

Complex Langevin simulation applied to a chiral model

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Complexification approaches to the sign problem

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Outline

- The sign problem
- Old & renewed approach:
 - Complex Langevin simulation
- New approach:
 - HMC simulation on Lefschetz thimble
 - No sign problem?
- Discussion and outlook

QCD partition fn & sign problem

$$Z(T, \mu) = \text{Tr} e^{-\beta(H - \mu N)} = \sum_N e^{-\beta E_N} 2 \cosh(\beta \mu N)$$

→ is real positive, and a function of μ^2

$$Z(T, \mu) = \int dU d\psi d\bar{\psi} e^{-S} = \int dU e^{-S_B} \det D$$

→ Importance sampling works if “ $e^{-S} \det D$ ” > 0

→ At finite μ , $\det D(\mu) = \det D(-\mu)^*$ is complex: sign problem

→ Attempts to overcome the problem

→ Taylor expansion at $\mu=0$, Imaginary μ , Re-weighting,

→ Density of states, ...

Old & new complexification approaches to the sign problem

- Complex Langevin simulation
- Simulation on the Lefschetz thimble

Langevin dynamics

- Statistical sampling w/o explicit weight fn (the Fokker-Planck eqn is associated)
- Equilibrium state is thermal (Brown motion)

$$\frac{d}{dt}v_i(t) = -\underbrace{\gamma}_{\text{friction}}v_i(t) + \underbrace{\eta_i(t)}_{\text{noise}} \quad \langle \eta_i(t)\eta_j(t') \rangle = 2kT\gamma\delta_{ij}\delta(t-t')$$

$$\lim_{t \rightarrow \infty} \frac{1}{2} \langle v_i(t)v_j(t) \rangle = \frac{1}{2} \delta_{ij} kT$$

Langevin dynamics

- Statistical sampling w/o explicit weight fn
(the Fokker-Planck eqn is associated)
- Equilibrium state is the quantum vacuum

Parisi-Wu

$$\frac{\partial \phi(x, \theta)}{\partial \theta} = -\frac{\delta S[\phi]}{\delta \phi(x, \theta)} + \eta(x, \theta) \quad \langle \eta(x, \theta) \eta(x', \theta') \rangle = 2\delta(x - x')\delta(\theta - \theta')$$

force

noise

Complex Langevin dynamics

- Langevin algorithm is simple
- No obvious problem with complex action S

Parisi-Klauder

$$\frac{\partial \phi(x, \theta)}{\partial \theta} = - \frac{\delta S[\phi]}{\delta \phi(x, \theta)} + \eta(x, \theta) \quad \langle \eta(x, \theta) \eta(x', \theta') \rangle = 2\delta(x - x')\delta(\theta - \theta')$$

force noise

- Price to pay:
 - Complex “force” $dS/d\phi$ makes ϕ also complex
 - True equilibration is not formally guaranteed

Results in ϕ^4 theory

Aarts et al.

- S becomes complex at finite μ

$$S = \int d^4x \left[|\partial_\nu \phi|^2 + (m^2 - \mu^2) |\phi|^2 + \mu (\phi^* \partial_4 \phi - \partial_4 \phi^* \phi) + \lambda |\phi|^4 \right]$$

Results in ϕ^4 theory

Aarts et al.

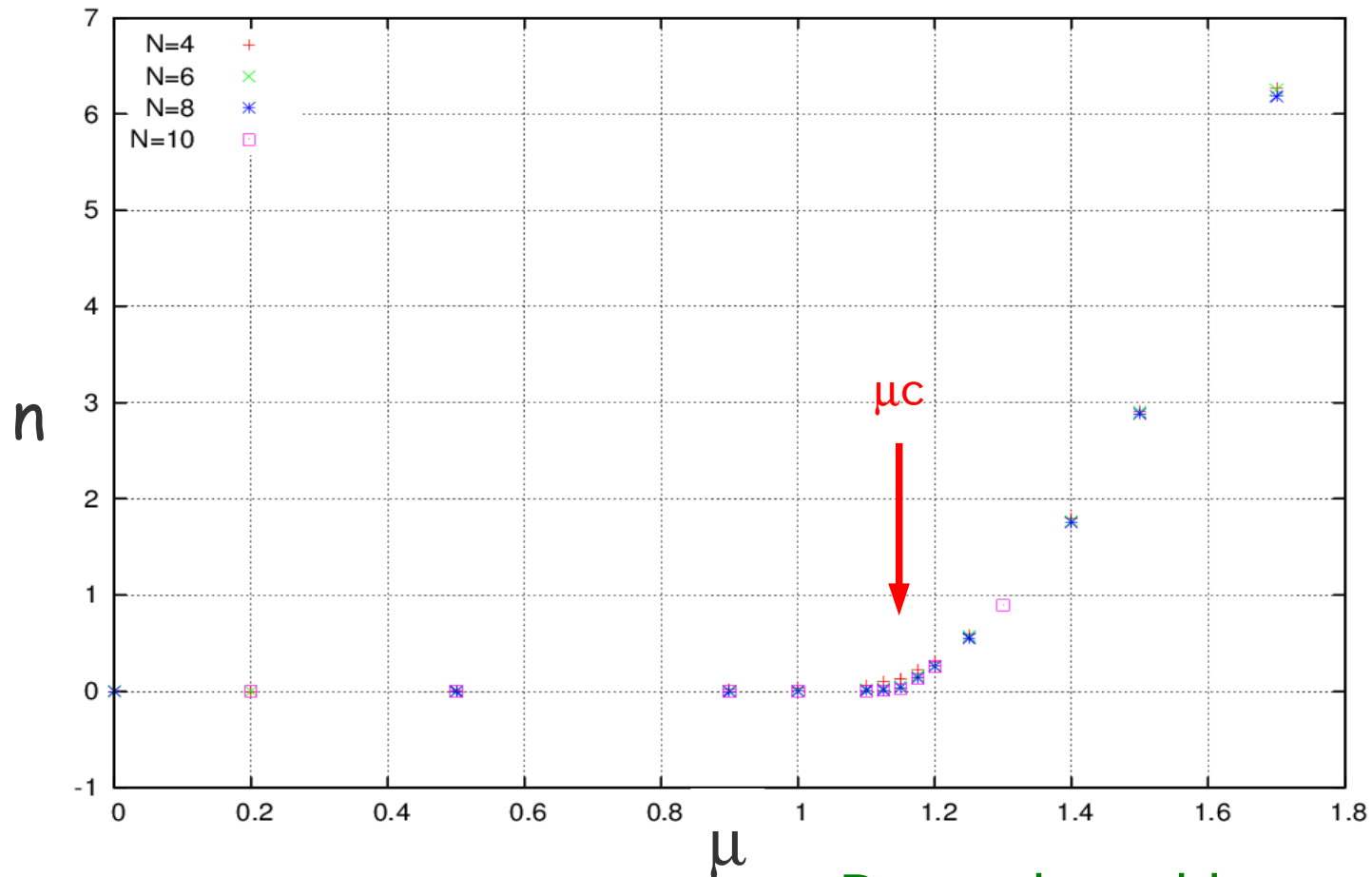
- S becomes complex at finite μ

$$S = \sum_{x \in \mathbb{L}^n} \left[-\phi_1(x) \left[\phi_1(x + \hat{0}) \cosh(\mu) - \phi_2(x + \hat{0}) \sinh(\mu) I \right] \right. \\ \left. - \phi_2(x) \left[\phi_2(x + \hat{0}) \cosh(\mu) + \phi_1(x + \hat{0}) \sinh(\mu) I \right] \right. \\ \left. - \sum_{\hat{k}} \left(\phi_1(x) \phi_1(x + \hat{k}) + \phi_2(x) \phi_2(x + \hat{k}) \right) \right. \\ \left. + \left(D + \frac{1}{2} \kappa \right) (\phi_1(x) \phi_1(x) + \phi_2(x) \phi_2(x)) + \frac{1}{4} \lambda (\phi_1(x) \phi_1(x) + \phi_2(x) \phi_2(x))^2 \right]$$

Results in ϕ^4 theory

Aarts et al.

- Density n stays zero up to $\mu=\mu_c$; Silver Blaze



Reproduced by ourselves

When Complex Langevin works?

- Longstanding problems
 - instability - only numerical? Aarts et al
 - wrong equilibrium - what's the key physics?
- $\text{TrLog}(D)$ is unique to fermion theories, whose effects are to be studied
 - Chiral Random Matrix model (see Sano's talk)
 - Nambu-Jona-Lasinio model (in progress)
 - QCD, ..., etc.

Path-integral in complexified phase space

- Complex Langevin = sampling algorithm in complexified phase space
- In complex space, one can choose the integration contour on which $\text{Im}S = \text{const}$!
 - Method of steepest descent - deform the path around critical points, $dS/dz=0$

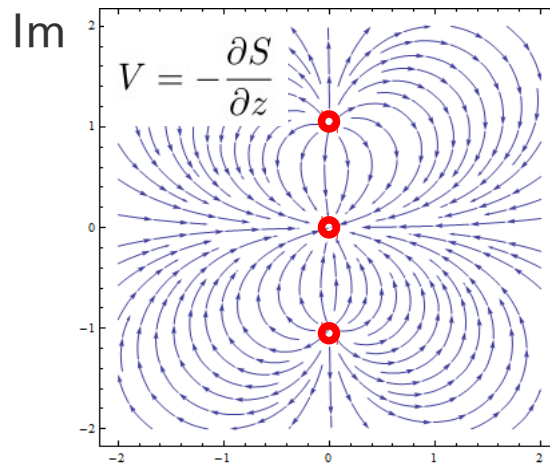
$$\int_{-\infty}^{\infty} dx e^{i\kappa x^2} = \int_c dz e^{i\kappa z^2} = e^{i\pi/4} \int_{-\infty}^{\infty} dt e^{-\kappa t^2}$$

Path-integral in complexified phase space

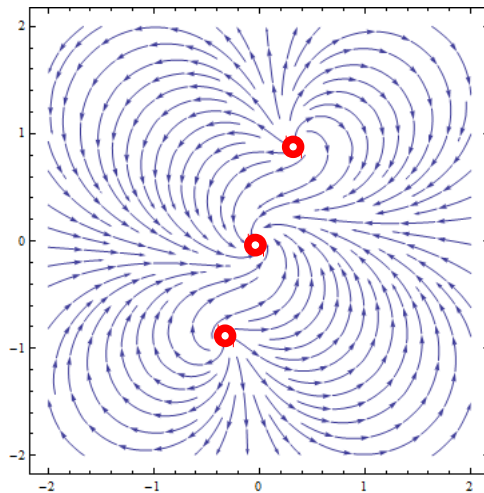
- Illustration $S = \frac{\kappa}{2}x^2 + \frac{\lambda}{4}x^4 \rightarrow \frac{\kappa}{2}z^2 + \frac{\lambda}{4}z^4 \quad \kappa \in \mathbb{C}$

Complex Langevin

$\kappa=1$



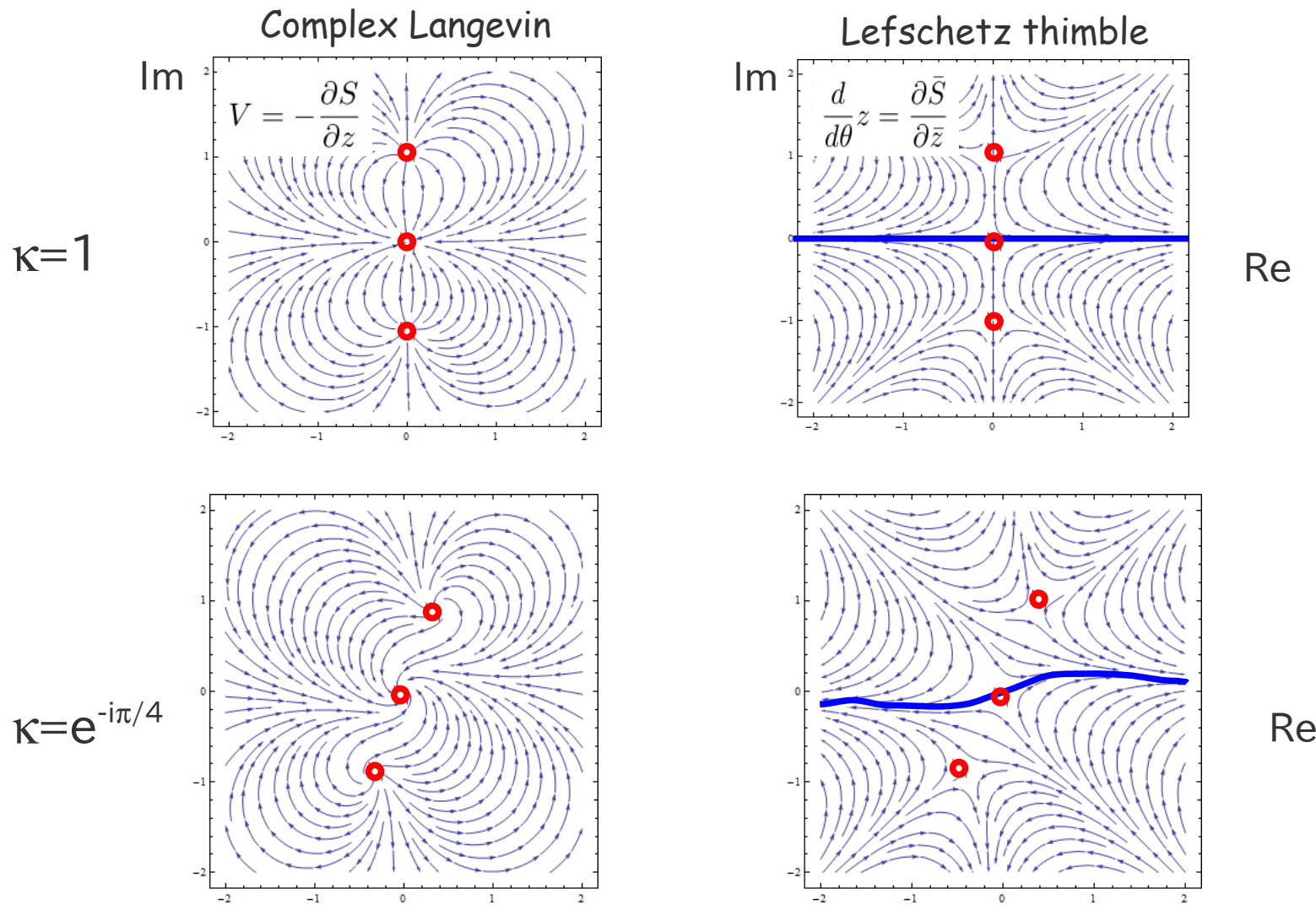
$\kappa=e^{-i\pi/4}$



Path-integral in complexified phase space

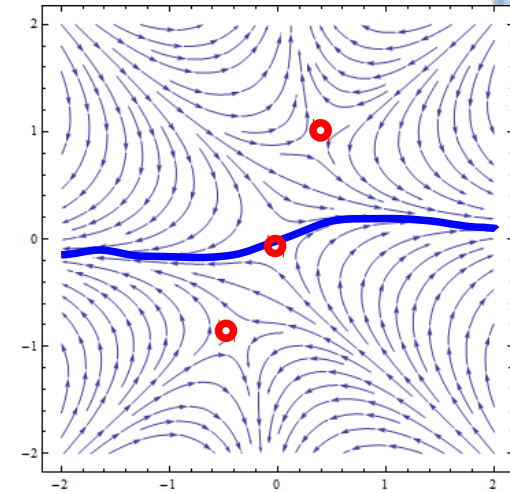
- Illustration

$$S = \frac{\kappa}{2}x^2 + \frac{\lambda}{4}x^4 \rightarrow \frac{\kappa}{2}z^2 + \frac{\lambda}{4}z^4 \quad \kappa \in \mathbb{C}$$



Path integral on Lefschetz thimble

- Flow eqn: $\frac{d}{dt}z(t) = \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}}, \quad \frac{d}{dt}\bar{z}(t) = \frac{\partial S[z]}{\partial z},$
- Along flow: $d(\text{Re}S)/dt > 0 \quad d(\text{Im}S)/dt=0$
- Critical pt.: $\left. \frac{\partial S[z]}{\partial z} \right|_{z=z_\sigma} = 0.$



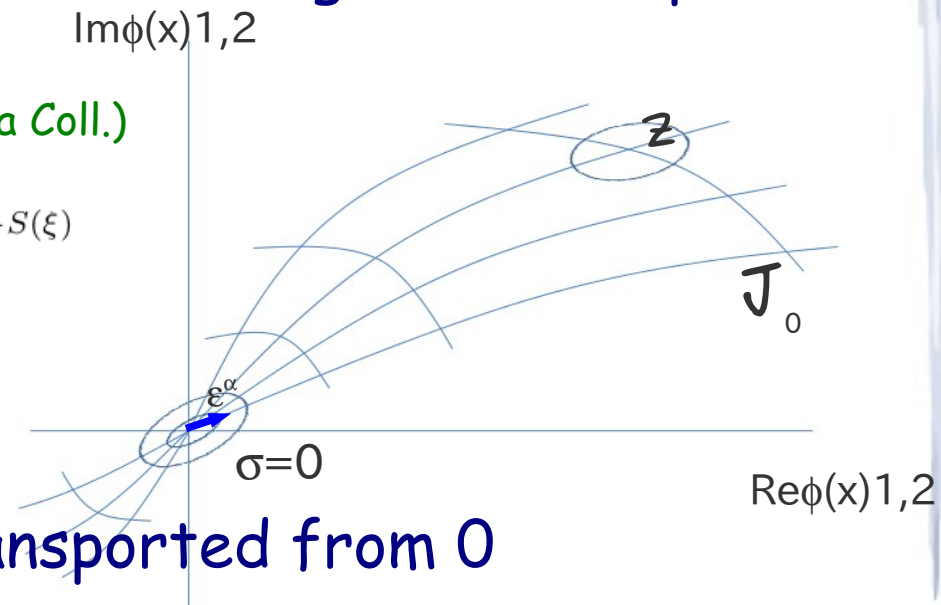
- Lefschetz thimble \mathcal{J}_σ : a union of downward flows from σ
- Morse theory shows: $\int_{\mathbb{R}^n} dx_1 \cdots dx_n g(x) e^{f(x)} = \int_{\sum n_\sigma \mathcal{J}_\sigma} g(z) e^{f(z)}$
- \mathcal{J}_0 from $z=0$ is a natural choice for integration contour, on which $\text{Im}S=0!!$ - No sign problem!?

Path integral on Lefschetz thimble

- Coordinates on J_0
 - Thimble is \mathbb{R}^n dimensional, the same as the original
 - For any point z on J_0 , there is a unique flow by τ starting at $z_0 = \varepsilon^\alpha V^a(0)$ near 0: **natural coordinates** $(\tau, \varepsilon^\alpha)$
 - We need Jacobian **$\det(V(z))$** , which is in general complex: **residual sign problem**

Cristoforetti et al (Aurora Coll.)

$$\int d\phi e^{-S(\phi)} = \int_{J_0} dz e^{-S(z)} = \int d\xi \left| \frac{dz}{d\xi} \right| e^{-S(\xi)}$$



- $\{V(z)\}$ needs to be parallel-transported from 0

HMC algorithm on Lefschetz thimble J_0

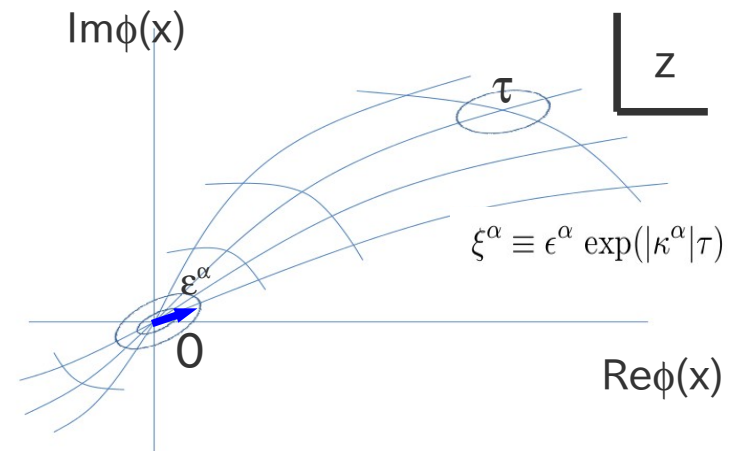
- Pick up an initial pt randomly:

$$z = \epsilon^\alpha V_i^\alpha(0) + \int_0^\tau dt \bar{\partial} \bar{S}[\bar{z}(t)] \equiv z[\epsilon^\alpha, \tau]$$

- Use coordinates $\xi^\alpha(\epsilon^\alpha, \tau)$

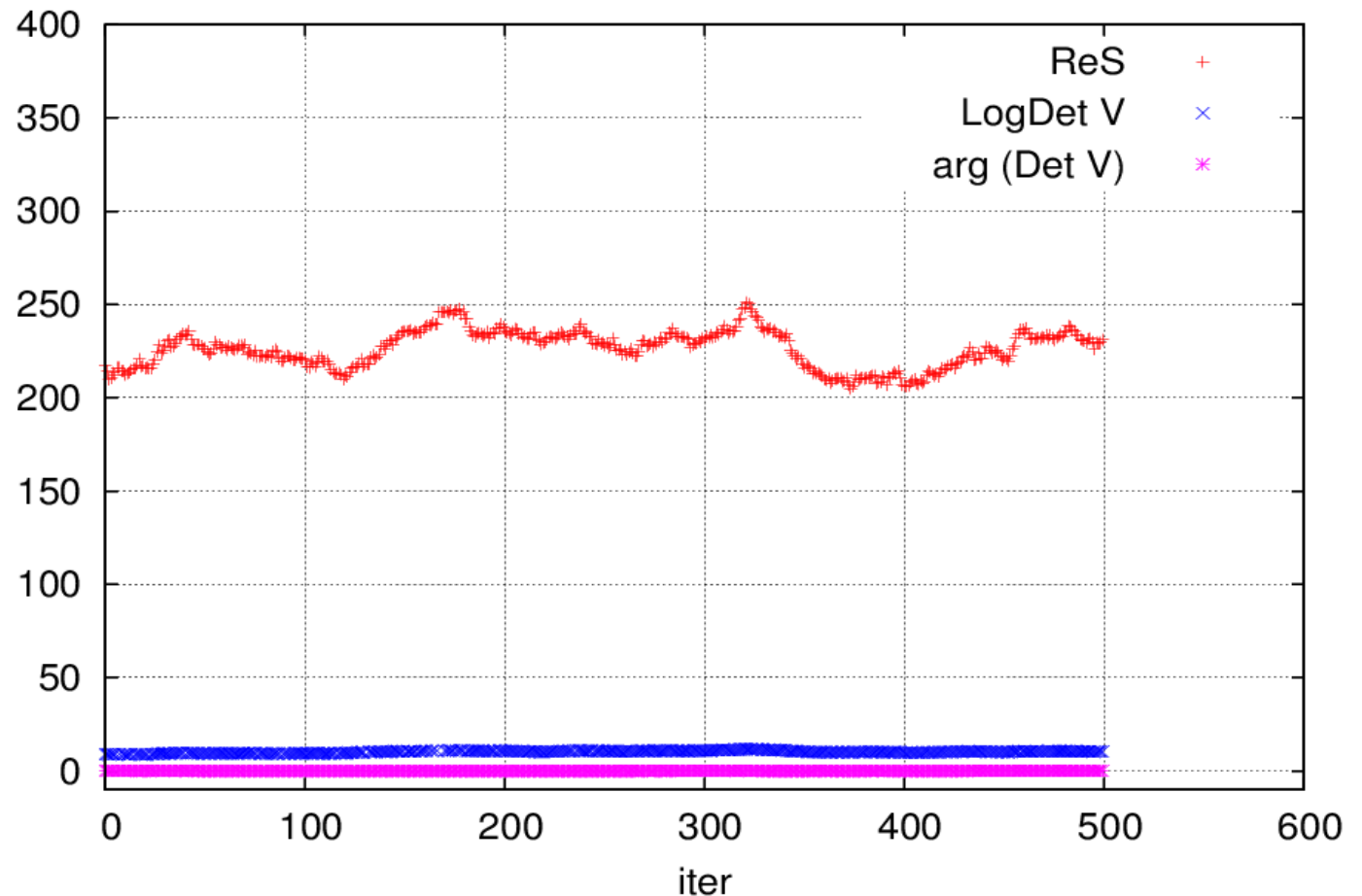
$$\begin{aligned} \dot{\xi}^\alpha &= p^\alpha \\ \dot{p}^\alpha &= -\frac{\partial S}{\partial \xi^\alpha} = -\frac{1}{2} \{ \partial_i S[z] V_i^\alpha(\tau) + \bar{\partial}_i \bar{S}[\bar{z}] \bar{V}_i^\alpha(\tau) \} \exp(-|\kappa^\alpha| \tau) \end{aligned}$$

- HMC needs (Field conf “z” & tangent vecs “V $^\alpha$ ”)
- Prepare (z , {V $^\alpha$ }) at (ϵ^α, τ) by solving flow eqn (parallel-transport of {V $^\alpha(0)$ })
- Jacobian det{V} should also be included
- Repeat HMC towards thermalization



First trial look at HMC on J_0 of ϕ^4

- $\kappa=\lambda=1, \mu=0.3, N=4$
- The HMC code runs!



- Trajectory length=0.08, step size=0.008 (very rough)

HMC on Lefschetz thimble J_0 of ϕ^4

- Time consuming: several min for one trajectory
 - Core i7 PC w/ C2070 GPU
- Residual sign problem seems numerically almost absent!
 - If exact!?, physical reasoning & proof should be possible (by Honda, Kato, Komatsu + us)
 - Unlike the Fresnel integral, $Z(\mu)$ is real positive and respects Charge Conjugation symmetry

Discussion and outlook

- Complex Langevin
 - does sampling in enlarged complexified space
 - works beautifully in some cases
 - more realistic cases with fermions, phase transitions, to be examined
- Lefschetz thimble
 - functional version of steepest descent method
 - time consuming to handle thimble geometry
 - But sign problem may be almost absent!