

Worldvolume Hybrid Monte Carlo method for lattice gauge theories

Masafumi Fukuma (Dept Phys, Kyoto Univ)

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[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

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Examples

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(strongly correlated electron systems, frustrated spin systems)
- finite θ term (topological term) **LGT**
- real-time dynamics of quantum many-body systems

WV-HMC for the doped Hubbard model

[MF-Namekawa, 2507.23748, 2508.02659]



Today's talk

Formulation of Worldvolume HMC for pure LGTs

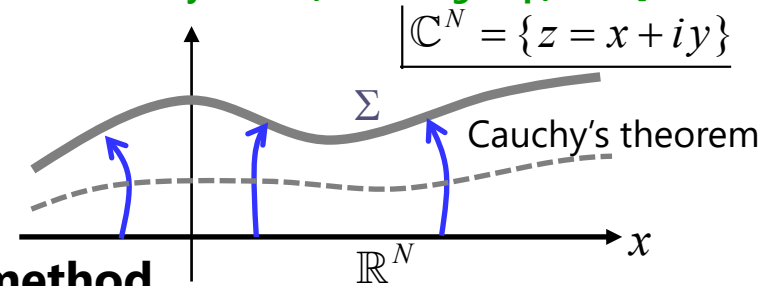
(with a new GPU-oriented codebase built from scratch)

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]

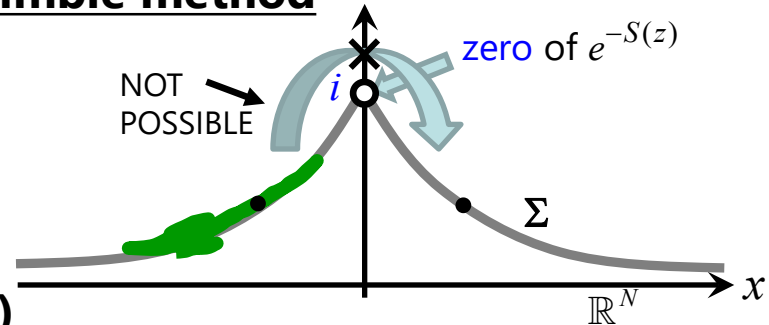
Deform the integ surface $\mathbb{R}^N$ into $\Sigma (\in \mathbb{C}^N)$
on which the oscillatory behavior is mild



■ Ergodicity problem in the Lefschetz thimble method

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

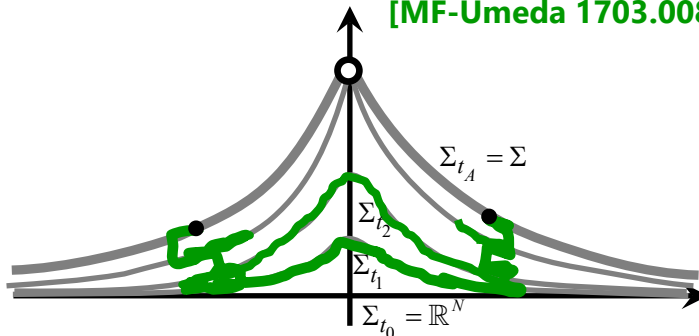
zero of the Boltzmann weight
 $\Leftrightarrow$ infinitely high potential barrier



■ Solution : prepare detours (tempering)

Tempered Lefschetz thimble method

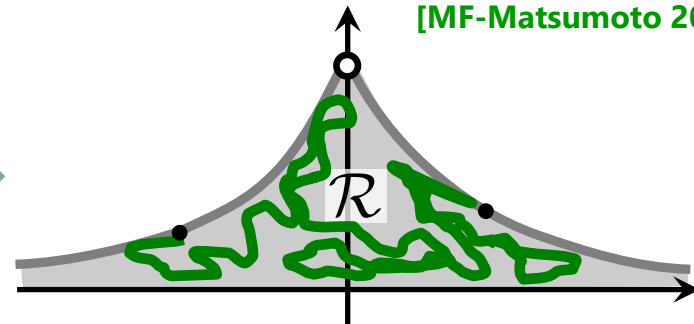
[MF-Umeda 1703.00861]



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

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 [2/11]

Picard-Lefschetz theory for group manifolds

[MF 2506.12002]

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

We want to evaluate:

$$\langle \mathcal{O} \rangle \equiv \frac{\int_G (dU_0) e^{-S(U_0)} \mathcal{O}(U_0)}{\int_G (dU_0) e^{-S(U_0)}} \quad \left(\begin{array}{l} U_0 \in G : \text{dynamical variable} \\ S(U_0) \in \mathbb{C} : \text{complex action} \end{array} \right)$$

Haar measure

$G^{\mathbb{C}}$: complexification of G

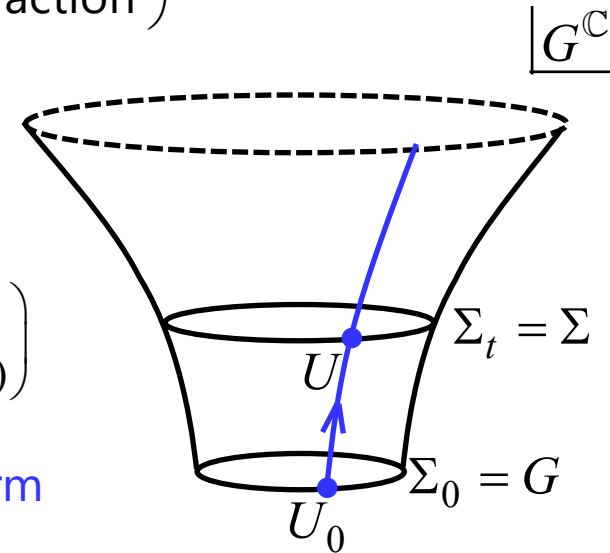
$$\left(\begin{array}{l} \mathfrak{g} = \bigoplus_a \mathbb{R} T_a \Rightarrow \mathfrak{g}^{\mathbb{C}} = \bigoplus_a \mathbb{C} T_a \\ G^{\mathbb{C}} \equiv \{e^Z e^{Z'} \cdots e^{Z''} \mid Z, Z', \dots, Z'' \in \mathfrak{g}^{\mathbb{C}}\} \end{array} \right) \quad \left(\begin{array}{l} G = SU(n) \\ \Rightarrow G^{\mathbb{C}} = SL(n, \mathbb{C}) \end{array} \right)$$

Cauchy's theorem

Haar measure

holomorphic N -form

$$\langle \mathcal{O} \rangle = \frac{\int_G (dU_0) e^{-S(U_0)} \mathcal{O}(U_0)}{\int_G (dU_0) e^{-S(U_0)}} = \frac{\int_{\Sigma} (dU)_{\Sigma} e^{-S(U)} \mathcal{O}(U)}{\int_{\Sigma} (dU)_{\Sigma} e^{-S(U)}} \quad \left(\begin{array}{l} \theta = dU U^{-1} = T_a \theta^a \text{ (Maurer-Cartan)} \\ \Rightarrow (dU)_{\Sigma} \equiv \theta^1 \wedge \cdots \wedge \theta^N \end{array} \right)$$



anti-holomorphic gradient flow

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

Path integral over the worldvolume

same as [MF-Matsumoto 2012.08468]

[MF 2506.12002]

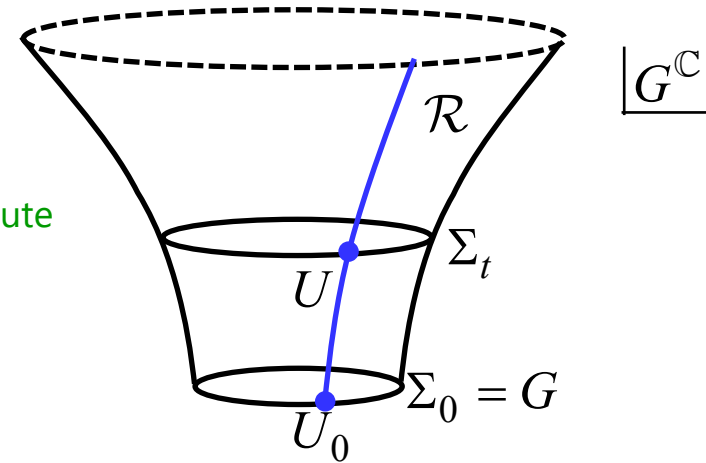
$$\langle \mathcal{O} \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t} e^{-S(U)} \mathcal{O}(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t} e^{-S(U)}} \quad \leftarrow t\text{-independent}$$

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

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

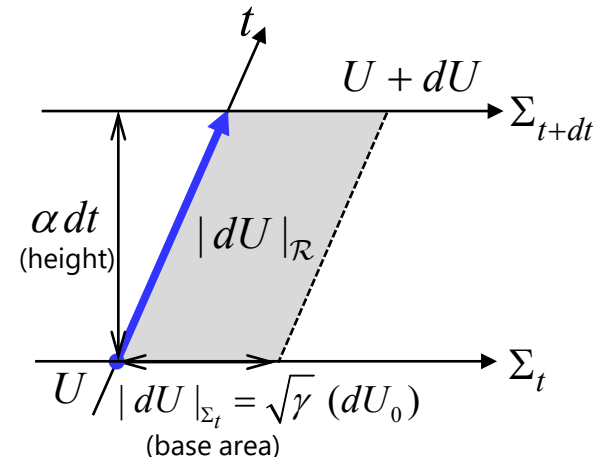
$$= \frac{\int_{\mathcal{R}} |dU|_{\mathcal{R}} e^{-V(U)} \mathcal{F}(U) \mathcal{O}(U)}{\int_{\mathcal{R}} |dU|_{\mathcal{R}} e^{-V(U)} \mathcal{F}(U)}$$

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



introduce momentum (velocity) π

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



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 $\omega = d\langle \pi, dUU^{-1} \rangle \Rightarrow$ symplectic volume form $d\Omega = \frac{1}{(N+1)!} \omega^{N+1}$ [4/11]

[MF 2506.12002]

[5/11]

Molecular dynamics over $T\mathcal{R}$

Algorithm

(i) initial momentum

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

$$\textcircled{2} \quad \tilde{\pi} \rightarrow \pi \in T_U \mathcal{R}$$

(ii) constrained MD (RATTLE)

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

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

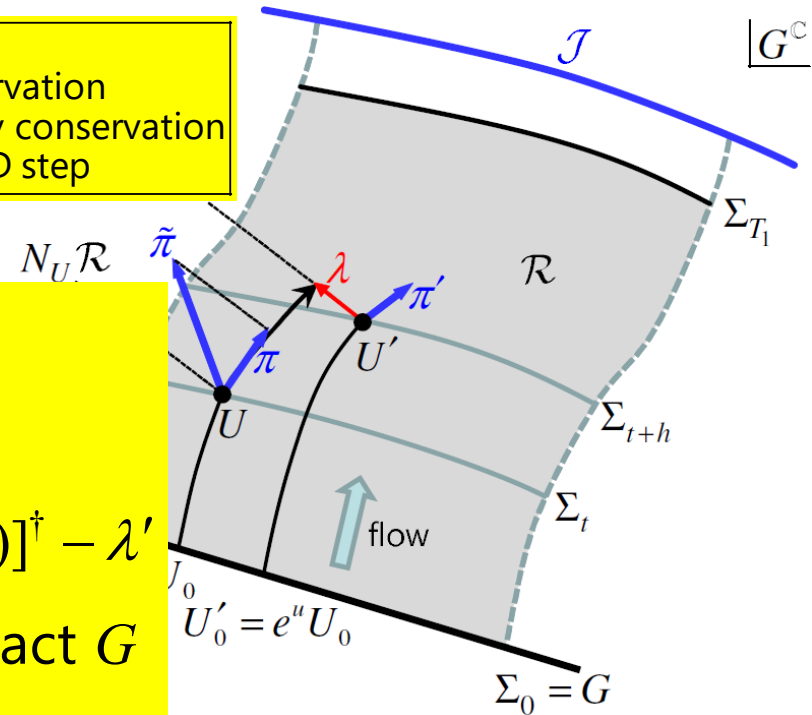
after repeating MD,

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

(iv) measurement

we estimate observables from the subsample

in a subregion $\widetilde{\mathcal{R}} = \{U \in \mathcal{R} \mid \tilde{T}_0 \leq t(U) \leq \tilde{T}_1\}$



Group-manifold structure in lattice gauge theory

[MF (in prep)]

Gauge group

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

Configuration space in LGT : **product group**

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

Partition function

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

Gauge invariance

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

Gauge transformation group $\{g_x \in \bar{G} \mid x\}$: "redundancy"

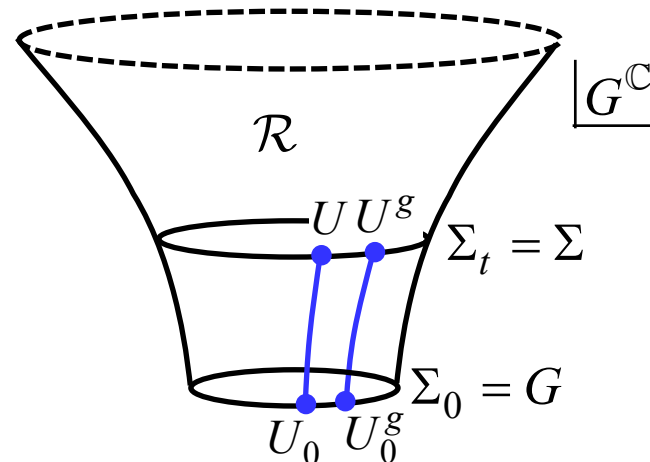
Gauge invariance in WV-HMC

[MF (in prep)]

Anti-holomorphic gradient flow

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

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



Gauge invariance for flowed configurations [MF]

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

NOT $\bar{G}^C$ same redundancy!



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

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

has the same gauge invariance as the original PI!

Application to pure lattice gauge theory

[MF (in prep)]

$$S(U) \equiv S_W(U) + S_\theta(U)$$

Wilson

$$S_W(U) \equiv \beta \sum_x e_x$$

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

θ term (clover)

$$S_\theta(U) \equiv -i\theta \sum_x q_x$$

(only for 4D)

$$\left(\begin{aligned} q_x &\equiv \frac{1}{32\pi^2} \sum_{\mu,\nu,\rho,\sigma} \epsilon_{\mu\nu\rho\sigma} \text{tr} F_{x,\mu,\nu} F_{x,\rho,\sigma} \\ F_{x,\mu,\nu} &\equiv \frac{1}{8} \left(U_{x,\mu,\nu} + U_{x,\nu,-\mu} + U_{x,-\mu,-\nu} + U_{x,-\nu,\mu} - (\mu \leftrightarrow \nu) \right) \end{aligned} \right)$$

Anti-holomorphic gradient flow

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

local



Hessian of S : sparse



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

$$\begin{cases} \text{configuration : } \dot{U} = (\textcolor{blue}{DS})^\dagger U \\ \text{tangent vector : } \dot{v} = \textcolor{brown}{D}_v \textcolor{blue}{DS} + [(\textcolor{blue}{DS})^\dagger, v] \\ \text{normal vector : } \dot{n} = -\textcolor{brown}{DD}_n \textcolor{blue}{S} - [\textcolor{blue}{DS}, n] \end{cases}$$

[MF 2311.10663]

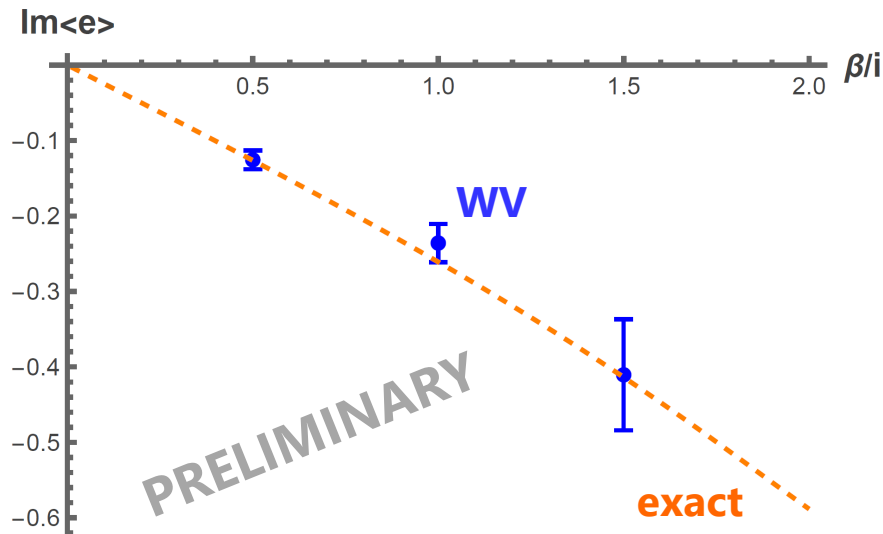
Check of algorithm

[MF (in prep)]

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

2D : 2x2 (Nconf=200)

(CPU : grid={2,2})

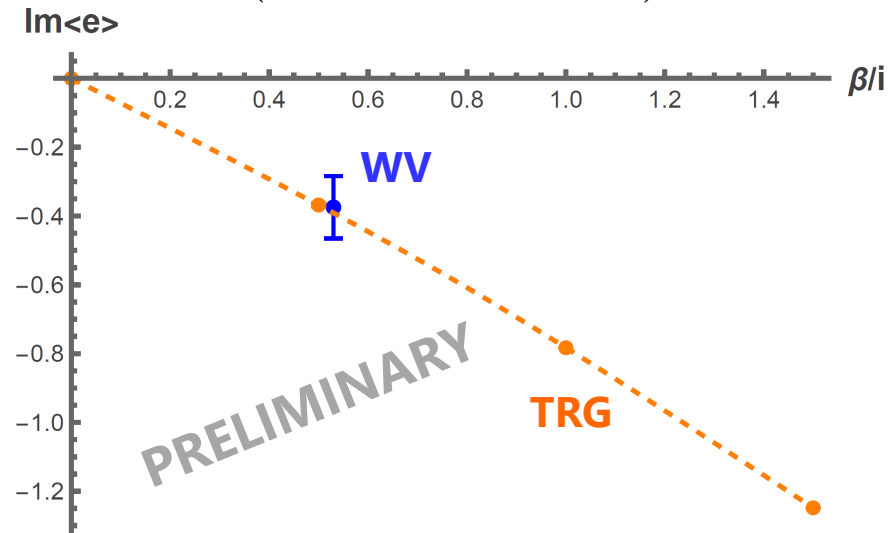


compared with exact values

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

3D : 2x2x2 (Nconf=100)

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



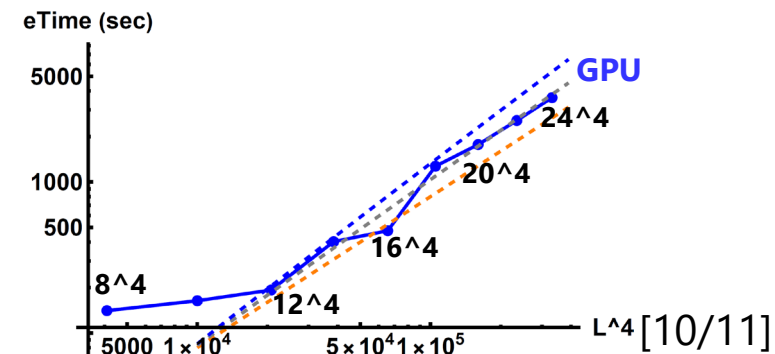
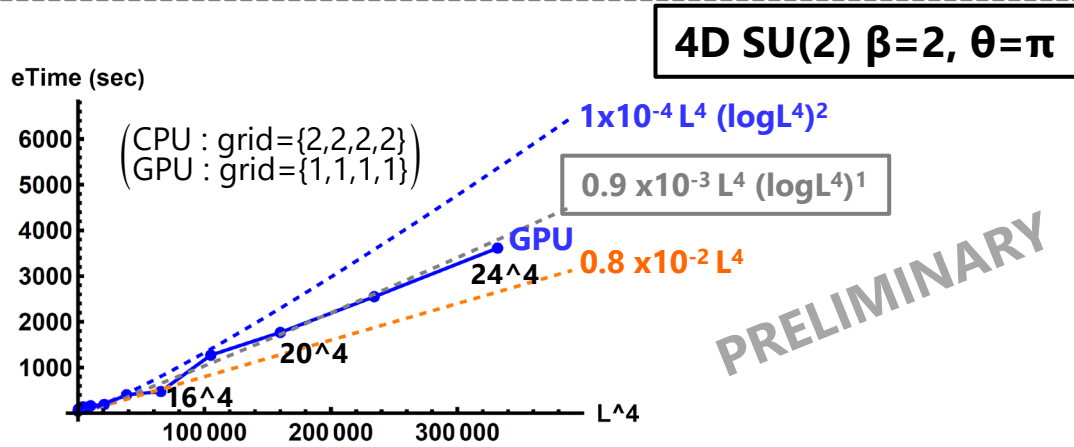
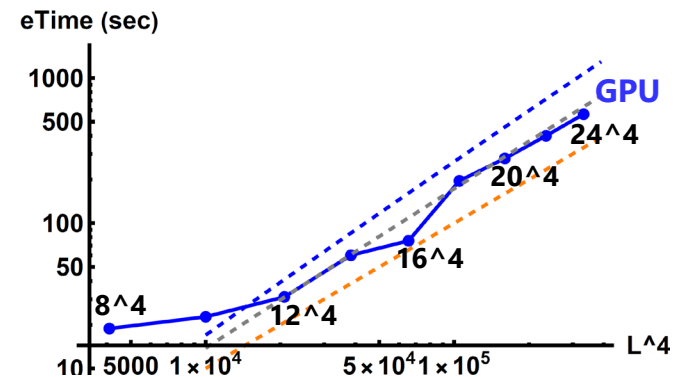
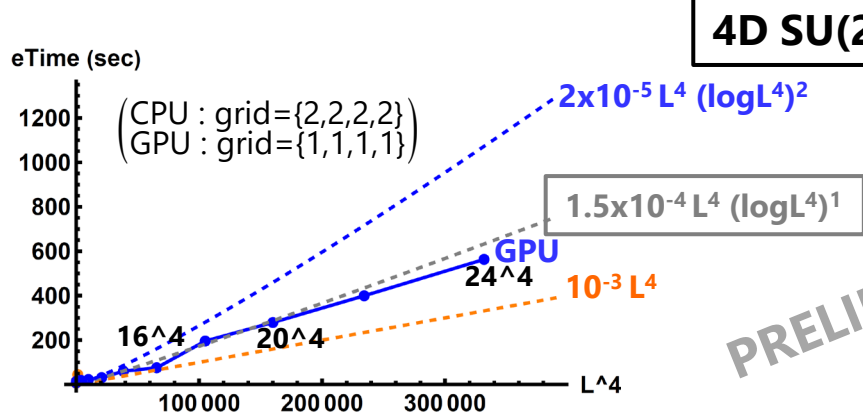
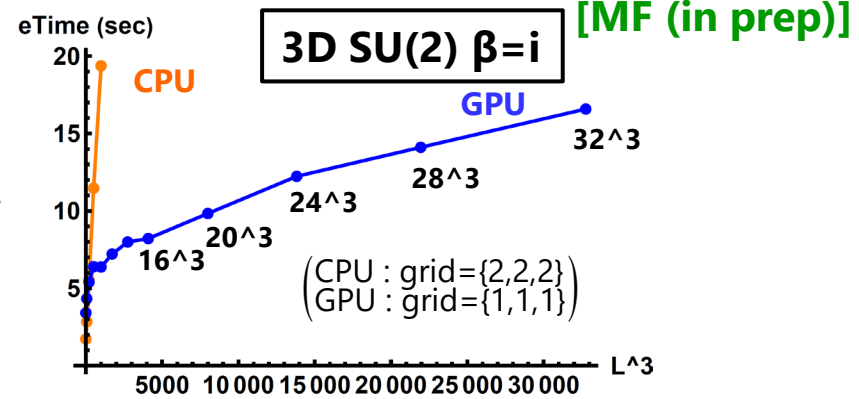
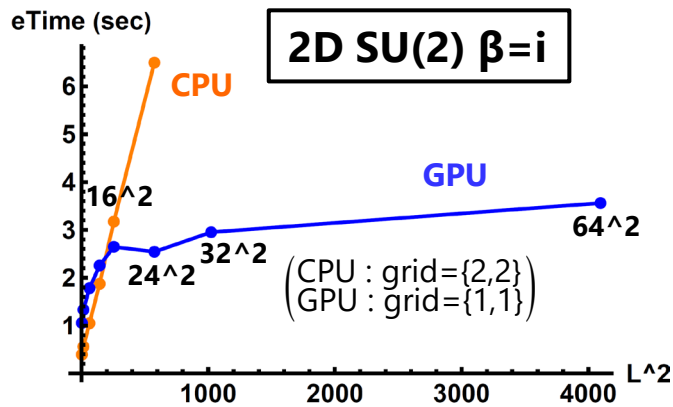
compared with **Tensor RG** results

[MF-Kuwahara (in prep)]



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

Computational cost scaling



Summary and outlook

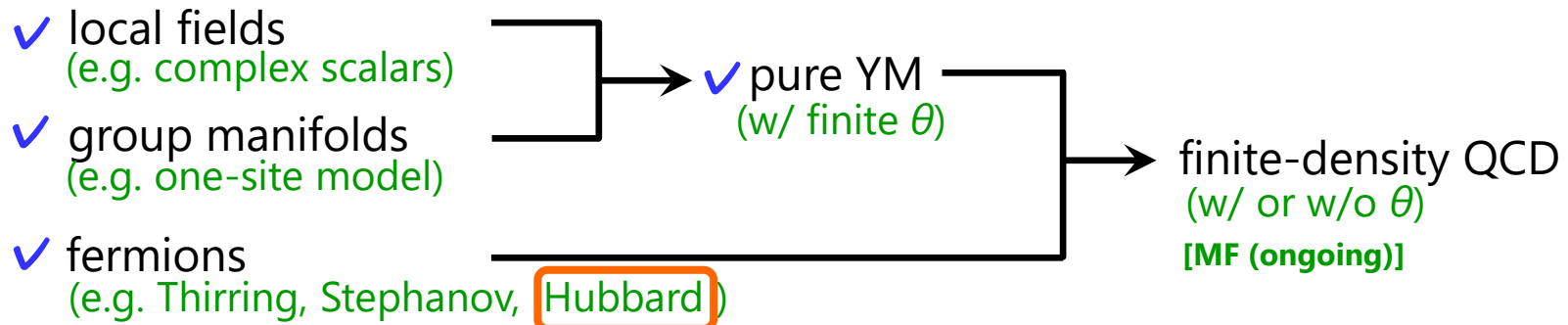
■ **Summary** : Formulated WV-HMC for LGTs using WV algorithm for group manifolds

- 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 code set

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

■ Outlook

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



▼ 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

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

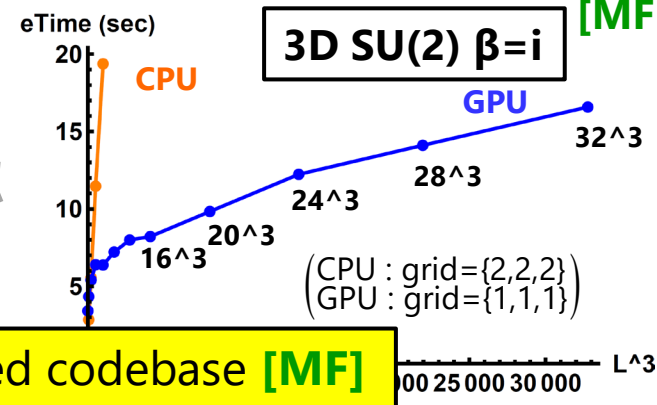
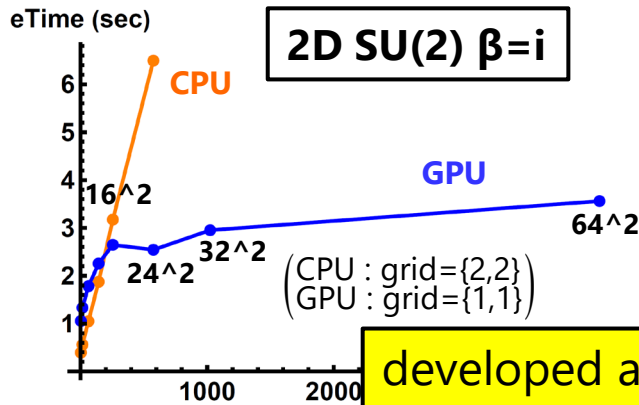
- real-time correlators at finite temperature ⇒ transport coefficients
- light-cone correlators ⇒ PDFs and their generalizations
- non-equilibrium processes

16:30, Friday, July 31
Algorithms and AI

Thank you.

Appendix

Computational cost scaling



developed a new GPU-oriented codebase [MF]

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

