formulated WV-HMC for LGTs using WV algorithm for group manifolds

- exact reversibility & volume preservation $H' = H + O(\Delta s^3)$
- approximate energy conservation to $O(\Delta s^2)$ at one MD step
- w/ a GPU-oriented codebase

$$\begin{pmatrix} G = \prod_{x,\mu} G_{x,\mu} \quad \left(G_{x,\mu} = SU(n)\right) \\ \mathfrak{g} = \bigoplus_{x,\mu} \mathfrak{g}_{x,\mu} \end{pmatrix}$$

■ **Outlook**

▼ Roadmap to **finite-density QCD** with WV-HMC :

✓ local fields (e.g. complex scalars)
✓ group manifolds (e.g. one-site model)
→ ✓ pure YM (w/ finite θ)

✓ fermions (e.g. Thirring, Stephanov, Hubbard)

→ finite-density QCD (w/ or w/o θ) **[MF (ongoing)]**

▼ Developing the algorithm itself **[MF (ongoing)]**

- incorporation of machine learning technique
- incorporation of other algorithm(s)

(e.g.) tensor RG (non-MC) **cf) TRG for YM: [MF-Kadoh-Matsumoto 2107.14149, ..., MF-Kuwahara (in prep)]**

⇨ **Kuwahara's talk**
16:30, Friday, July 31
Algorithms and AI

▼ **Real-time dynamics** of quantum many-body systems **[MF (ongoing)]**

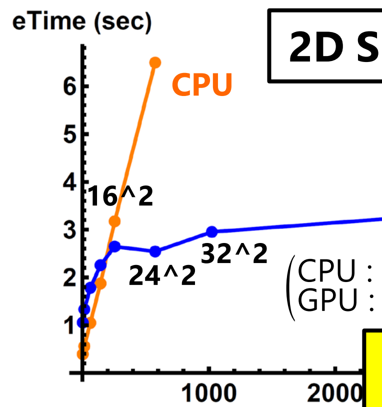
- real-time correlators at finite temperature ⇒ transport coefficients
- light-cone correlators ⇒ PDFs and their generalizations
- non-equilibrium processes

Thank you.

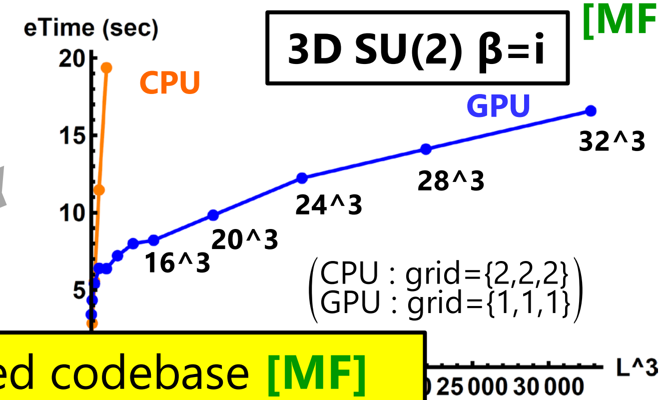
Appendix

Computational cost scaling

2D SU(2) β=i



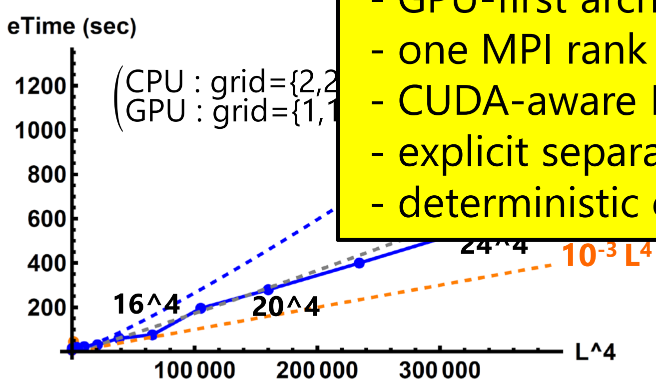
3D SU(2) β=i [MF (in prep)]

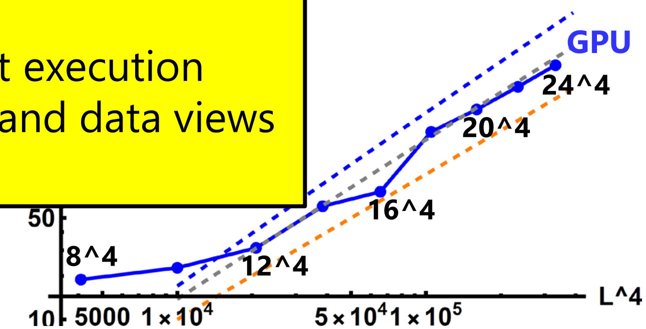


PRELIMINARY

developed a new GPU-oriented codebase **[MF]**

- designed primarily for WV-HMC
- GPU-first architecture built from scratch in C++17
- one MPI rank per GPU
- CUDA-aware MPI with device-resident execution
- explicit separation of data ownership and data views
- deterministic counter-based RNG





PRELIMINARY

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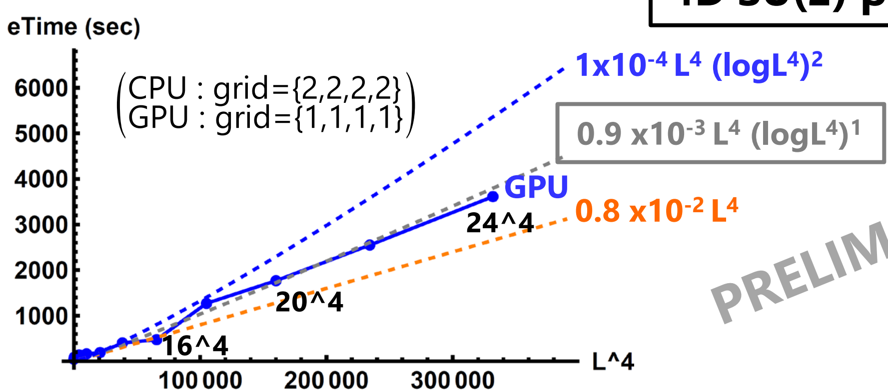

PRELIMINARY