Simulation of dynamical (u,d,s,c) overlap/DW quarks at the physical point

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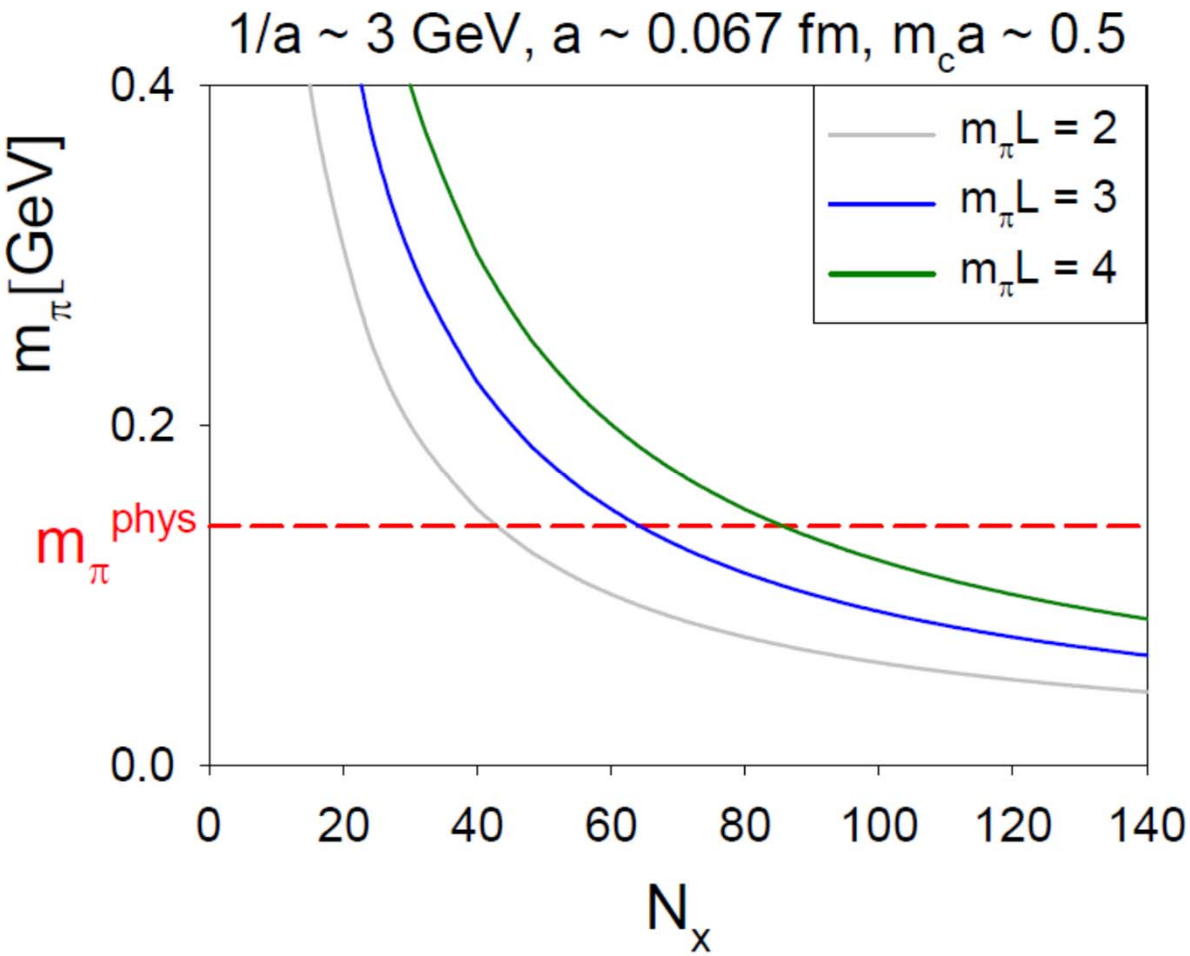
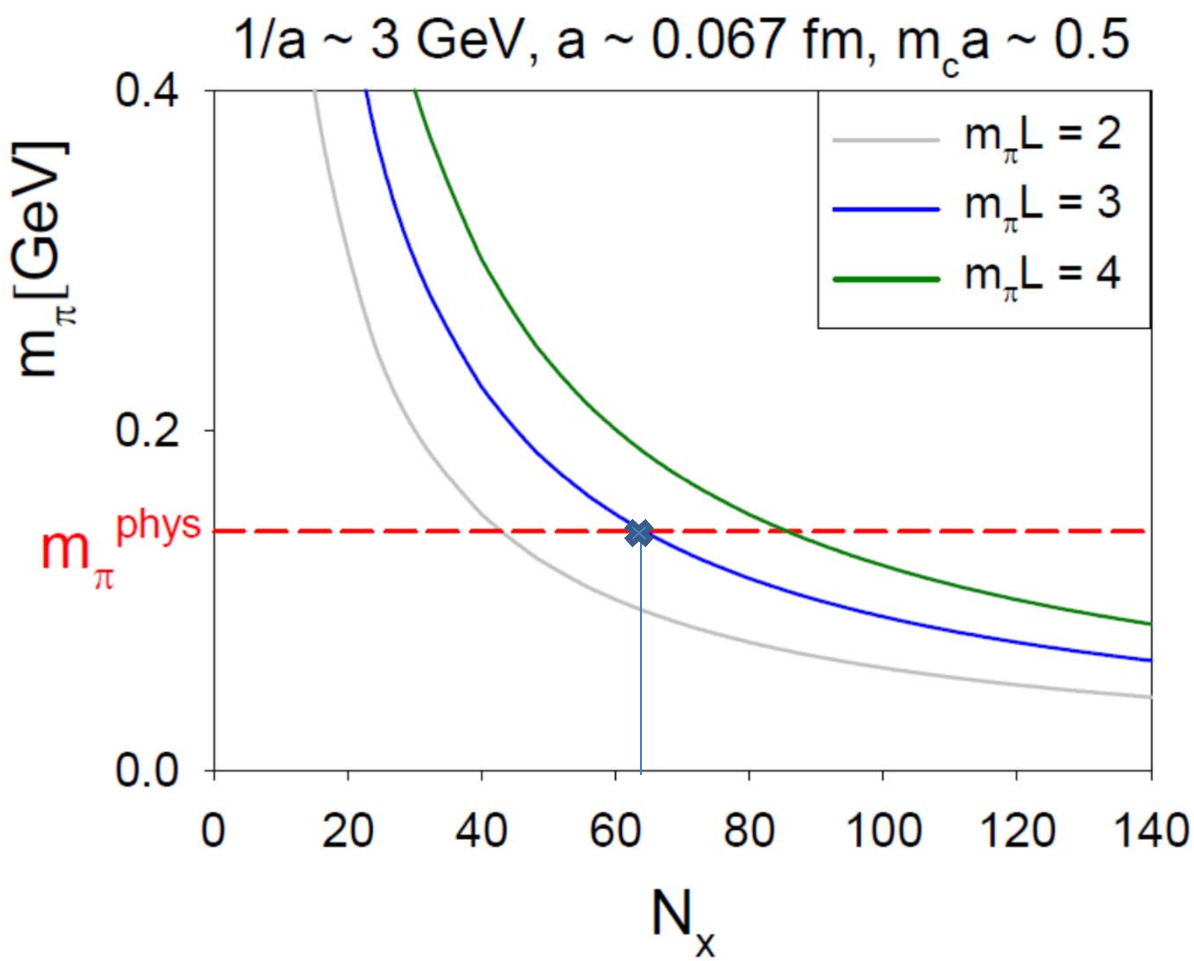
Outline

- 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
- Nvidia DGX-1
- Lattice setup and simulation parameters
- Salient features of the simulation
- Preliminary results of meson spectrum
- Conclusion and outlook

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



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



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

- 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**.

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- 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

Domain-Wall Fermion

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

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

$$\boxed{\begin{aligned}\rho_s&=c\omega_s+d\\ \sigma_s&=c\omega_s-d\\ c,d&\ \text{(constants)}\end{aligned}}$$

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

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

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

with boundary conditions

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

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

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]

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

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

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

2+1+1 = 2+2+1

For domain-wall fermions

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

$$=\underbrace{\left(\frac{\det D(m_{u/d})}{\det D(m_{PV})}\right)^2}_{\text{2-flavor}}\underbrace{\left(\frac{\det D(m_c)}{\det D(m_{PV})}\right)^2}_{\text{2-flavor}}\underbrace{\frac{\det D(m_s)}{\det D(m_c)}}_{\text{1-flavor}}$$

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

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

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

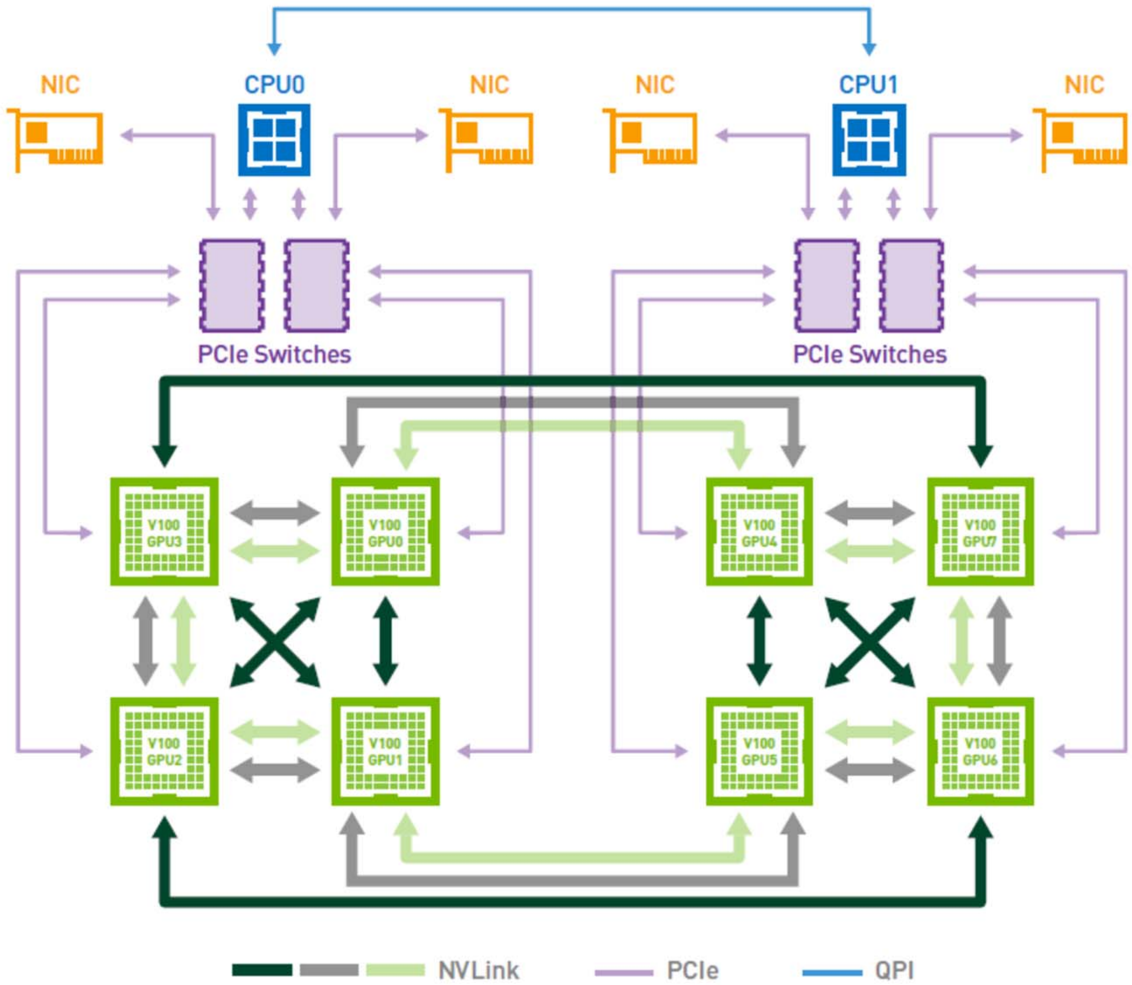
$L_\pm(m)$ are matrices in the fifth dimension, with dependence on quark mass.

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)

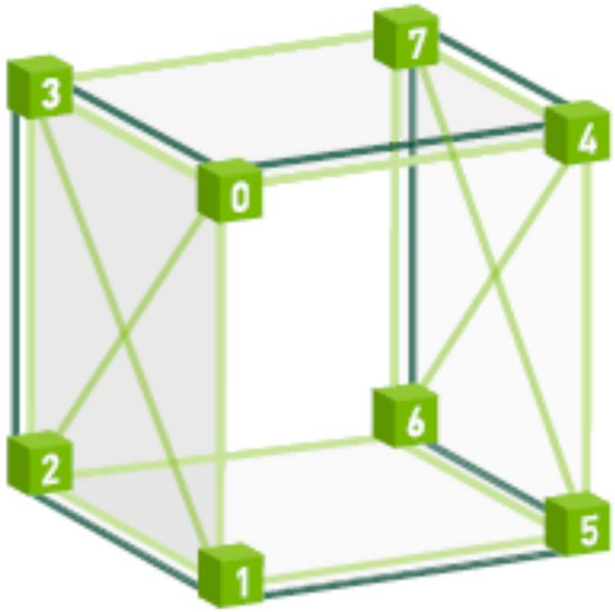
Figure taken from the White Paper
NVIDIA DGX-1 With Tesla V100 System Architecture



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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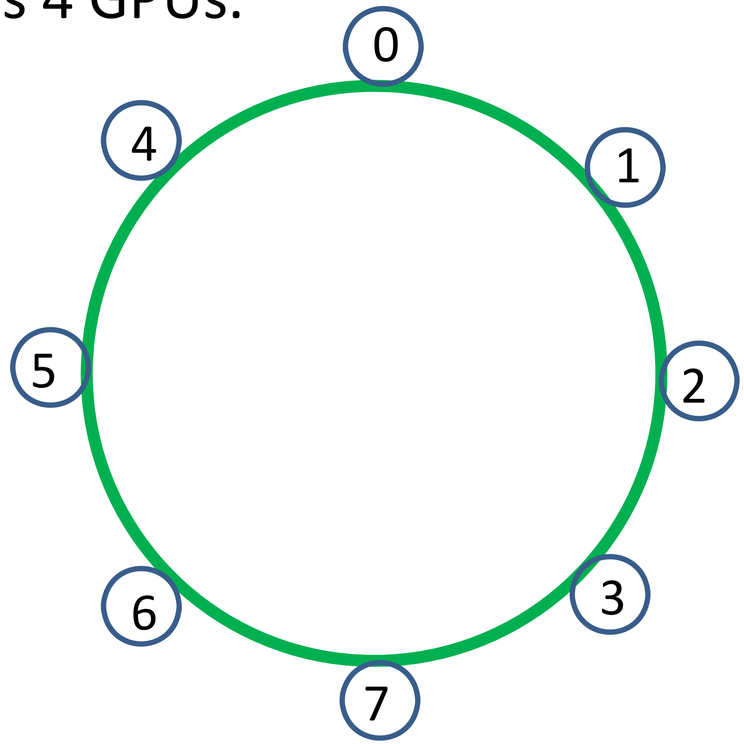
Nvidia DGX-1(8 V100+NVLink)

- **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

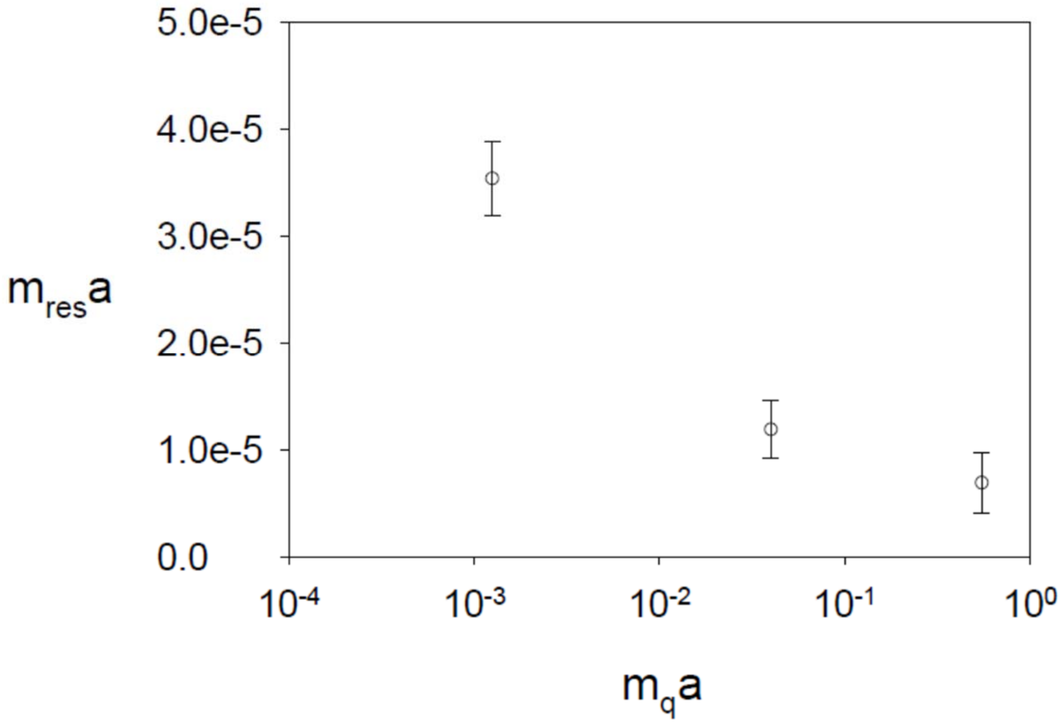
- What is chiral symmetry breaking due to finite Ns ?
  What are the residue masses for (u, d, s, c) quarks ?

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

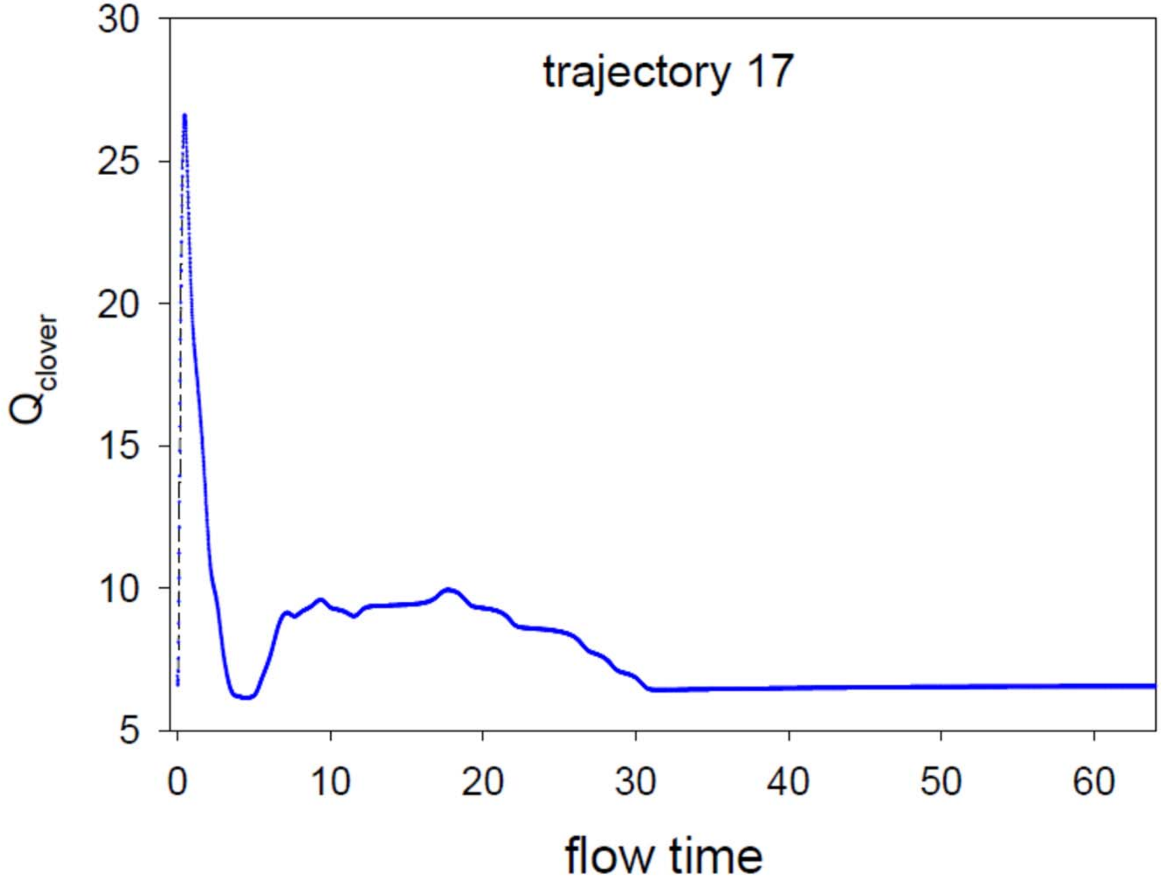


- Residual mass: $m_{res}a = 3.75(34)\times 10^{-5},\ 1.25(22)\times 10^{-5},\ 0.64(22)\times 10^{-5}$

  $\approx\ 0.1$ MeV, ≈ 0.04 MeV, ≈ 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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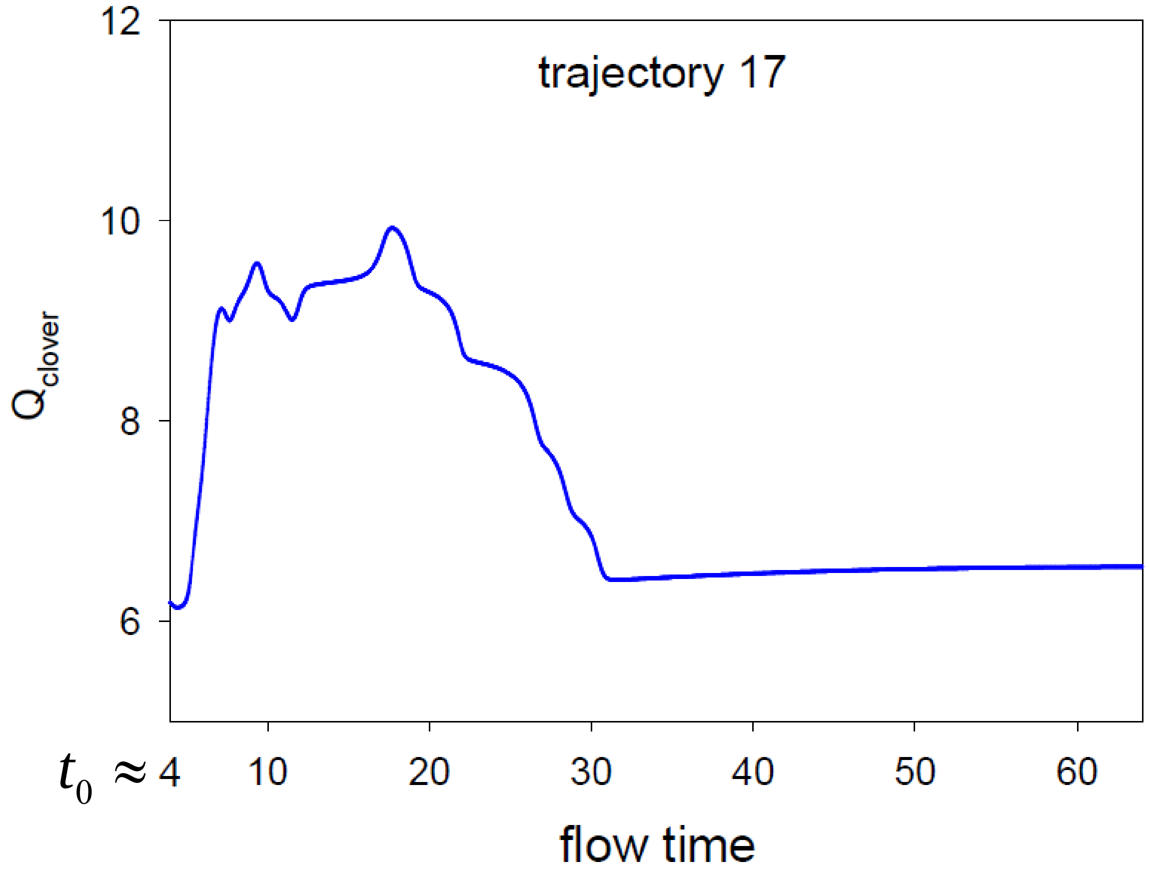

The most reliable topological charge seems to be at t=64

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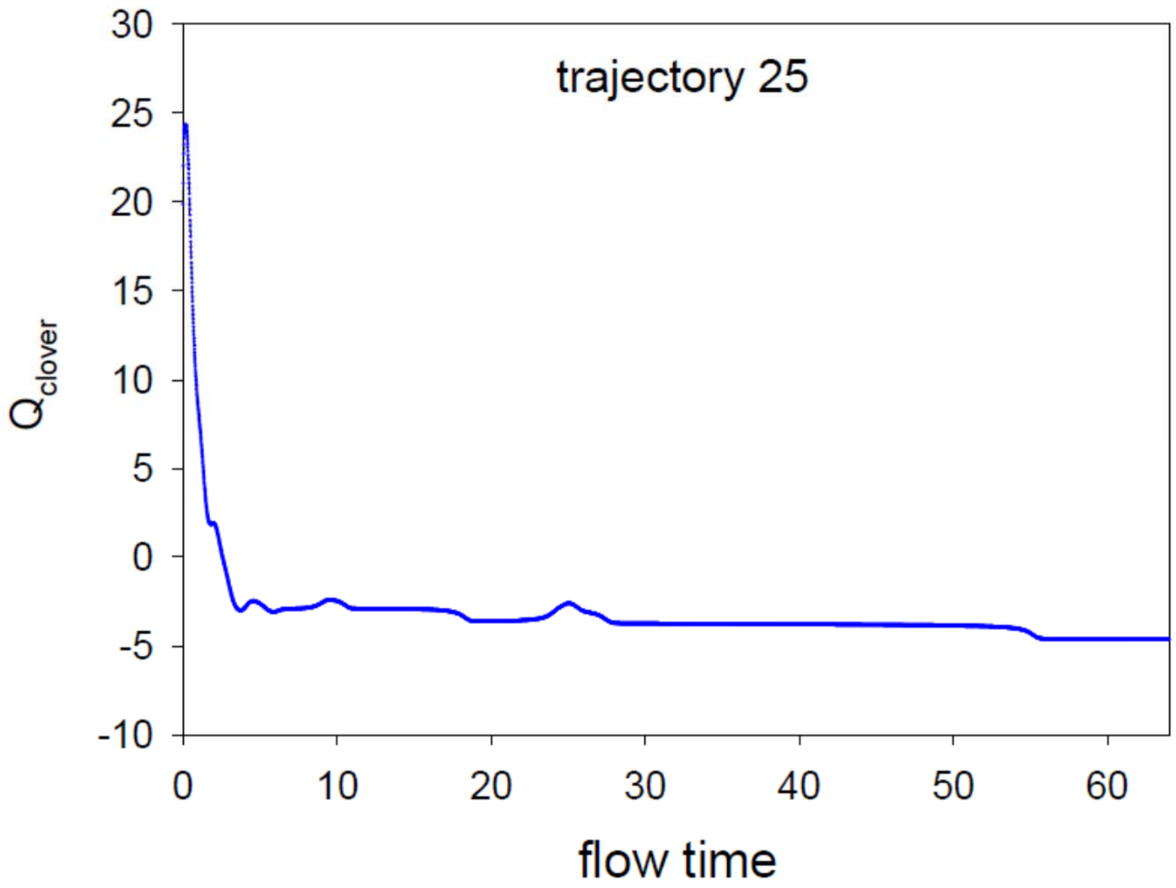

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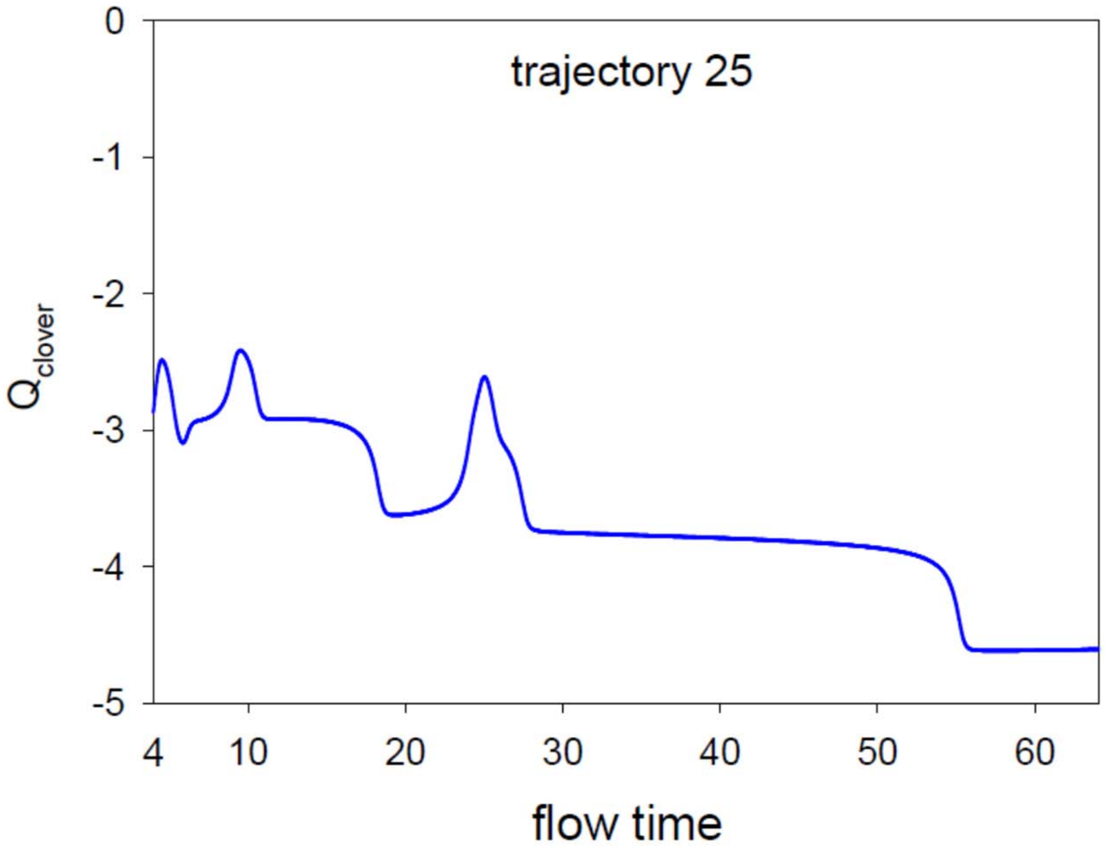

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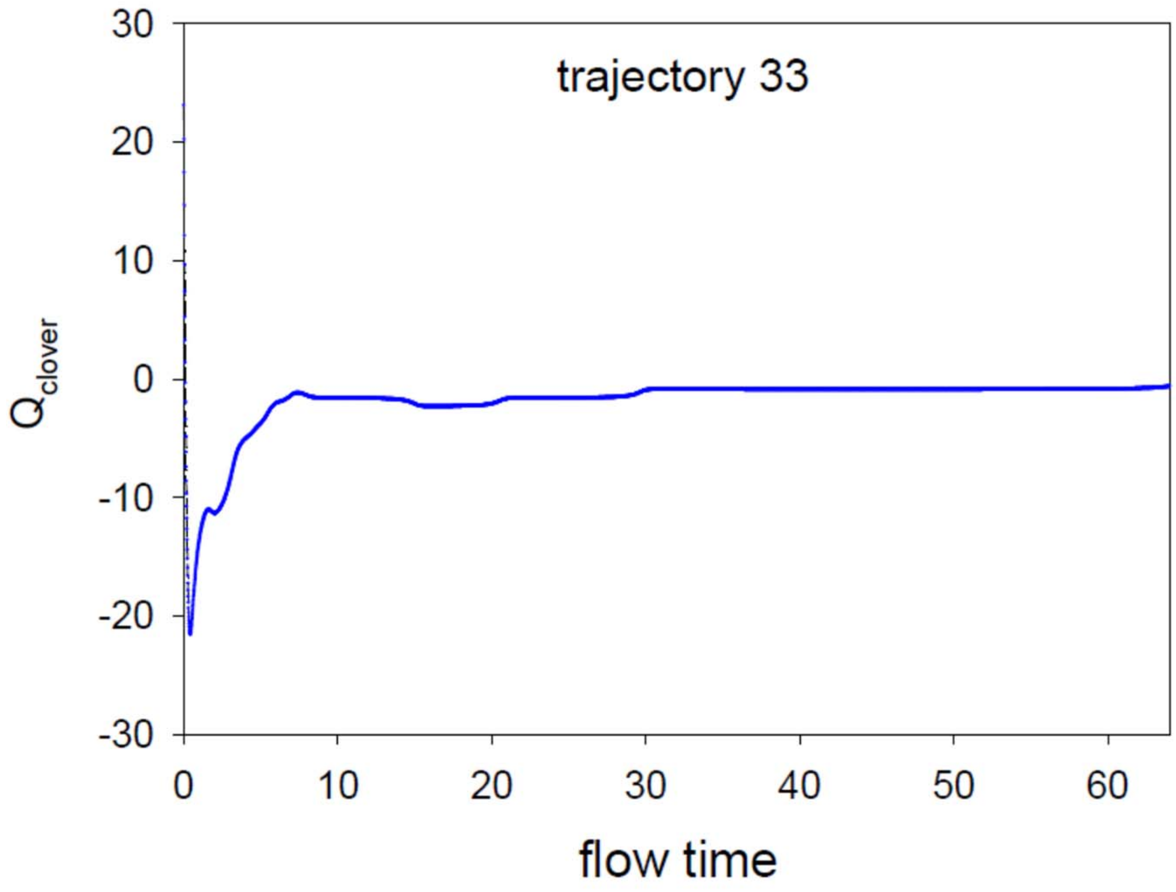

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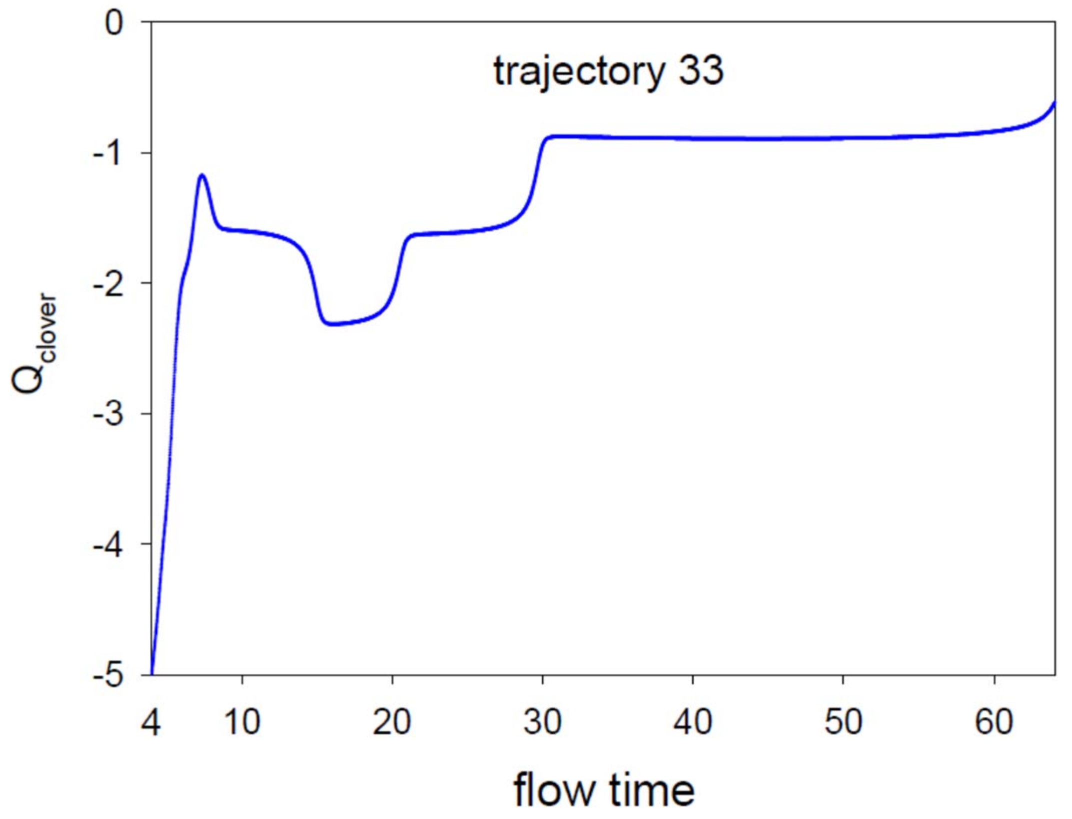
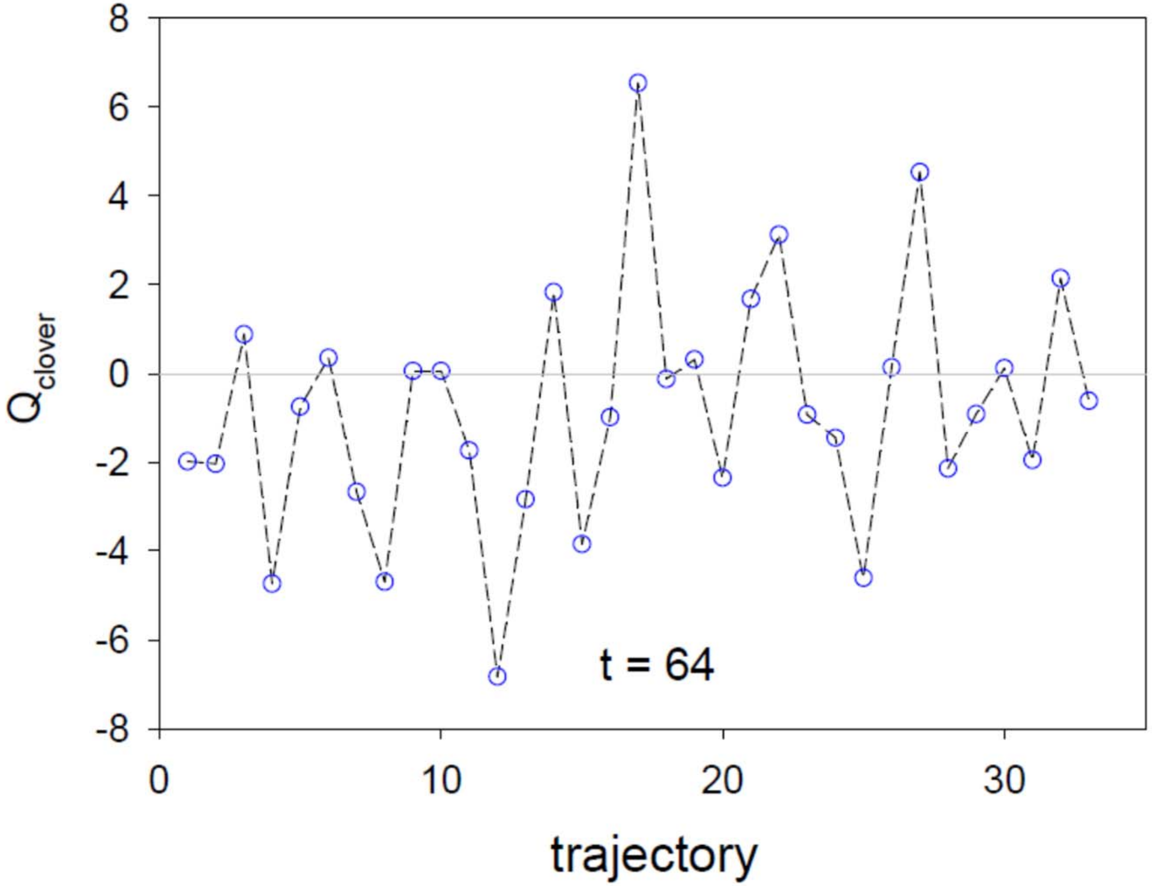


The most reliable topological charge seems to be at t=64

Topological Ergodicity

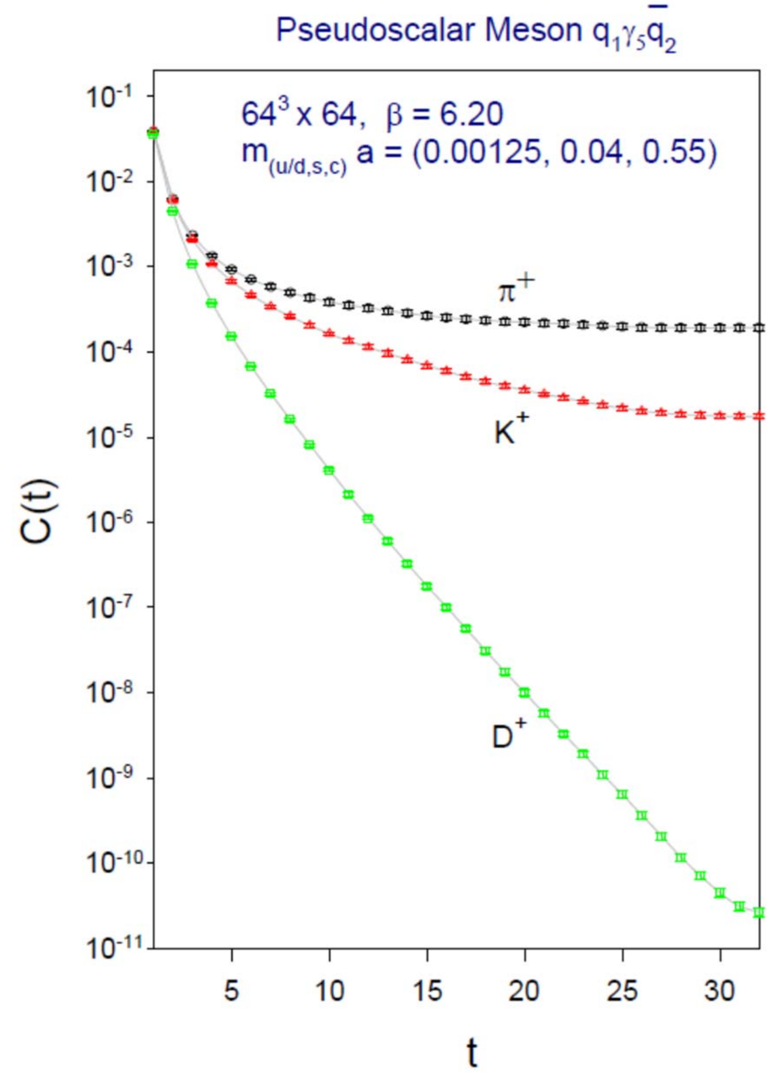
Clover topological charge of 33 successive trajectories,
at the Wilson flow time t=64.

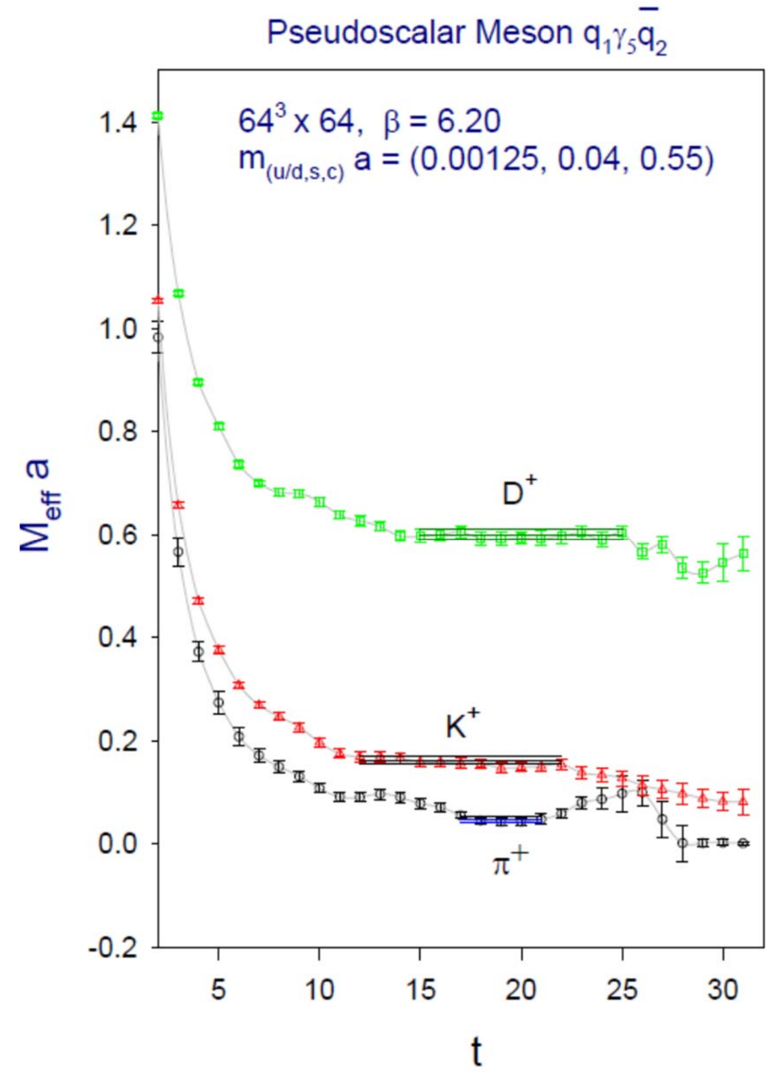


It confirms that the HMC does not suffer from the topology freezing.

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 $64^3 \times (64,\ 20,\ 16,\ 12,\ 10,\ 8,\ 6)$, with $T \approx (150,\ 188,\ 250,\ 300,\ 375,\ 500)$ MeV.

Conclusion and Outlook

- With the new DGX-1 with 8*V100(32 GB)+NVLink, (or compatible platforms), we will generate gauge ensemble with physical (u,d,s,c) overlap/DW quarks on the $64^3 \times 128$ lattice.