Lattice QCD with (u,d,s,c) overlap/DW quarks at the physical point

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Outline

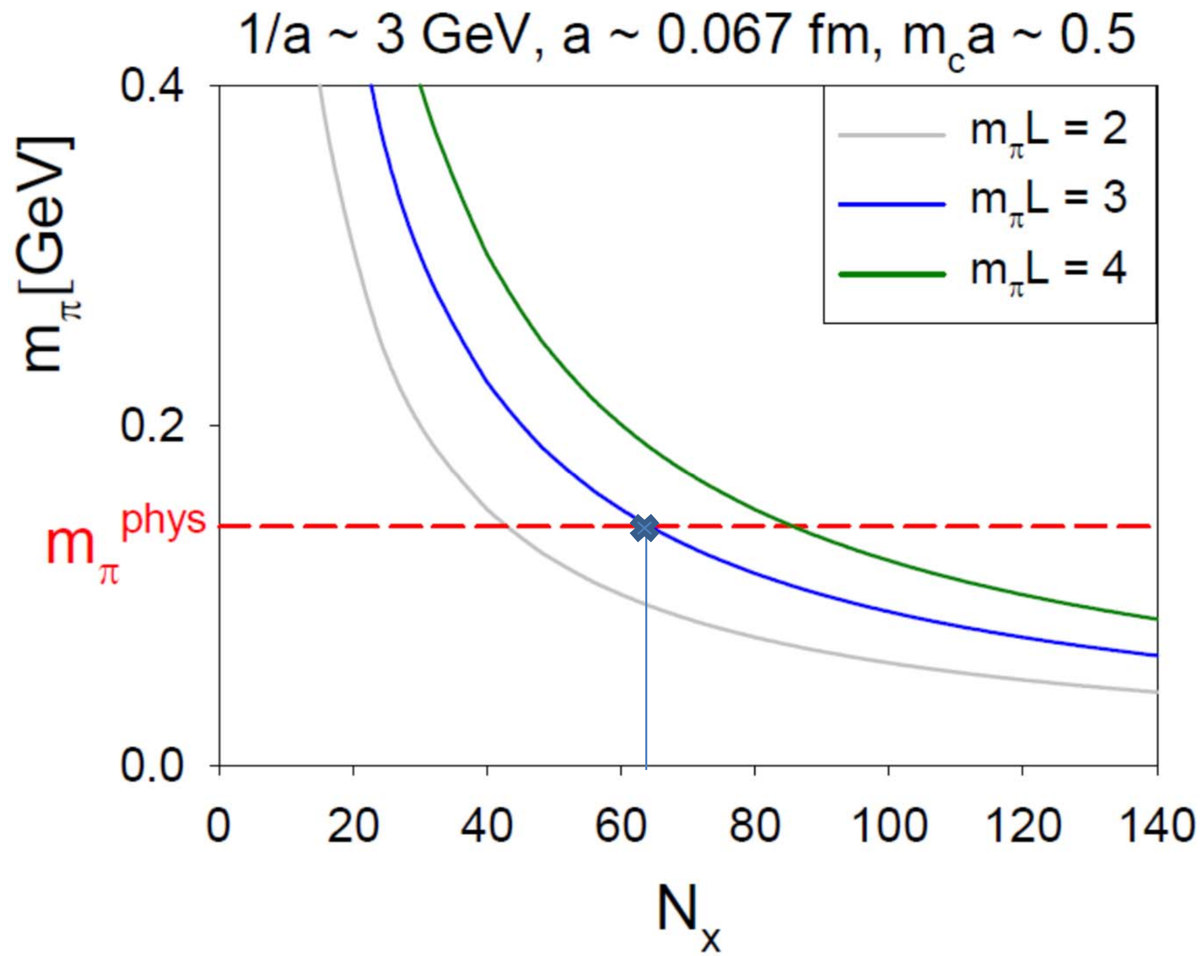
- Current status of lattice QCD at the physical point
- Design lattice QCD with physical (u,d,s,c) quarks
- Lattice QCD with overlap/DW quarks
- Simulate LQCD with physical (u,d,s,c) overlap/DWQ
- Computational platform - Nvidia DGX-1
- Lattice setup and simulation parameters
- Salient features of the simulation
- Preliminary results of the meson spectrum
- Conclusion and outlook

Current Status of lattice QCD at the physical point

The holy grail of lattice QCD is to simulate QCD with all quarks at their physical masses, with sufficiently large volume and fine lattice spacing, then to extract physics from these gauge ensembles.

Collaboration	Lattice Fermion	u/d	u/d, s	u/d, s, c	u, d, s, c	u/d, s, c, b
MILC	highly improved staggered fermion		X	X		
PACS-CS	Improved Wilson fermion		X			
tmQCD	twisted mass Wilson fermion	X	X	X		
RBC/UKQCD	DWF (Shamir, Möbius)		X			
TWQCD	optimal DWF			X		

Design lattice QCD with physical (u,d,s,c) quarks



For the $L^3 \times T = 64^3 \times 128$ lattice, $M_\pi L \approx 3$, $M_\pi \approx 140$ MeV, $L \approx 4.3$ fm

Lattice Fermions

- It took 24 years (1974 ~1998) to realize that **Lattice QCD with Exact Chiral Symmetry** is the ideal theoretical framework to study the nonperturbative physics from the first principles of **QCD**.
- **It is challenging to perform the Monte Carlo simulation** such that the chiral symmetry is preserved to very high precision and all topological sectors are sampled ergodically, and all quarks at their physical masses.
- The computational requirement for **Lattice QCD with overlap/DW quarks** is ~**10-100 times** more than their counterparts with traditional lattice fermions (e.g., Wilson, staggered, and their variants).

Lattice QCD with Exact Chiral Symmetry

The Nelson-Ninomiya theorem (1981) asserts that it is impossible to have massless lattice Dirac fermion which possesses the continuum chiral symmetry without violating some basic properties (e.g., locality, doubler-free, ...) of the Dirac fermion.

The best way to break the chiral symmetry on the lattice is given by

$$D\gamma_5 + \gamma_5 D = 2rD\gamma_5 D$$ Ginsparg-Wilson relation (1982)

$$\Leftrightarrow D^{-1}_{xy}\gamma_5 + \gamma_5 D^{-1}_{xy} = 2r\gamma_5\delta_{xy}$$ Chiral symmetry is broken by a contact term

$$\Leftrightarrow D^{-1}_{xy}\gamma_5 + \gamma_5 D^{-1}_{xy} = 0,$$ for $x \neq y$, exactly the same in continuum

Explicit realization of the GW relation

$$D = \frac{1}{2r}\left(1 + \gamma_5 \frac{H}{\sqrt{H^2}}\right),$$ overlap Dirac op. (Neuberger 1997)

Topology on the lattice

Axial anomaly

$$\mathrm{tr}\left[\gamma_5(1-rD)_{x,x}\right] \xrightarrow{a\to 0} \frac{1}{32\pi^2}\varepsilon^{\mu\nu\lambda\sigma}\mathrm{tr}\left(F_{\mu\nu}F_{\lambda\sigma}\right)$$

Index Theorem

$$\mathrm{Tr}\left[\gamma_5(1-rD)\right] = n_+ - n_- = Q_{\mathrm{top}} = \int d^4x \frac{1}{32\pi^2}\varepsilon^{\mu\nu\lambda\sigma}\mathrm{tr}\left(F_{\mu\nu}F_{\lambda\sigma}\right)$$

Salient features of lattice QCD with exact chiral symmetry

Difficulties of Simulating LQCD with Overlap Fermion

$$D = m_q + \frac{(1 - r m_q)}{2r}\left[1 + \gamma_5 H (H^2)^{-1/2}\right],$$

$$r = 1/\left[2m_0(1 - d m_0)\right], \quad m_0 \in (0, 2).$$

$H = c H_w (1 + d \gamma_5 H_w)^{-1}$, c and d are constants

$$\det D = \begin{cases} (r m_q)^{n_+} \det \mathcal{H}_-^2 = (r m_q)^{-n_+} \det \mathcal{H}_+^2, & n_+ \geq 0, \\ (r m_q)^{n_-} \det \mathcal{H}_+^2 = (r m_q)^{-n_-} \det \mathcal{H}_-^2, & n_- \geq 0, \end{cases}$$

where $\mathcal{H}_\pm^2 = P_\pm (D^\dagger D)$, and $P_\pm = (1 \pm \gamma_5)/2$.

HMC requires the computation of $\delta n_\pm$ at each step of the MD, prohibitively expensive even for a small lattice (e.g., $16^3 \times 32$).

Difficulties of Simulating LQCD with Overlap Fermion

$$D = m_q + \frac{(1 - rm_q)}{2r}\left[1 + \gamma_5 H (H^2)^{-1/2}\right],$$

$$r = 1/\left[2m_0(1 - dm_0)\right], \quad m_0 \in (0, 2).$$

$$H = cH_w(1 + d\gamma_5 H_w)^{-1}, \ c \text{ and } d \text{ are constants}$$

$$\det D = \begin{cases} (rm_q)^{n_+} \det \mathcal{H}_-^2 = (rm_q)^{-n_+} \det \mathcal{H}_+^2, & n_+ \geq 0, \\ (rm_q)^{n_-} \det \mathcal{H}_+^2 = (rm_q)^{-n_-} \det \mathcal{H}_-^2, & n_- \geq 0, \end{cases}$$

where $\mathcal{H}_\pm^2 = P_\pm(D^\dagger D)$, and $P_\pm = (1 \pm \gamma_5)/2$.

Moreover, the discontinuity of the $\det D$ at the topological boundary highly suppresses the crossing rate between different topological sectors, thus renders HMC failing to sample all topological sectors ergodically.

Difficulties of Simulating LQCD with Overlap Fermion

These difficulties can be circumvented as follows.

(I) Any positive Dirac operator satisfying $\gamma_5 D \gamma_5 = D^\dagger$ possesses a positive-definite pseudofermion action for one-flavor fermion, without explicit dependence on $n_\pm$.

(II) The step function of the fermion determinant at the topological boundary can be smoothed out by using DWF with finite $N_s (= 16)$, then the HMC on the 5-dimensional lattice can sample all topological sectors ergodically and also keep the chiral symmetry at a good precision (e.g., the residual mass less than 5% of the bare quark mass).

Effective 4D Dirac op. of DWF ⟺ overlap Dirac op.

Domain-Wall Fermion

$$A_{\rm dwf} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}_{x,s} \left[\left(I + \rho_s D_w \right)_{x,x'} \delta_{s,s'} - \left(I - \sigma_s D_w \right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \psi_{x',s'}$$

$$\equiv \bar{\Psi} D_{\rm dwf} \Psi$$

$$D_w = \sum_{\mu=1}^{4} \gamma_\mu t_\mu + W - m_0, \qquad m_0 \in (0,2)$$

$$\rho_s = c\omega_s + d$$
$$\sigma_s = c\omega_s - d$$
$$c, d \ \text{(constants)}$$

$$t_\mu(x,x') = \frac{1}{2} \left[U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

$$W(x,x') = \sum_{\mu=1}^{4} \frac{1}{2} \left[2\delta_{x,x'} - U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

with boundary conditions

$$P_+ \psi(x,0) = -r m_q P_+ \psi(x,N_s), \quad m_q\text{: bare mass}, \quad r = 1/[2m_0(1-dm_0)]$$

$$P_- \psi(x,N_s+1) = -r m_q P_- \psi(x,1), \qquad P_\pm = \frac{1}{2}(1 \pm \gamma_5)$$

Domain-Wall Fermion (cont)

The action for Pauli-Villars fields is

$$A_{PV} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\phi}_{x,s} \left[\left(I + \rho_s D_w \right)_{x,x'} \delta_{s,s'} - \left(I - \sigma_s D_w \right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \phi_{x',s'}$$

with boundary conditions:

$$P_+ \phi(x,0) = -P_+ \phi(x, N_s),$$
$$P_- \phi(x, N_s + 1) = -P_- \phi(x,1)$$

$$\int [d\bar{\psi}][d\psi][d\bar{\phi}][d\phi] \exp\left(-A_{\text{odwf}} - A_{\text{PV}}\right) = \frac{\det D_{\text{odwf}}(m_q)}{\det D_{\text{odwf}}(m_{PV})} = \det D(m_q)$$

$$m_{PV} = 2m_0(1 - dm_0)$$

The effective 4D Dirac operator

$$D(m_q) = m_q + \left(m_0(1 - dm_0) - \frac{m_q}{2} \right) \left[1 + \gamma_5 S(H) \right], \quad H = cH_w (1 + d\gamma_5 H_w)^{-1}$$

$$\lim_{N_s \to \infty} S(H) = \frac{H}{\sqrt{H^2}}$$

Variants of Domain-Wall Fermion

Sharmir DWF: $c = d = \frac{1}{2}, \; \omega_s = 1, \; H = H_w (2 + \gamma_5 H_w)^{-1}, \; S(H) = \text{polar approx. of } \frac{H}{\sqrt{H^2}}$

Möbius DWF: $d = \frac{1}{2}, \; \omega_s = 1, \; H = 2cH_w (2 + \gamma_5 H_w)^{-1}, \; S(H) = \text{polar approx. of } \frac{H}{\sqrt{H^2}}$

Borici DWF: $c = 1, \; d = 0, \; \omega_s = 1, \; H = H_w, \; S(H) = \text{polar approx. of } \frac{H_w}{\sqrt{H_w^2}}$

Optimal DWF: $c = 1, \; d = 0, \; H = H_w,$ [TWC, Phys. Rev. Lett. 90 (2003) 071601]

$$\omega_s = \frac{1}{\lambda_{\min}} \sqrt{1 - \kappa'^2 sn^2(v_s; \kappa')}, \quad s = 1, \cdots, N_s$$

$$S(H) = \text{Zolotarev optimal rational approximation of } \frac{H_w}{\sqrt{H_w^2}}$$

ODWF can keep the residual mass very small, for both light and heavy quarks.

2+1+1 = 2+2+1

For domain-wall fermions

$$\frac{\det D(m_{u/d})}{\det D(m_{PV})}\frac{\det D(m_{u/d})}{\det D(m_{PV})}\frac{\det D(m_s)}{\det D(m_{PV})}\frac{\det D(m_c)}{\det D(m_{PV})}$$

$$=\left(\frac{\det D(m_{u/d})}{\det D(m_{PV})}\right)^2\left(\frac{\det D(m_c)}{\det D(m_{PV})}\right)^2\frac{\det D(m_s)}{\det D(m_c)}$$

2-flavor | 2-flavor | 1-flavor

- For the one-flavor, use the exact pseudofermion action for one-flavor DWF [Y.C. Chen & TWC, Phys. Lett. B738 (2014) 55; TWC, Phys. Lett. B744 (2015) 95]
- For the 2-flavor part, use the two-flavors algorithm for DWF [TWC, T.H. Hsieh, Y.Y. Mao, Phys. Lett. B702 (2012) 131]

Exact One-Flavor Pseudofermion Action (EOFA)

[Y.C. Chen & TWC, Phys. Lett. B738 (2014) 55; TWC, Phys. Lett. B744 (2015) 95]

The exact pseudofermion action for one-flavor DWF can be written as

$$S_{pf} = \begin{pmatrix} 0 & {\phi_1}^\dagger \end{pmatrix} \left[I - k{v_-}^T \omega^{-1/2} \frac{1}{H\,(m)} \omega^{-1/2} v_- \right] \begin{pmatrix} 0 \\ \phi_1 \end{pmatrix}$$

$$+ \begin{pmatrix} {\phi_2}^\dagger & 0 \end{pmatrix} \left[I + k{v_+}^T \omega^{-1/2} \frac{1}{H(1) - \Delta_+(m) P_+} \omega^{-1/2} v_+ \right] \begin{pmatrix} \phi_2 \\ 0 \end{pmatrix}$$

where $H(m) = \gamma_5 R_5 D(m),\ R_5 = \delta_{s',N_s+1-s}$

$$\Delta_\pm(m) = k\omega^{-1/2} v_\pm {v_\pm}^T \omega^{-1/2}$$

$$k = \frac{c}{1 - c\lambda} \frac{1 - m}{1 + m(1 - 2c\lambda)}$$

which is Hermitian and positive-definite.

Salient Features of EOFA

- It is an exact, Hermitian and positive-definite pseudofermion action for HMC of one-flavor DWF, without taking square root.
- It can be used for all variants of DWF, and for any approximations (polar or Zolotarev) of the sign function.
- The memory consumption of EOFA is much smaller than that of RHMC. This feature is crucial for using GPUs to simulate QCD.
- The efficiency of HMC with EOFA is more than 3 times faster than that using RHMC.

2-flavors algorithm for DWF

By even-odd preconditioning (see next page)

$$\mathcal{D}(m_q) = S_1^{-1} \begin{pmatrix} 1 & M_5 D_w^{\mathrm{EO}} \\ M_5 D_w^{\mathrm{OE}} & 1 \end{pmatrix} S_2^{-1}$$

Schur decomposition

$$\mathcal{D}(m_q) = S_1^{-1} \begin{pmatrix} 1 & 0 \\ M_5 D_w^{\mathrm{OE}} & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & C \end{pmatrix} \begin{pmatrix} 1 & M_5 D_w^{\mathrm{EO}} \\ 0 & 1 \end{pmatrix} S_2^{-1}$$

$$C \equiv 1 - M_5 D_w^{\mathrm{OE}} M_5 D_w^{\mathrm{EO}}$$

Since $\det \mathcal{D} = \det S_1^{-1} \cdot \det C \cdot \det S_2^{-1}$
and S_1 and S_2 do not depend on the gauge field,
we can just use C in the Monte Carlo simulation.

For 2-flavors QCD, the pseudofermion action can be written as

$$S_{pf}^{2\mathrm{F}} = \phi^\dagger C_{PV}^\dagger (CC^\dagger)^{-1} C_{PV} \phi, \qquad C_{PV} = C(m_q = 1/r).$$

Even-Odd Preconditioning for the Lattice Dirac operator of DWF

In general,

$$\mathcal{D}(m_q) = D_w[c\omega(1+L)+d(1-L)]+(1-L), \qquad (L \text{ is defined in the next page})$$

$$= \begin{pmatrix} 4-m_0 & D_w^{\text{EO}} \\ D_w^{\text{OE}} & 4-m_0 \end{pmatrix} [c\omega(1+L)+d(1-L)]+(1-L)$$

$$= \begin{pmatrix} (4-m_0)[c\omega(1+L)+d(1-L)]+(1-L) & D_w^{\text{EO}}[c\omega(1+L)+(1-L)] \\ D_w^{\text{OE}}[c\omega(1+L)+d(1-L)] & (4-m_0)[c\omega(1+L)+d(1-L)]+(1-L) \end{pmatrix}$$

$$\equiv \begin{pmatrix} X & D_w^{\text{EO}}Y \\ D_w^{\text{OE}}Y & X \end{pmatrix} \equiv S_1^{-1} \begin{pmatrix} 1 & M_5 D_w^{\text{EO}} \\ M_5 D_w^{\text{OE}} & 1 \end{pmatrix} S_2^{-1},$$

$$M_5 \equiv \sqrt{\omega}^{-1} Y X^{-1} \sqrt{\omega} = \left\{ (4-m_0) + \sqrt{\omega}^{-1} [c(1-L)(1+L)^{-1} + d\omega^{-1}]^{-1} \sqrt{\omega}^{-1} \right\}^{-1}$$

$$S_1 \equiv \sqrt{\omega}^{-1} Y X^{-1} = M_5 \sqrt{\omega}^{-1}, \qquad S_2 \equiv Y^{-1}\sqrt{\omega}$$

Even-Odd Preconditioning for the Lattice Dirac operator of DWF (cont)

$$L(m) = P_+ L_+(m) + P_- L_-(m) = \begin{pmatrix} L_+(m) & 0 \\ 0 & L_-(m) \end{pmatrix}_{Dirac}$$

$$L_+(m)_{s,s'} = \begin{cases} \delta_{s',s-1} & , 1 < s \le N_s \\ -m\delta_{s',N_s} & , s = 1, \end{cases} \quad m = r m_q \,, \; r = 1/[2m_0(1 - d m_0)]$$

$$L_-(m) = L_+(m)^T$$

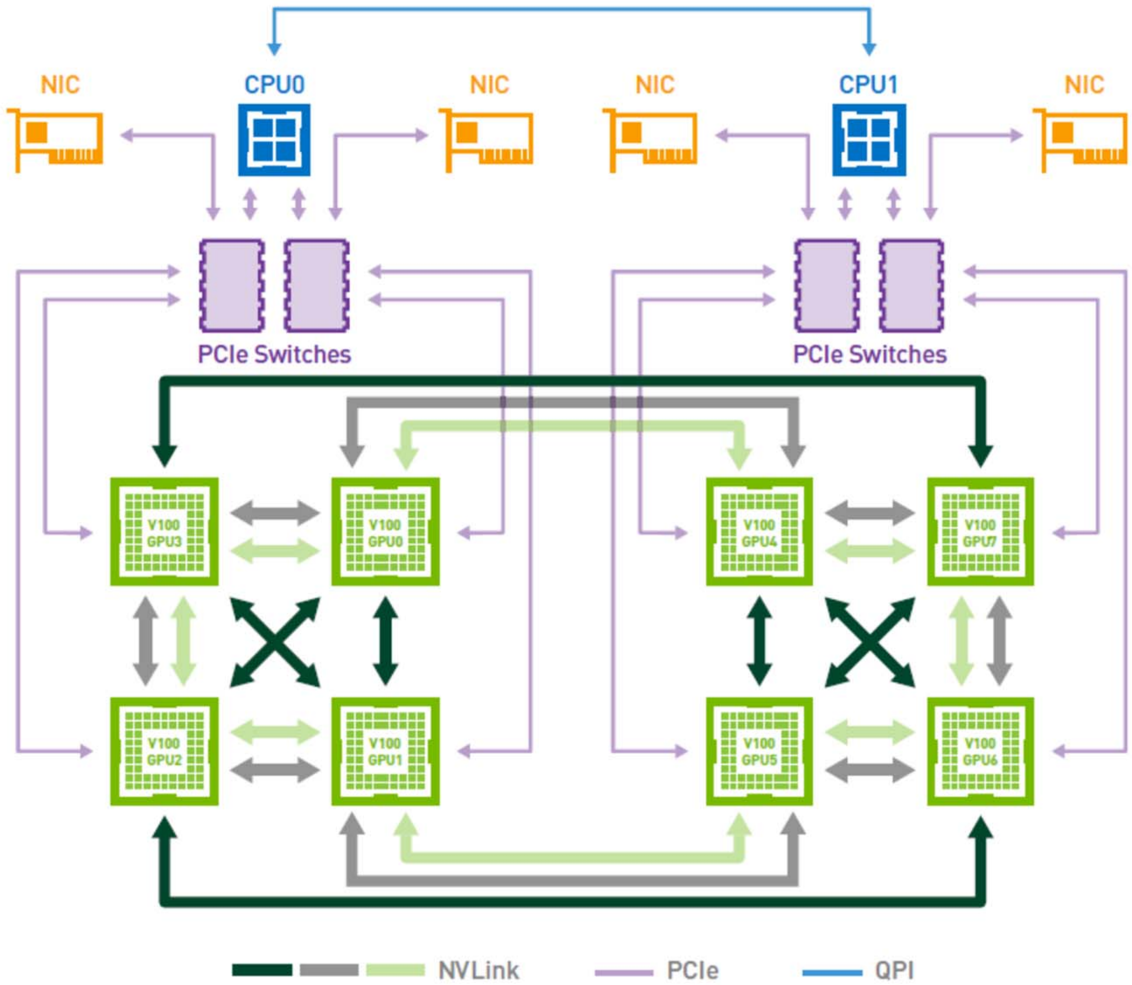
$L_\pm(m)$ are matrices in the fifth dimension, with dependence on quark mass.

How much does it take to simulate lattice QCD with physical (u,d,s,c) overlap/DW quarks ?

- To satisfy $M_\pi L \approx 3$, $M_\pi \approx 140$ MeV, $a^{-1} \approx 3$ GeV, $m_c a \approx 0.5$, the lattice size must be at least $64^3 \times 64$.
- For overlap/DW quarks with N_s=16, the 5D lattice is $64^3 \times 64 \times 16$, and the HMC (using EOFA) requires a memory space at least 128 GB.
- For DWF with good chiral symmetry ($m_{res} a < 5 \times 10^{-5}$), it requires >10 Tflops/s (sustained) to generate > 1 trajectory/day with $P_{\text{accept}} \approx 70\%$
- A GPU cluster with PCIe/infiniband-switch cannot attain this goal, due to the bottleneck of PCIe/internode communications.
- Currently, only Nvidia DGX-1, DGX-2, ... (or compatible systems with NVLink) can meet the requirements: device memory >128 GB, and sustained speed > 10 Tflops/s.

Nvidia DGX-1(8 V100+NVLink)

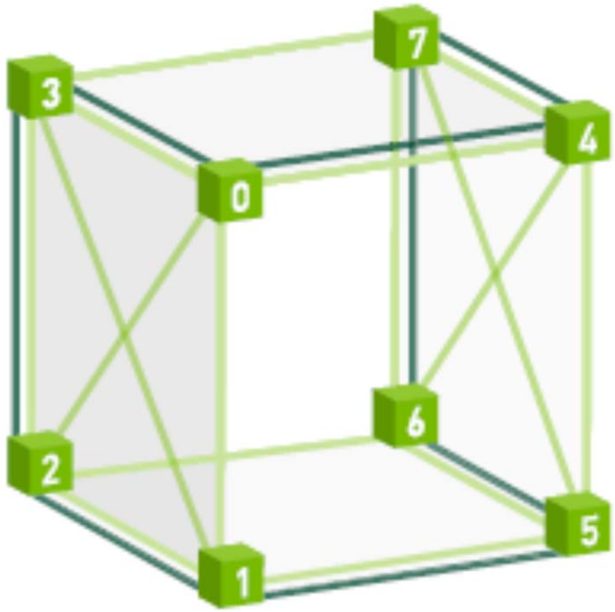
Figure taken from the White Paper
NVIDIA DGX-1 With Tesla V100 System Architecture



NVLink 2.0, data rate ~ 300 GB/s

Nvidia DGX-1(8 V100+NVLink)

➢ **Connection topology**: with 8 GPUs sitting at the corners of a cube, NVLink only connects the edges and 2 face diagonals.



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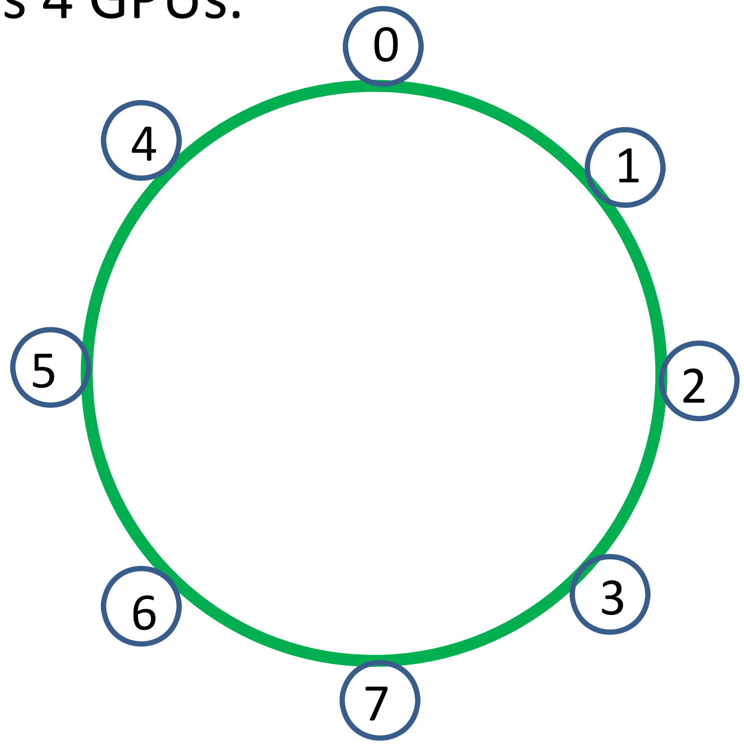
NVIDIA DGX-1 With Tesla V100 System Architecture

Nvidia DGX-1(8 V100+NVLink)

- **Connection topology**: with 8 GPUs sitting at the corners of a cube, NVLink only connects the edges and 2 face diagonals.
- export OpenMP environment to re-map 8 GPUs in a circle such that each GPU can access its neighbors P2P through NVLink, and each CPU handles 4 GPUs.



Lattice Setup and Simulation Parameters

- The gauge ensemble is generated on the $64^3 \times 64$ lattice with $N_s = 16$, and with the plaquette gauge action at $\beta = 6/g^2 = 6.20$
- Parameters for optimal DWF: $m_0 = 1.3$, $N_s = 16$, $\lambda_{\min}/\lambda_{\max} = 0.05/6.20$
- HMC with Multiple Time Scale Integration and Mass Preconditioning.
  [New mass preconditioning for EOFA, Y.C. Chen, TWC, arXiv:1710.09621]
- Omelyan Integrator for the Molecular Dynamics.
- Conjugate Gradient with Mixed Precision.
- For the one-flavor, use the Exact One-Flavor pseudofermion Action (EOFA)
  [Y.C. Chen & TWC, Phys. Lett. B738 (2014) 55; TWC, Phys. Lett. B744 (2015) 95]
- For the 2-flavor, use the two-flavor algorithm for DWF
  [TWC, T.H. Hsieh, Y.Y. Mao, Phys. Lett. B702 (2012) 131]

Lattice spacing and Quark masses

- The inverse lattice spacing ($a^{-1} \simeq 3.104 \pm 0.017$ GeV) is determined by the Wilson flow, using $\sqrt{t_0} = 0.1416(8)$ fm obtained by the MILC collaboration for $N_f = 2+1+1$.
- The masses of s and c quarks are fixed by the masses of $\phi(1020)$ and $J/\psi(3097)$ respectively, while the mass of u/d quarks by $M_\pi(140)$.
- Quark masses: $m_{u/d}a = 0.00125,\ m_s a = 0.04,\ m_c a = 0.55$

Basic Questions about the Simulation

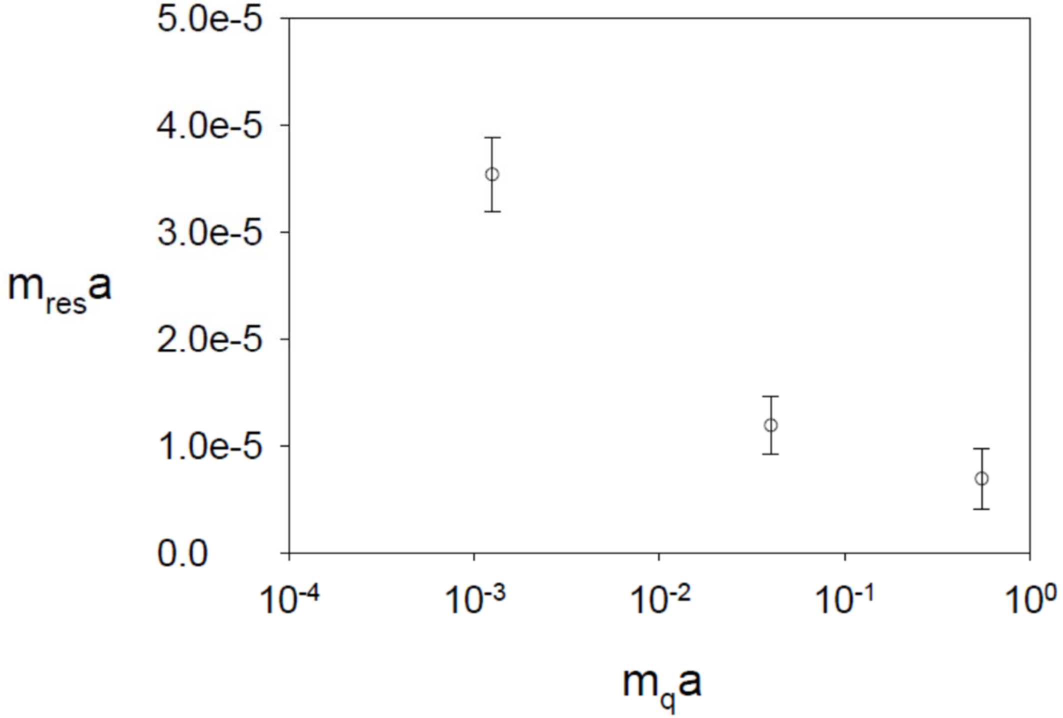
- What is chiral symmetry breaking due to finite Ns ?
  What are the residue masses for (u, d, s, c) quarks ?

- Does the simulation suffer from the topology freezing ?
  Does it sample all topological sectors ergodically ?

Chiral Symmetry Breaking due to finite Ns

Residual Mass

- Quark masses: $m_{u/d}a = 0.00125,\ m_s a = 0.04,\ m_c a = 0.55$

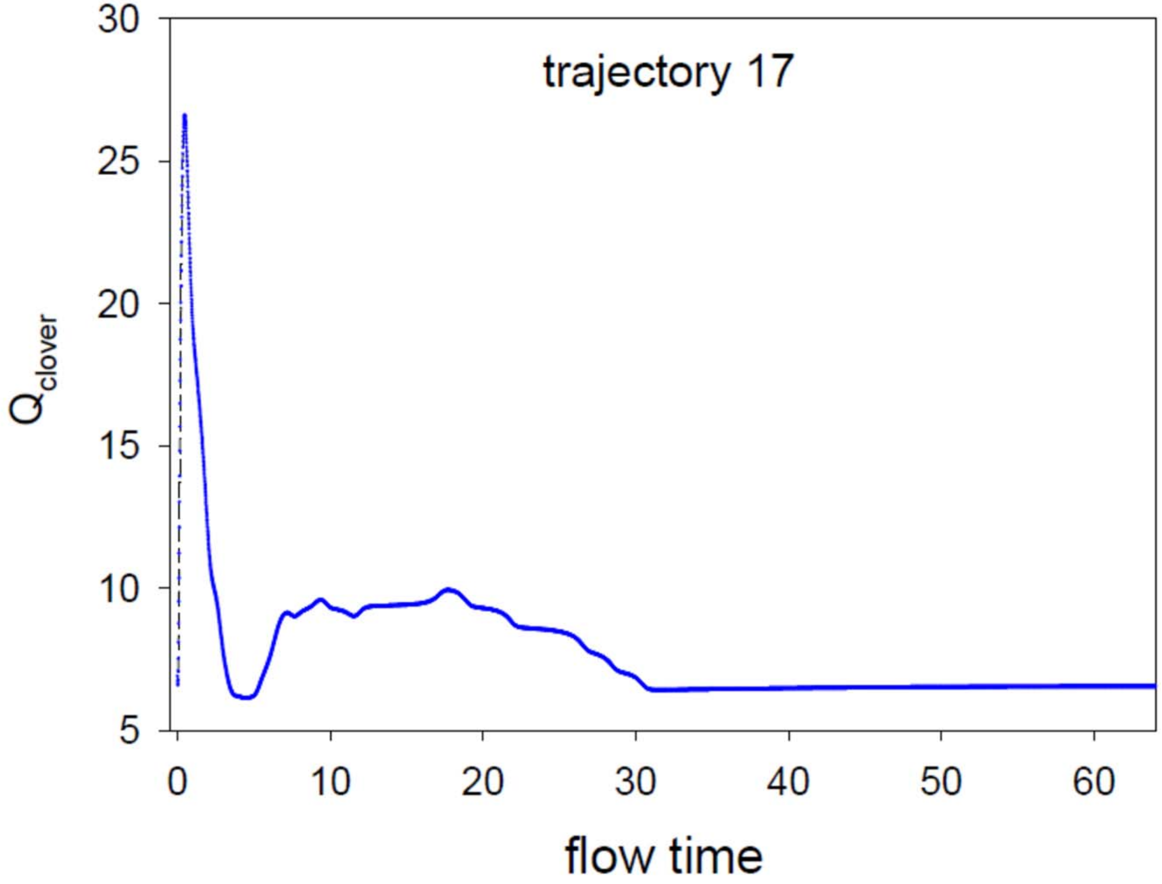


- Residual mass: $m_{res}a = 3.75(34)\times 10^{-5},\ 1.25(22)\times 10^{-5},\ 0.64(22)\times 10^{-5}$

$\approx$ 0.1 MeV, $\approx$ 0.04 MeV, $\approx$ 0.02 MeV

Clover Topological Charge from Wilson-Flow

At which flow time to measure the topological charge ?



The flow equation is integrated from $t = 0$ to $t = 64$ with $\Delta t = 0.01$

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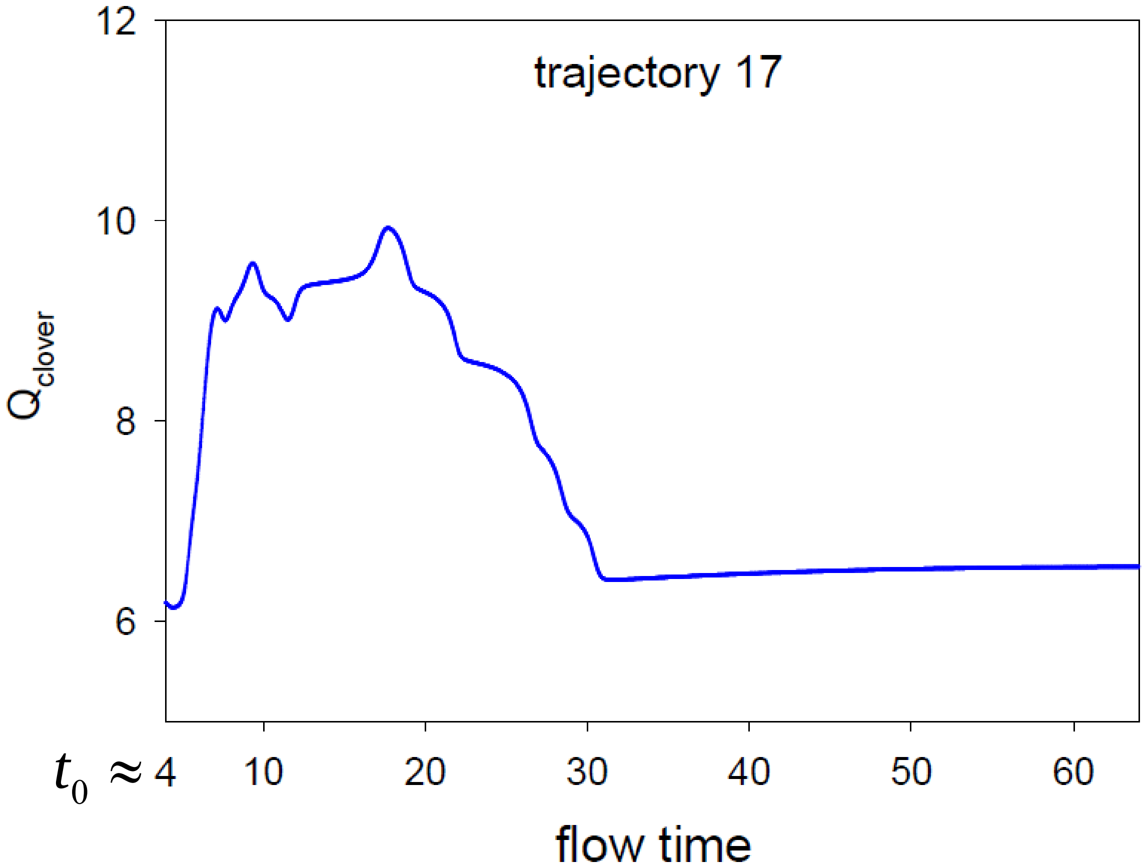

The most reliable topological charge seems to be at t=64

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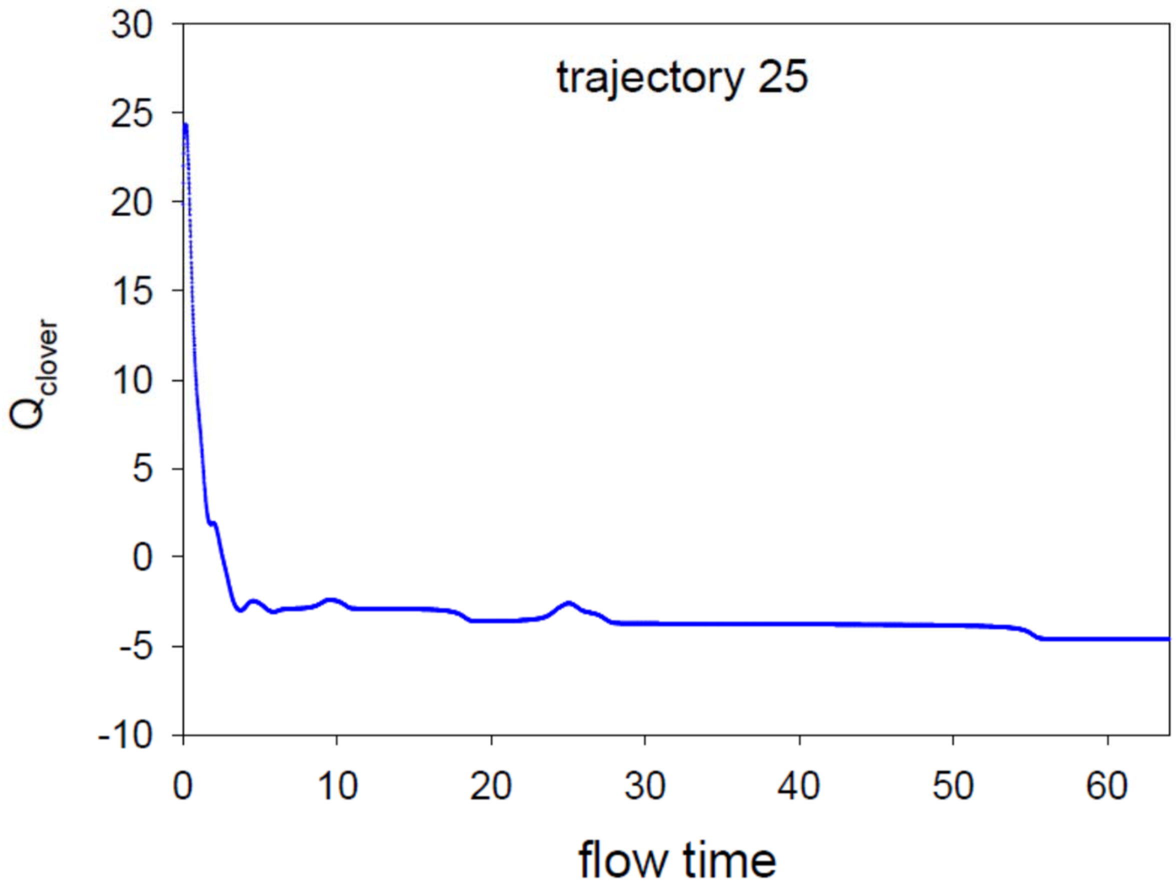

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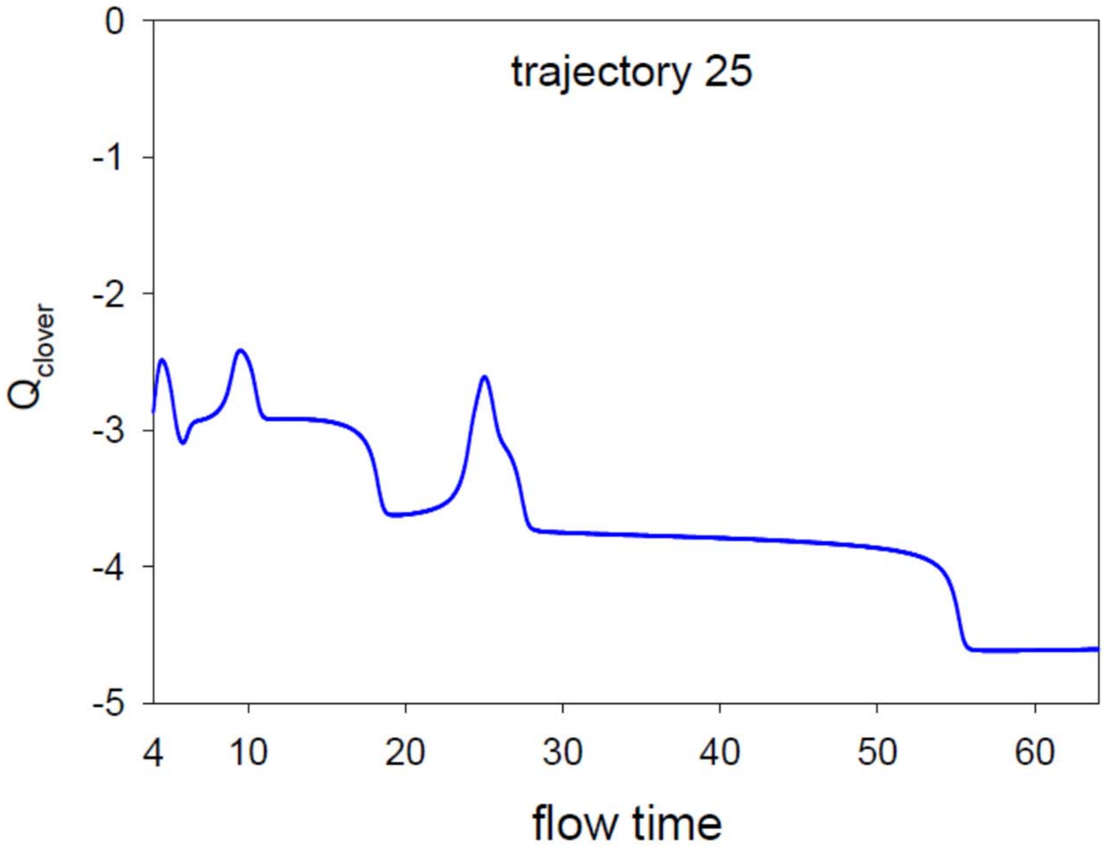

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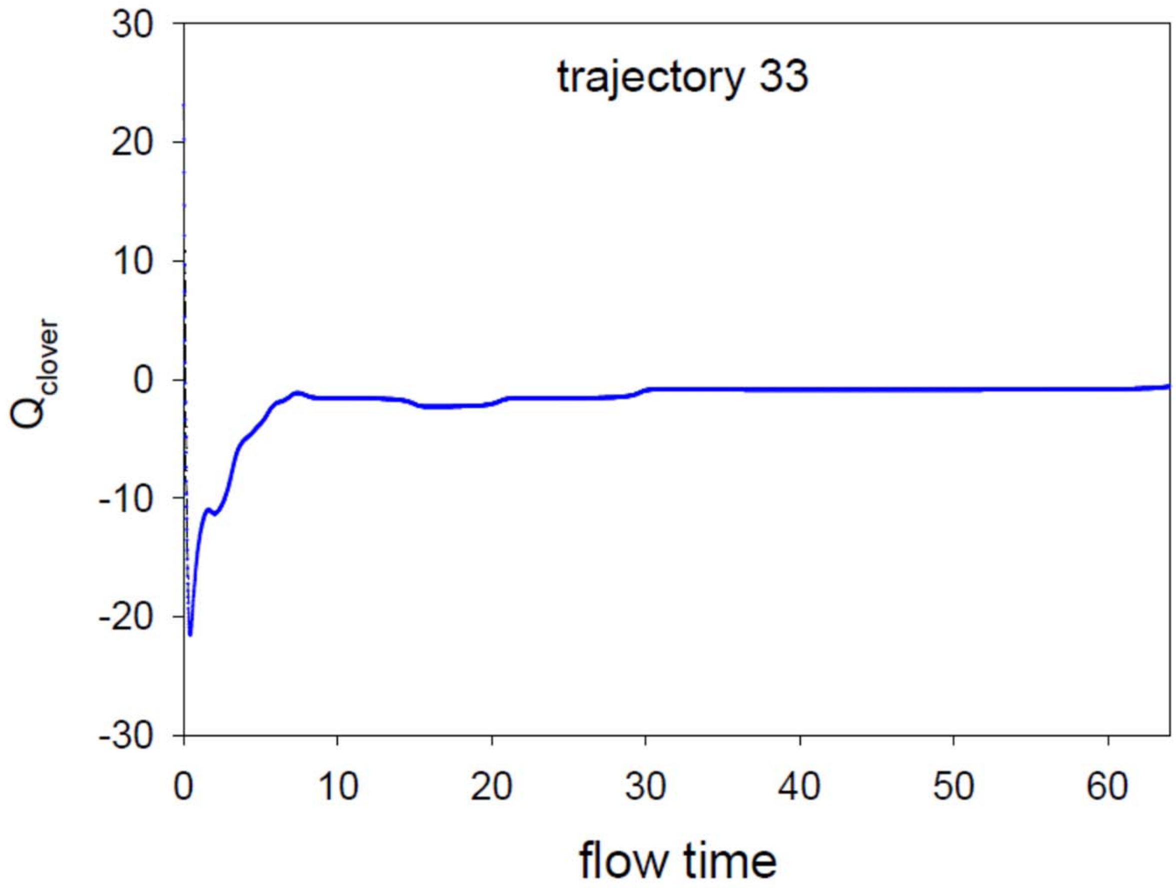

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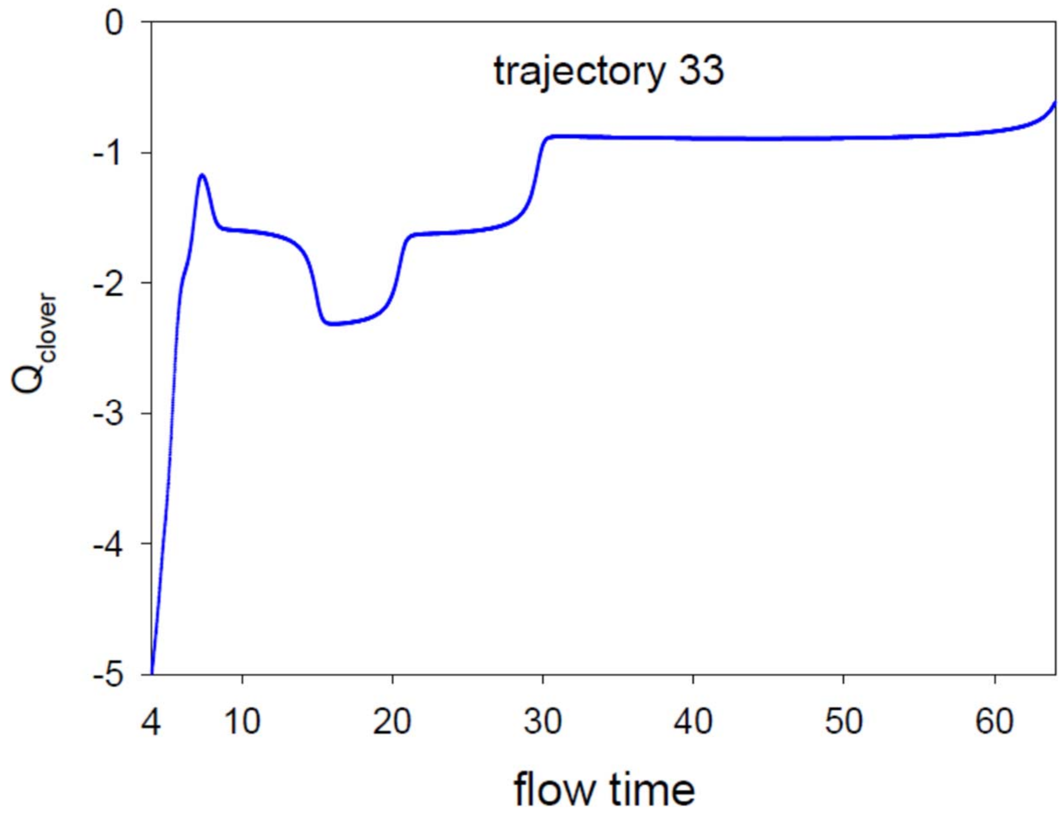
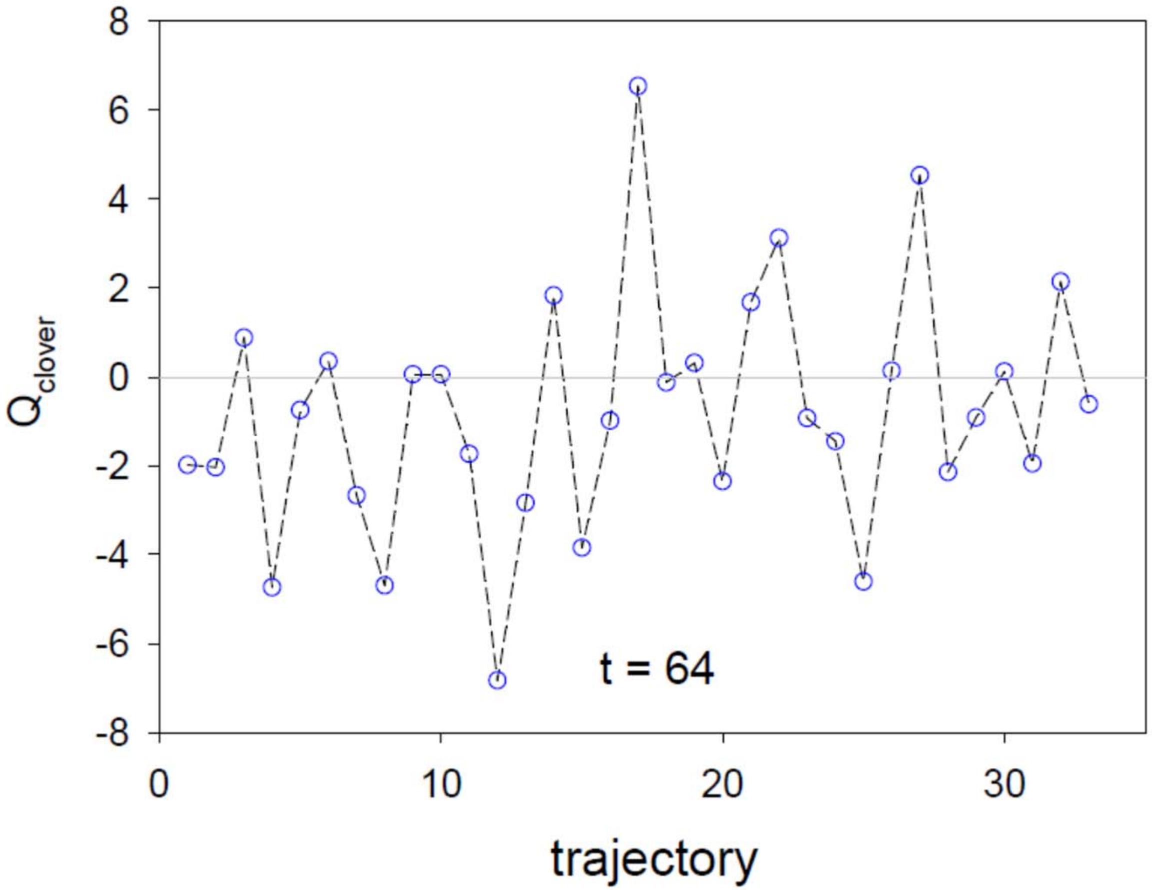


The most reliable topological charge seems to be at t=64

Topological Ergodicity

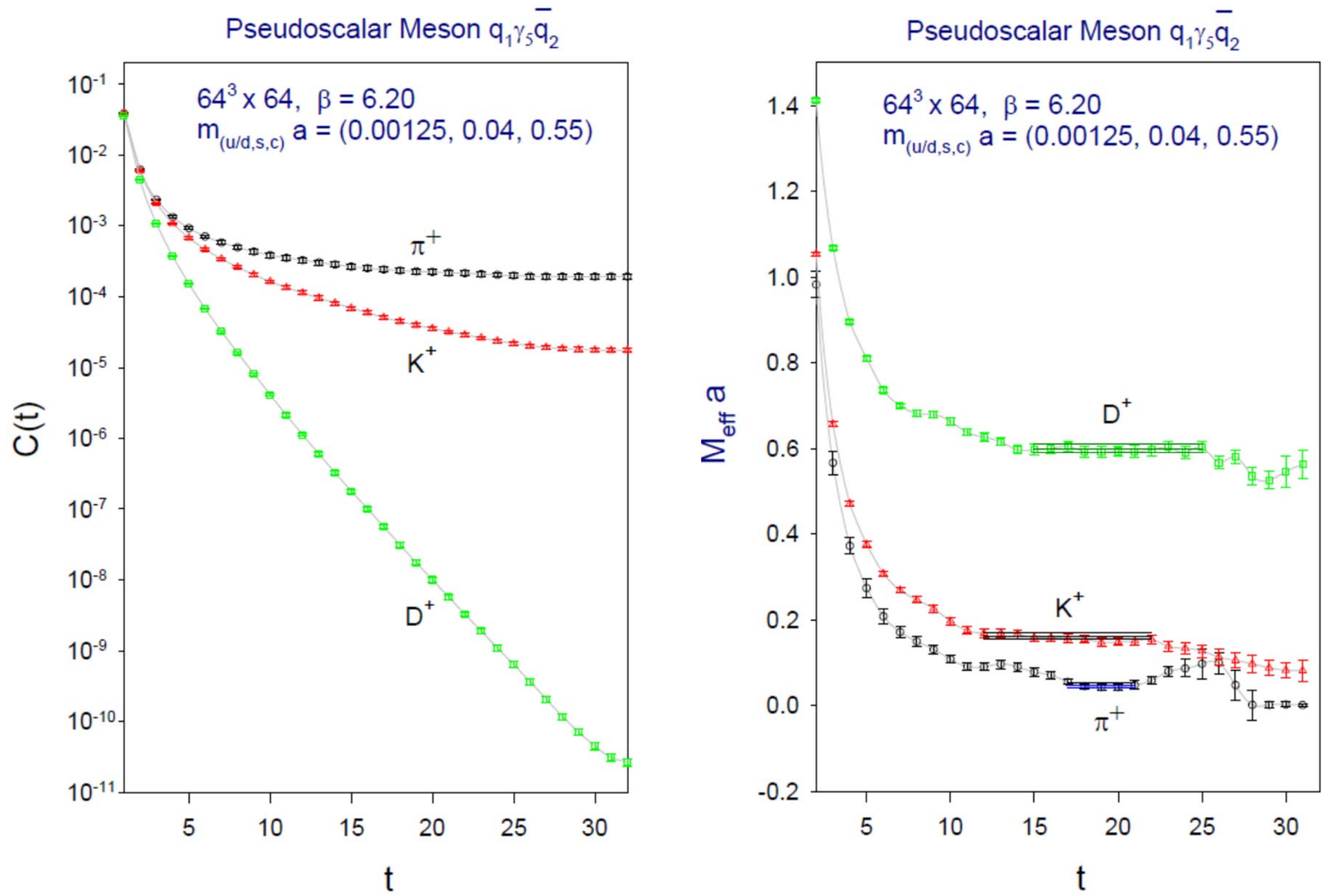
Clover topological charge of 33 successive trajectories, at the Wilson flow time t=64.



It confirms that the HMC does not suffer from the topology freezing.

Preliminary results of the meson spectrum

For 40 trajs after thermalization, sample one conf. every 5 trajs, resulting 8 confs.



Preliminary results of the meson spectrum (cont)

	$[t_1, t_2]$	χ^2/dof	Mass(MeV)	PDG(MeV)
$\pi^\pm$	[18, 21]	0.61	141(8)	140
$K^\pm$	[12, 18]	0.83	495(10)	494
$D^\pm$	[15, 22]	0.63	1874(18)	1870

Conclusion and Outlook

- We assert that it is feasible to simulate lattice QCD with physical (u, d, s, c) overlap/DW quarks, with good chiral symmetry, and sampling all topological sectors ergodically.
- The exact pseudofermion action for one-flavor DWF plays the crucial role in the simulation, not only to save the memory such that the HMC (on $64^4 \times 16$ lattice) can fit into the 128 GB device memory of DGX-1, but also to enhance the HMC efficiency significantly.
- Currently, we are generating gauge ensembles with physical (u, d, s, c) overlap/DW quarks, at zero and finite temperatures, on the lattices $64^3 \times (64,\ 24,\ 20,\ 16,\ 12,\ 10,\ 8,\ 6)$, with $T \approx (130,\ 150,\ 188,\ 250,\ 300,\ 375,\ 500)$ MeV.

Conclusion and Outlook

- With the new DGX-1 like platform with 8*V100(32 GB)+NVLink, we will generate gauge ensemble with physical (u, d, s, c) overlap/DW quarks on the $64^3 \times 128$ lattice.
- To generate gauge ensembeles with physical (u, d, s, c) quarks, we will be in a better position to extract the mass spectrum, decay constants, ..., as well as to understand some subtle nonperturbative physics, e.g, GIM mechanism, $\Delta I = 1/2$ rule, ...