#### Topology changing update algorithms for SU(3) gauge theory



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### Introduction

# Continuation of [2112.05188] 2D U(1) $\rightarrow$ 4D SU(3)

PS PROCEEDINGS OF SCIENCE	Metadynamics Surfing on Topology Ba in the Schwinger Hiddel Phily Inselect Income charge theory	
	Abstract	
	We present our investigation of introductions as a solution for topological frames on the state parage theory. The solution behavior of the independent way, where is considered with a determination in measurement of pro- sents as a considered with frames.	A Decision of the second
	International Transmission Research and the automatication takes the transmission of the automatication takes and the second at the automatication takes and the following the second at the following the second at the following the second at	$\mathbb{R}^{R^{1}}$
Comparison of topology changing update algorithms	$\theta = \frac{1}{2\pi} e_{\theta} \left[ \sum_{i=1}^{n} e_{i}(\theta) \right]$ (4)	and the second se
	where P and is the plaquette of the lattice site in the minimum large	
		The call are that the treat inpy failure with their respective the behavior further as the start behavior for any failed to restore against the behavior <i>EUTE-JUT TO</i>
		12
	apprint aligner or rates and a mapping the rates of the states of the second se	A
In modern lattice simulations, concentional splate algorithms do not affect for immediag between	In the Galaxinger analysis interaction patients and a possible range with both constraints of adaptements in patients. They instant metallysis is and dependent of the set of a post-order constraints of adaptements of a post-order constraints of the approximation of a post-order constraints. The post-order constraints of the approximation of a post-order constraints of a post-order constraints of the approximation of a post-order constraints. The post-order constraints of the approximation of a post-order constraints. The post-order constraints of the approximation of a post-order constraints. The post-order constraints of the post-order constraints of the post-order constraints. The post-order constraints of the post-order constraints of the post-order constraints. The post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints. The post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-order constraints of the post-	Dest of the later is
inpulsigical sectors at line latitor spanings. We compare the visibility of multiple laws commonly used algorithms (mutadynamics, instanton updates, and antiticade dormalization) with respect to	Heledownia	Print - 1 444 - 4
proper sampling of all inpulsiging senses in the followinger model. We briefly comment on the property of applicing these methods to 6 descentional IEO/8 simulations.	The approach of instally writes experience in characterise the ghose open in other top synthese. Are this take an at 1.0 support using a modified concerned of a modified processing of the state of the	and out he wan is fig. the stry an even polynomials
	$\psi_{mn} = \frac{1}{2\pi} m \left[\sum_{i} h_{ij}(h)\right]$ (4)	1074 64 14 44 141 19794
	which are all not continuous repringers charge, as it is not integer-solution arrayment, thereing a fract rate real transmission (in-any configuration a to address a strangementation and provide and provide and and a strangementation).	
	$V(\theta a a (t, t) - \sum_{i} \mu (\theta a a (t, -\theta a a b (t')))$ (4)	
	which is antibility over the gamma action an access thread with the a finance of the sound comparison between their barriers of the sound of the sound of the sound of the which is transfer and parameters as a solid or could interactive. Alternatively, and a processor as the data sound actions includes "subsequences, under the parameters in the data sound actions includes" subsequences and interactive parameters.	
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Paper and Statement Advantage of the Statement and the Statement and Statement	This has been done for the strangets (P), see Fig. 2(b). Observables will have been to be calculated on temportup	51 A Lais, 5 Municul and D1 5 Files Settlement
	$\rho_{1} = \frac{2 (R_{12} + 2 R_{22} + 2 R_{22})}{2 (-2) (R_{22} + 2 R_{22})}$ (4)	of a farmer, 6 had an

#### Related talks:

- Parallel tempering: [talk by Ruben Kara]
- Tempered boundaries: [talk by Claudio Bonanno]
- Multicanonical: [talk by Francesco D'Angelo]
- Many more in this session: [Algorithms I]
   [Algorithms II]
   [Algorithms III]
   [Algorithms IV]

#### Also see [poster by Philip Rouenhoff]

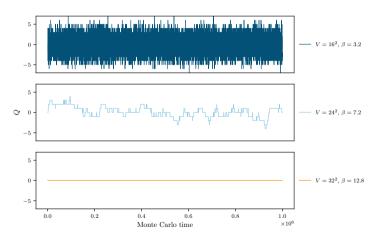




## MOTIVATION

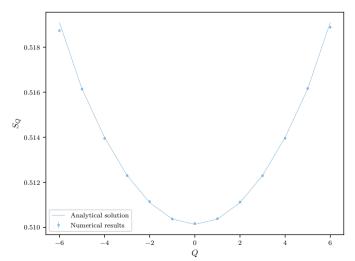
### Topological freezing in 2-dimensional U(1)

Not exclusive to QCD/SU(3) gauge theory





Slow topological modes couple to other observables!





#### Topological freezing in 4-dimensional SU(3) agora, la falla falla (b. el colarge) de adora de la falla. Mandales adora, el decisión de la grand factoria de la $V = 10^4$ , $\beta = 5.8980$ -5ő -5-5 20000 40000 60000 80000 100000 Monte Carlo time

Not yet completely frozen for the lattice spacings considered here



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 $V = 10^4, \beta = 5.8980$  $S^{(0)}$  $S^{(0)}$  $S^{(1)}$  $S^{(1)}$  $S^{(2)}$  $S^{(2)}$ 0.8 - 0.8  $S^{(3)}$  $S^{(3)}$  $S^{(4)}$  $S^{(4)}$ c(5)c(5)- 0.6  $S^{(6)}$ 0.6  $S^{(6)}$ . S(7)S(7) $|Q^{(0)}|$  $|O^{(0)}|$  $|Q^{(1)}|$  $|Q^{(1)}|$ 0.4 - 0.4  $|O^{(2)}|$  $|O^{(2)}|$  $Q^{(3)}$  $|O^{(3)}|$  $|O^{(4)}|$  $|O^{(4)}|$ 0.2 -0.2 $|Q^{(5)}|$  $|Q^{(5)}|$  $Q^{(6)}$  $|Q^{(6)}|$  $Q^{(7)}$  $|Q^{(7)}|$ 4° 4° 4° 4° 4° 4° 4° 4° 6° 6° 6° 6° 6° 6° 6° 6° 6° 6° 6° 6°

 $V = 22^4, \beta = 6.4035$ 

Weak but non-vanishing correlation between action and topological charge!

 $V = 10^4, \beta = 5.8980$  $V = 22^4, \beta = 6.4035$ 1.0  $W_2^{(0)}$  $W_{2}^{(0)}$  $W_2^{(1)}$  $W_2^{(1)}$  $W_{2}^{(2)}$  $W_{2}^{(2)}$ 0.8 - 0.8  $W_2^{(3)}$  $W_2^{(3)}$  $W_2^{(4)}$  $W_2^{(4)}$  $W_{2}^{(5)}$  $W_{2}^{(5)}$  $\mathcal{W}_2^{(6)}$  $W_{2}^{(6)}$ - 0.6 0.6  $W_{0}^{(7)}$  $W_{2}^{(7)}$  $|Q^{(0)}|$  $|O^{(0)}|$  $|Q^{(1)}|$  $|Q^{(1)}|$ - 0.4 0.4  $|O^{(2)}|$  $|O^{(2)}|$  $|Q^{(3)}|$  $|Q^{(3)}|$  $|O^{(4)}|$  $|O^{(4)}|$ - 0.2 0.2  $|Q^{(5)}|$  $|Q^{(5)}|$  $|Q^{(6)}|$  $|Q^{(6)}|$  $|Q^{(7)}|$  $|Q^{(7)}|$ 

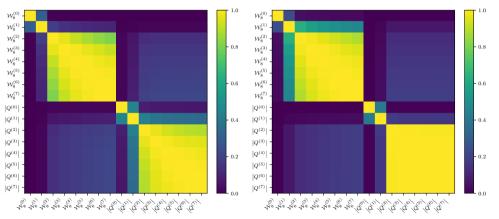
The same can be seen for Wilson loops (L = 2)

 $V = 10^4, \beta = 5.8980$ 1.0  $W_{4}^{(0)}$  $W_4^{(0)}$  $\mathcal{W}_4^{(1)}$  $W_4^{(1)}$  $W_4^{(2)}$  $\mathcal{W}_{i}^{(2)}$ - 0.8 - 0.8  $\mathcal{W}_4^{(3)}$  $W_4^{(3)}$  $\mathcal{W}_4^{(4)}$  $W_4^{(4)}$  $W_{4}^{(5)}$  $W_{4}^{(5)}$  $W_4^{(6)}$  $\mathcal{W}_4^{(6)}$ - 0.6 0.6  $\mathcal{W}_{t}^{(7)}$  $W_4^{(7)}$  $|Q^{(0)}|$  $|O^{(0)}|$  $|Q^{(1)}|$  $|Q^{(1)}|$ - 0.4 0.4  $|O^{(2)}|$  $|O^{(2)}|$  $|Q^{(3)}|$  $|Q^{(3)}|$  $|O^{(4)}|$  $|O^{(4)}|$ - 0.2 0.2  $|Q^{(5)}|$  $|Q^{(5)}|$  $|Q^{(6)}|$  $|Q^{(6)}|$  $|Q^{(7)}|$  $|Q^{(7)}|$ 

 $V = 22^4, \beta = 6.4035$ 

The same can be seen for Wilson loops (L = 4)

 $V = 10^4, \beta = 5.8980$ 



 $V = 22^4, \beta = 6.4035$ 

The same can be seen for Wilson loops (L = 8)

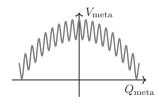


## **UPDATE ALGORITHMS**

#### Two approaches

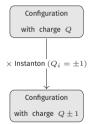
#### Metadynamics

[Laio et al '16] Add history-dependent bias potential to action



#### **Instanton updates**

[Fucito et al '84] Multiply configurations with instantons

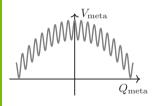




### Metadynamics

#### Metadynamics

#### [Laio et al '16] Add history-dependent bias potential to action



• Requires non-integer definition of Q:

$$Q_c = \frac{1}{32\pi^2} \sum_{n} \operatorname{tr}[\epsilon_{\mu\nu\rho\sigma} C_{\mu\nu}(n) C_{\rho\sigma}(n)]$$

Here: Clover-definition with under-smeared fields

- After every accepted update, also update  $V_{\rm meta}$
- Add bias potential to action

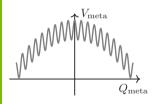
$$S_{\text{meta}} = S_g + V_{\text{meta}}$$

• Reweight observables back to desired distribution

### Metadynamics

#### Metadynamics

#### [Laio et al '16] Add history-dependent bias potential to action



- Local update algorithms not feasible:
  - Heatbath + Overrelaxation:

No force induced by Metadynamics, doesn't help with tunneling

• Metropolis:

Either compute  $\Delta Q_{meta}$  for every link update (too expensive) or after one sweep (low acceptance rate)

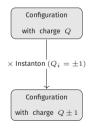
- Use global updates (Hybrid Monte Carlo):
  - $\Rightarrow$  Force given by sum of normal thin-link force and (fat-link) metadynamics-force:

$$\frac{\partial V_{\text{meta}}}{\partial Q_{\text{meta}}} \frac{\partial Q_{\text{meta}}}{U^{(n)}} \underbrace{\star \frac{\partial U^{(n)}}{\partial U^{(n-1)}} \dots \frac{\partial U^{(1)}}{\partial U}}_{\text{Stout force recursion}}$$

#### Instanton updates

#### **Instanton updates**

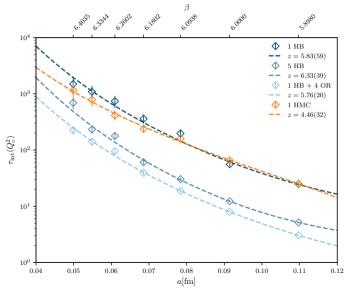
#### [Fucito et al '84] Multiply configurations with instantons



- Link-wise multiplication of initial configuration with  $Q_i = 1$  or  $Q_i = -1$  instanton
- Add Metropolis accept-reject step
- Works well in Schwinger model
   ⇒ Advantage: No need to pass through phase
   space regions with high action

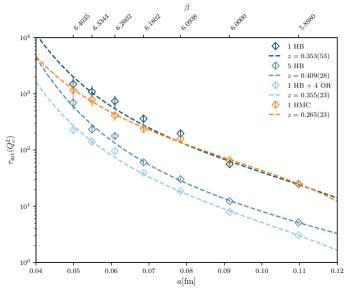


# RESULTS CONVENTIONAL UPDATES



- HB: Heatbath over 3 SU(2) subgroups
- OR: Overrelaxation over 3 SU(2) subgroups
- HMC: Unit length Hybrid Monte Carlo with 4th order minimum norm integrator
- **Topological charge**

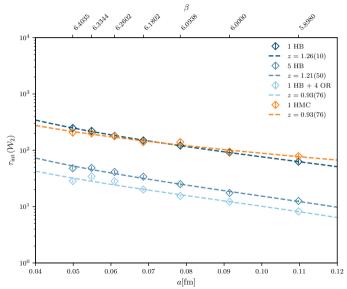
$$au_{\rm int}(Q_c^2) \propto a^-$$
  
 $z \approx 5 - 6?$ 



- HB: Heatbath over 3 SU(2) subgroups
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#### **Topological charge**

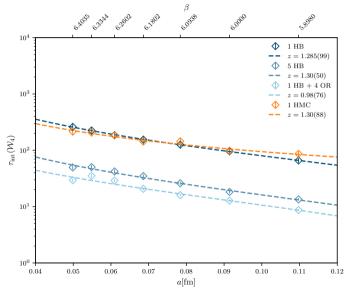
 $\tau_{\rm int}(Q_c^2) \propto e^{\frac{z}{a}}$  $z \approx 0.2 - 0.4?$ 



- HB: Heatbath over 3 SU(2) subgroups
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#### **Smeared Wilson loops**

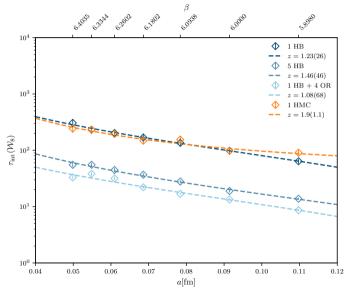
$$\tau_{\rm int}(\mathcal{W}_2) \propto a^{-1}$$
  
 $z \approx 1 - 2?$ 



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#### **Smeared Wilson loops**

$$au_{
m int}(\mathcal{W}_4) \propto a^{-z}$$
  
 $z \approx 1 - 2?$ 



- HB: Heatbath over 3 SU(2) subgroups
- OR: Overrelaxation over 3 SU(2) subgroups
- HMC: Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

#### **Smeared Wilson loops**

$$au_{
m int}(\mathcal{W}_8) \propto a^{-z}$$
  
 $z \approx 1 - 2?$ 

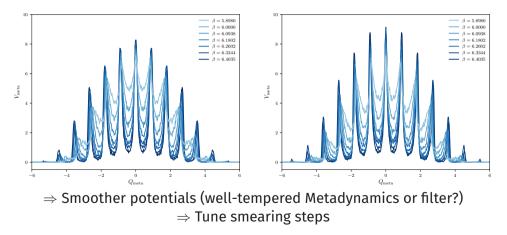


# RESULTS METADYNAMICS

### Scaling of metapotential

8 stout

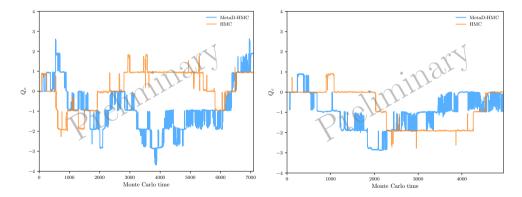
10 stout



### Metadynamics timeseries

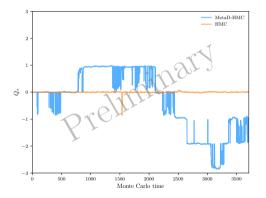
$$V = 18^4, \, \beta = 6.2602$$

$$V = 20^4, \, \beta = 6.3344$$



### Metadynamics timeseries

$$V = 22^4, \, \beta = 6.4035$$

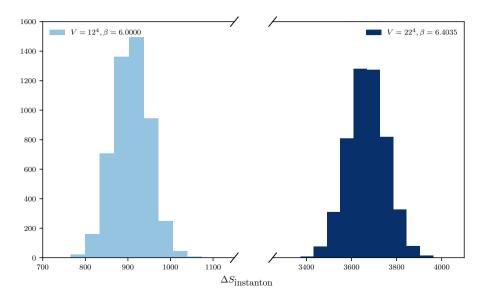


- Modest improvement compared to HMC
- Fluctuations between sectors (suboptimal parameters?)
- Lower acceptance rates HMC  $99\% \rightarrow 80\%$  MetaD-HMC
- Much higher computational cost (~ 20 times slower than HMC!)
  - $\Rightarrow$  Not that relevant for full QCD



# RESULTS INSTANTON UPDATES

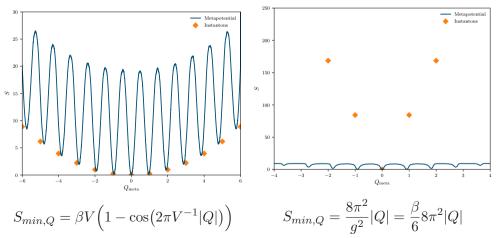
#### Instanton update - Action difference



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#### Instanton actions - U(1) vs SU(3)

2D U(1)  $V = 32^2, \beta = 12.8$  4D SU(3)  $V = 22^4, \beta = 6.4035$ 



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### Instanton updates + gradient flow

Combination of instanton updates and gradient flow?

- Apply gradient flow
- Multiply flowed configuration with instanton
- Flow back to flowtime o
- During accept-reject

 $p = \exp(-\Delta S + \ln(\det(\mathcal{J})))$ 

 $\Rightarrow$  Even lower acceptance probabilities than without flow



# OUTLOOK

### Outlook & Future plans

For now focus on Metadynamics

- More statistics and parameter tuning!
- Study metadynamics for improved actions
- Guess/fit potential
- Well-tempered Metadynamics (weight changes adaptively  $\Rightarrow$  usually better convergence of potential)
- Choosing a better collective variable:
  - Build up variational basis of observables at different scales
  - GEVP to extract leading modes of Markov chain
  - Collective variable from linear combination?
- Multiple timescale integration?

## Thank you for your attention!

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## **BACKUP SLIDES**

### Well-tempered Metadynamics

[Barducci' 08]

• Original Metadynamics

$$V_{t+1}(Q) = V_t(Q) + w \exp\left(-\frac{(Q_t - Q)^2}{2\sigma^2}\right)$$

• Well-tempered Metadynamics

$$V_{t+1}(Q) = V_t(Q) + \exp\left(-\frac{V_t(Q)}{\Delta T}\right) w \exp\left(-\frac{(Q_t - Q)^2}{2\sigma^2}\right)$$

#### Tunable parameter $\Delta T$ :

- $\circ \Delta T \rightarrow 0$ : No Metadynamics
- $\circ \ \Delta T \rightarrow \infty$ : Original metadynamics

### Construction of SU(3) instantons

Based on [Jahn' 19]

- Construction of instanton with radius  $\rho$  centered around z
- Embed SU(2) BPST instantons into SU(3)
- In singular gauge the vector potential is given by

$$A_{\mu} = \eta_{a\mu\nu} \frac{\rho^2 (x_{\nu} - z_{\nu})\tau_a}{(x - z)^2 ((x - z)^2 + \rho^2)}$$

- Deal with periodicity/boundary effects by applying 150 stout smearing sweeps with  $\rho_{\rm stout}=0.12$
- For an anti-instanton replace the 't Hooft symbol  $\eta_{a\mu\nu}$  with an anti 't Hooft symbol  $\bar\eta_{a\mu\nu}$