

Zimányi School 2022

Stabilizing complex Langevin for real-time YM theory

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Paul Hotzy

in collaboration with Kirill Boguslavski and David I. Müller

Institute for Theoretical Physics, TU Wien

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- 1 Introduction to CL for real-time simulations
- 2 Numerical solution of the CL equation
- 3 Results: Systematic improvement of stability
- 4 Conclusion & Outlook

Schwinger-Keldysh formalism for Yang-Mills theory

Expectation values

- Gauge fields on SK-contour

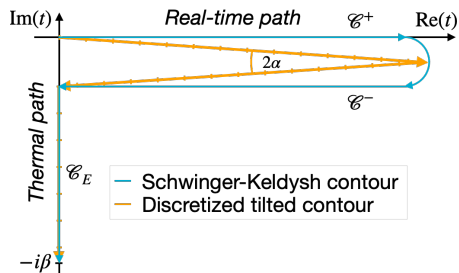
$$\langle \mathcal{O}[A] \rangle = \frac{1}{Z} \int \mathcal{D}A_E e^{-S_E[A_E]} \int \mathcal{D}A_+ \mathcal{D}A_- e^{iS[A_+, A_-]} \mathcal{O}(x)$$

- Periodic boundary conditions

$$A_\mu^a(t=0) = A_\mu^a(t=-i\beta)$$

- Yang-Mills action

$$S_{\text{YM}} = -\frac{1}{4} \int_{\mathcal{C}} d^4x F_a^{\mu\nu} F_{\mu\nu}^a$$



Complex weight function leads to the sign problem

- Real-time contour leads to complex weight function
- Direct calculation of oscillatory integrals is not feasible

$$\langle \mathcal{O}[A] \rangle = \frac{1}{Z} \int \mathcal{D}A_E e^{-S_E[A_E]} \int \mathcal{D}A_+ \mathcal{D}A_- e^{iS[A_+, A_-]} \mathcal{O}(x)$$

- Numerical integration methods exponentially costly

Alternative integration methods needed

- Reweighting, Contour deformation, Analytic continuation, Taylor expansion, Lefschetz thimbles, **Complex Langevin method**, ...

Complex Langevin method for gauge fields

- Introduction of (auxiliary) Langevin time θ
- CL equation for gauge fields [1]

$$\partial_\theta A_\mu^a(\theta, x) = i \frac{\delta S_{\text{YM}}}{\delta A_\mu^a(t, x)} + \eta_\mu^a(\theta, x), \quad A_\mu(\theta, x) \in \mathfrak{sl}(N_c, \mathbb{C})$$

- Gaussian distributed noise term

$$\begin{aligned} \langle \eta_\mu^a(\theta, t, \mathbf{x}) \rangle &= 0, \\ \langle \eta_\mu^a(\theta, t, \mathbf{x}) \eta_\nu^b(\theta', t', \mathbf{x}') \rangle &= 2\delta(\theta - \theta')\delta(t - t')\delta^{(d-1)}(\mathbf{x} - \mathbf{x}')\delta^{ab}\delta_{\mu\nu} \end{aligned}$$

Goal: Overcoming the sign problem

- CL bypasses the sign problem by sampling at late θ

$$\langle \mathcal{O}[A] \rangle \approx \lim_{\theta_0 \rightarrow \infty} \frac{1}{T} \int_{\theta_0}^{\theta_0+T} d\theta \mathcal{O}[A(\theta)]$$

CL suffers from instabilities

- Runaway instabilities \rightarrow numerical blow-up
 - Wrong-convergence instabilities \rightarrow distorted expectation values
 - Severity of the instabilities increase with shrinking tilt-angles
-
- Discretized path integral is regularized for tilted contours
 - Complex time contours leads to ambiguous noise correlator expression (δ -distribution for complex arguments)
 - ▶ Ambiguities are resolved by a parametrization dependent CL formulation

$$t : [a, b] \mapsto \mathbb{C}, \quad t(a) = 0, \quad t(b) = -i\beta$$

- ▶ Noise correlator in terms of λ

$$\delta(t(\lambda) - t(\lambda')) \rightsquigarrow \delta(\lambda - \lambda')$$

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- Link variables and plaquette variables

$$U_{x,\mu} \simeq \exp [iga_\mu A_\mu(x + \hat{\mu}/2)] \in \text{SU}(N_c) \rightsquigarrow \text{SL}(N_c, \mathbb{C}),$$
$$U_{x,\mu\nu} = U_{x,\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu}^{-1} U_{x,\nu}^{-1}$$

- Wilson plaquette action

$$S_W[U] = \frac{1}{2N_c} \sum_{k,\mathbf{x},\mu \neq \nu} \beta_{\mu\nu} \text{Tr} [U_{x,\mu\nu} - 1],$$

- Coupling constants

$$\beta_{0i} = -\frac{2N_c}{g^2} \frac{a_s}{a_{t,k}}, \quad \beta_{ij} = +\frac{2N_c}{g^2} \frac{\bar{a}_{t,k}}{a_s}$$

- Time reversibility is retained by averaged spacing

$$\bar{a}_{t,k} = (a_{t,k} + a_{t,k+1})/2$$

CL update step for link variables on a SK-contour

- Additional lattice spacing factors compared to common CL-step [2]

$$U_{x,t}(\theta + \epsilon) = \exp \left(it^a \left[i\epsilon \frac{a_{\lambda,k}}{a_s} \frac{\delta S_W}{\delta \tilde{A}_{x,t}^a} \Big|_{\theta} + \sqrt{\epsilon} \sqrt{\frac{a_{\lambda,k}}{a_s}} \eta_{x,\lambda}^a(\theta) \right] \right) U_{x,t}(\theta)$$

$$U_{x,i}(\theta + \epsilon) = \exp \left(it^a \left[i\epsilon \frac{a_s}{\bar{a}_{\lambda,k}} \frac{\delta S_W}{\delta \tilde{A}_{x,i}^a} \Big|_{\theta} + \sqrt{\epsilon} \sqrt{\frac{a_s}{\bar{a}_{\lambda,k}}} \eta_{x,i}^a(\theta) \right] \right) U_{x,i}(\theta)$$

- Langevin time step $\epsilon \rightarrow 0$
- Noise is approximated by a Gaussian function

Stabilization techniques

- **Gauge cooling [3]:** Exploit gauge freedom to minimize non-unitarity measured by a functional $F[U]$

$$U_{x,\mu} \mapsto U_{x,\mu}^V = V_x U_{x,\mu} V_{x+\mu}^{-1}, \quad F[U] \geq F[U^V]$$

- **Adaptive stepsize [4]:** Regulate large drift terms which lead to instabilities

$$\epsilon \mapsto \tilde{\epsilon} = \epsilon \min \left(1, \frac{B}{\max_{x,\mu,a} |K_{x,\mu}^a|} \right)$$

- **Dynamical stabilization [5]:** Penalize drift terms depending on the local non-unitarity of the configuration

$$K_{x,\mu}^a \mapsto \tilde{K}_{x,\mu}^a = K_{x,\mu}^a + i\alpha_{\text{DS}} M_x^a$$

We introduce an anisotropic kernel to improve stability!

Field-independent Kernel Freedom [1]

- *Kerneled Langevin equation* yields same limiting density function

$$\partial_{\theta} A_{\mu}^a(\theta, x) = i \int dx' \Gamma_{\mu\nu}^{ab}(x, x') \frac{\delta S}{\delta A_{\nu}^b(x')} + \int dx' \tilde{\Gamma}_{\mu\nu}^{ab}(x, x') \eta_{\nu}^b(\theta, x')$$

- $\Gamma_{\mu\nu}^{ab}(x, x')$ is required to be factorizable

$$\Gamma_{\mu\nu}^{ab}(x, x') = \int dx'' \tilde{\Gamma}_{\mu\sigma}^{ac}(x, x'') \tilde{\Gamma}_{\nu\sigma}^{bc}(x', x'')$$

- Kerneled Langevin equations correspond to the same Fokker-Plank equation
- *In practice:* Kernels may aggravate or mitigate instabilities

Kerneled CL update step

- Rescaling of Langevin time for temporal and spatial d.o.f.

$$U_{x,t}(\theta + \epsilon) = \exp \left(it^a \left[i\epsilon \left(\frac{a_{\lambda,k}}{a_s} \right)^2 \frac{\delta S_W}{\delta \tilde{A}_{x,t}^a} \Big|_{\theta} + \sqrt{\epsilon} \frac{a_{\lambda,k}}{a_s} \eta_{x,\lambda}^a(\theta) \right] \right) U_{x,t}(\theta)$$

$$U_{x,i}(\theta + \epsilon) = \exp \left(it^a \left[i\epsilon \frac{\delta S_W}{\delta \tilde{A}_{x,i}^a} \Big|_{\theta} + \sqrt{\epsilon} \eta_{x,i}^a(\theta) \right] \right) U_{x,i}(\theta)$$

- Noise of spatial update blows up for $a_{\lambda,k} \rightarrow 0 \rightsquigarrow \theta \mapsto \frac{\bar{a}_{\lambda,k}}{a_s} \theta$
- Temporal plaquette shows only slow dynamics $\rightsquigarrow \theta \mapsto \frac{a_{\lambda,k}}{a_s} \theta$

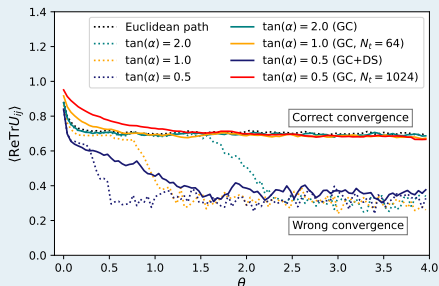
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- We simulate $SU(2)$ gauge theory on a $N_t \times 4^3$ lattice
- Coupling constant $g = 1$
- Inverse temperature of the system $\beta = 4.0$
- Simulations are initialized with identity matrices
- Same seed for random number generator for noise

Correct expectation values of one-point functions

Trace of average spatial plaquette

- **Kernels successfully stabilizes even small tilt angles**
- Existing methods not enough for stabilizing simulations



- Avg. spatial plaquette (considered in earlier studies [2]):

$$\mathcal{O}[U] = \frac{1}{N_t N_s^3} \sum_x \frac{1}{3} \sum_{i < j} \frac{1}{N_c} \text{ReTr} U_{x,ij}$$

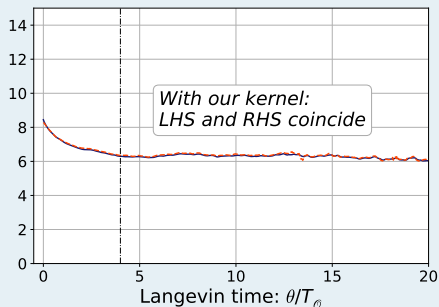
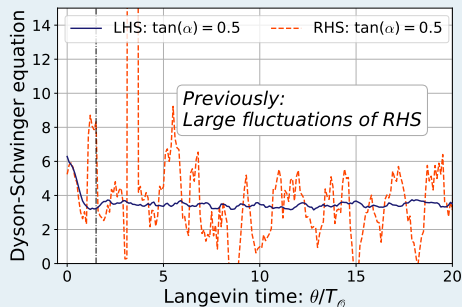
- Time translation inv. allows comparison to Euclidean results

Results for average spatial plaquette $\langle \mathcal{O} \rangle$ via CL:

$\tan(\alpha)$	Stabilization techniques	N_t	$\langle \mathcal{O} \rangle$
Euclidean	None	16	0.704 ± 0.002
2.0	AS, GC	16	0.701 ± 0.002
1.0	AS, GC, DS	16	0.678 ± 0.002
0.5	AS, GC, DS	16	0.318 ± 0.007
2.0	AS, GC, Γ	16	0.701 ± 0.003
1.0	AS, GC, Γ	64	0.703 ± 0.003
0.5	AS, GC, Γ	1024	0.705 ± 0.004

Dyson-Schwinger equations

DSE for spatial plaquettes



- Self-consistency check of link configuration
- Derivation from first principles \rightsquigarrow sampling process is “physical”

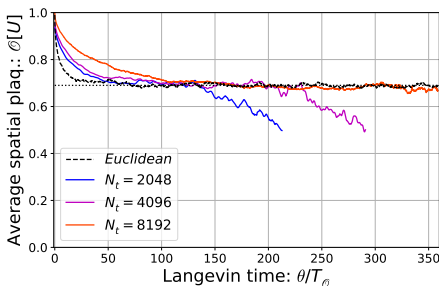
$$\frac{2(N_c^2 - 1)}{N_c} \langle \text{ReTr}(U_{x,ij}) \rangle = \frac{i}{2N_c} \sum_{|\rho| \neq i} \beta_{i\rho} \left\langle \text{ReTr} \left[(U_{x,i\rho} + U_{x,i\rho}^{-1}) U_{x,ij} \right] \right\rangle$$

Systematic improvement of CL instabilities

Anisotropic kernel systematically stabilizes CL

- Our kernel allows simulations even for $\max \text{Re}(t) > \beta$
- Stability is systematically improved for partial continuum limit
⇒ **Calculation of real-time observables may be feasible!**

- Stability region grows faster than auto-correlation time w.r.t. N_t
- Computational cost grows linearly with N_t



Tilt angle: $\tan(\alpha) = 0.4$






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Conclusion

- Stabilization techniques extend the applicability of CL
- We found an approach to systematically improve stability
- Anisotropic kernel enables simulations of $\max \text{Re}(t) > \beta$
 - ↪ Extrapolation to Schwinger-Keldysh contour might be possible
 - ↪ Application to real-time observables

Outlook

- Calculation of unequal time correlation functions
- Development of further stabilization techniques
- Criterion of correctness and boundary terms
- Non-thermal quantum systems (future prospect)

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