First dynamical symulations with minimally doubled fermions

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in collaboration with
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Motivation

For simulating two light flavors dynamically at $T \neq 0,\ \mu \neq 0$ one can choose from several discretizations:

- Wilson fermions
  Explicit breaking of chiral simmetry $\rightarrow$ at $T = 0$ OK.
- Overlap fermions
  Computationally costly.
- Staggered fermions
  Rooting is ambiguous for $\mu \neq 0$. (For more details see C. H. Wong's talk)
- Minimally doubled fermions
  A remnant chiral simmetry is present, rooting is not needed.
  Do we have O(a) discretization errors?

Karsten-Wilczek fermions

Our choice for a minimally doubled action is the so-called Karsten-Wilczek (KW) action [L.H. Karsten 1981, F. Wilczek 1987].

$$S_F^{KW} = S_F^N + \sum_x \sum_{j=1}^{3} \bar{\psi}(x) \frac{i\zeta}{2} \gamma^\alpha \left(2\psi(x) - U_j(x)\psi(x+\hat{j}) - U_j^\dagger(x)\psi(x-\hat{j}) \right),$$

Where S_F^N is the naive fermion action, the $U_\mu(x)$ are the links in diretion μ at lattice site x. ζ is the Wilczek parameter, with $|\zeta| > 1/2$. S_F^{KW} breaks hypercubic symmetry, thus we need three counter-terms for renormalization (coefficients were determined perturbatively [S. Capitani et.al. (2009)])

$$S^{3f} = c \sum_x \bar{\psi}(x) i\gamma^\alpha \psi(x),$$

$$S^{4f} = d \sum_x \bar{\psi}(x) \frac{1}{2} \gamma^\alpha \left(U_\alpha(x)\psi(x+\hat{\alpha}) - U_\alpha^\dagger(x-\hat{\alpha})\psi(x-\hat{\alpha}) \right),$$

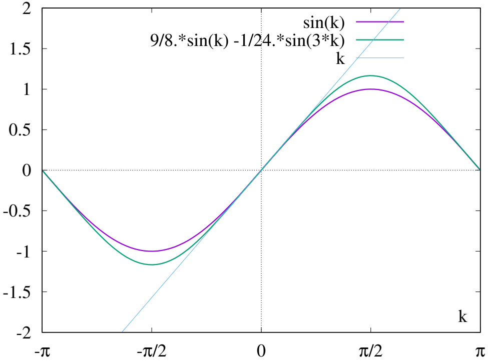
$$S^{4g} = d_G \sum_x \sum_{\mu \neq \alpha} \mathrm{Re}\,\mathrm{Tr}\left(1 - \mathcal{P}_{\mu\alpha}(x)\right),$$

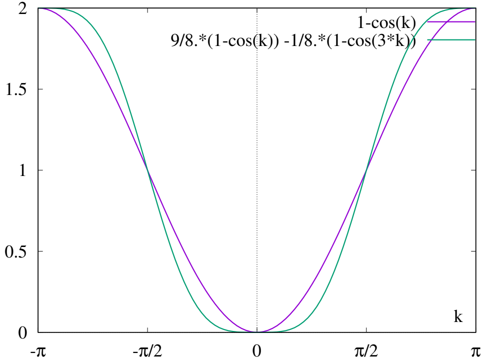
In our case $\alpha \equiv t$.

Karsten-Wilczek Dirac operator in momentum space

In momentum space the Dirac operator reads

$$D_{\mathrm{KW}}(k) = \frac{i}{a}\left[\sum_{\mu=0}^{3}\gamma_\mu\xi_\mu \sin\, ak_\mu + \zeta\gamma_0\sum_{j=1}^{3}(1-\cos\, ak_j)\right]$$





Karsten-Wilczek Dirac operator in position space

The KW Dirac operator in position space acts on a fermion fied the following way

$$D^{KW}\psi[s] \equiv \sum_{\mu}\Big[c_\mu(s)\ \Gamma^\mu\ U_\mu(s)\ \psi[s+\mu] - c_\mu^{-1}(s-\mu)\ \Gamma^{\mu\dagger} U_\mu^\dagger(s-\mu)\psi[s-\mu]\Big]$$
$$+ (2m + 2i(3\zeta + c)\gamma^\alpha)\psi[s]$$

$$\Gamma^\mu = \begin{cases}\gamma^\mu - i\zeta\gamma^\alpha & ,\mu \neq \alpha \text{ "}\textit{spatial}\text{"}\\ (1+d)\gamma^\mu & ,\mu = \alpha \text{ "}\textit{temporal}\text{"}\end{cases}$$

Where $(1+d)$ is structurally the same as an anisotropy parameter, thus we will use the notation $\xi \equiv (1+d)$ and also $\xi_\beta \equiv (1+d_G)$.

$c_\mu(s) = e^{\frac{\mu_q}{N_t}\ \delta_{\mu,t}}\Phi(s)$, with boundary condition $\Phi(s) = \pm 1$,

($\mu \in \{0,1,2,3\}$ which are equivalent to directions $\{t,z,y,x\}$.)

Naik improvement

The KW term is first order in the lattice spacing a. Thus for a better approach of the continuum limit we introduced improvement in the Dirac operator.

$$D_{\mathrm{KW}}(k) = \frac{i}{a}\left[\sum_{\mu=0}^{3} \gamma_\mu \xi_\mu \sin\, ak_\mu + \zeta \gamma_0 \sum_{j=1}^{3} (1 - \cos\, ak_j)\right]$$

The $sin(ak_\mu)$ term corresponds to the Nabla and the $(1 - cos(ak_j))$ corresponds to the Laplacian.
We can elimininate the $\mathcal{O}(k^2)$ term in this expression by realizing improvement of the Laplacian

$$(1 - \cos\, ak_j) \to c_1(1 - \cos\, ak_j) + c_3(1 - \cos\, 3ak_j)$$

with the special choice $c_1 = 9/8$, $c_3 = -1/8$.

Naik improvement

In position space we have the following improved expression

$$D^{KW}\psi[s] \equiv \sum_\mu \xi_\mu \Big[c_\mu(s)\ \Gamma^\mu_{(1)}\ U_\mu(s)\ \psi[s+\mu] - c_\mu^{-1}(s-\mu)\ \Gamma^{\mu\dagger}_{(1)} U^\dagger_\mu(s-\mu)\psi[s-\mu]$$
$$+ c_\mu(s)c_\mu(s+\mu)c_\mu(s+2\mu)\ \Gamma^\mu_{(3)}\ U_\mu(s)U_\mu(s+\mu)U_\mu(s+2\mu)\ \psi[s+3\mu]$$
$$-c_\mu^{-1}(s-\mu)c_\mu^{-1}(s-2\mu)c_\mu^{-1}(s-3\mu)\ \Gamma^{\mu\dagger}_{(3)} U^\dagger_\mu(s\mu)U^\dagger_\mu(s-2\mu)U^\dagger_\mu(s-3\mu)\psi[s-3\mu]\Big]$$
$$+ (2m + 2i(3\zeta + c)\gamma^0)\ \psi[s]$$

Where

$$\Gamma^0_{(1)} = \gamma^0, \qquad \Gamma^\mu_{(1)} = \bar{s}_1\gamma^\mu - i\bar{c}_1\gamma^0 \quad (\mu \neq 0)$$
$$\Gamma^0_{(3)} = 0, \qquad \Gamma^\mu_{(3)} = \bar{s}_3\gamma^\mu - i\bar{c}_3\gamma^0 \quad (\mu \neq 0)$$
$$1 = \bar{s}_1 + 3\bar{s}_3, \quad \zeta = \bar{c}_1 + \bar{c}_3$$

The relation to the momentum space c_1 and c_3 is $c_1 = \zeta\bar{c}_1,\ c_3 = \zeta\bar{c}_3$.

Half vector trick

- We want to use only 2 Dirac components instead of 4 $\rightarrow$ half as many operations.
- If $\bar{s}_1 = \bar{c}_1$ and $\bar{s}_3 = \bar{c}_3$, then $\Gamma^{\mu}_{(1),(3)} = \gamma_j + i\gamma_0$ are projectors. This allows the half vector trick.
- By the following choice of parameters criteria for the half vector trick and Laplacian improvement are satisfied

$$\bar{s}_1 = \bar{c}_1 = 1.5$$
$$\bar{s}_3 = \bar{c}_3 = -1/6$$
$$\zeta = 4/3$$

- Because of the Laplacian improvement the action is $\mathcal{O}(a)$ improved even in this case.

Properties of the Dirac operator

The KW Dirac operator $D^{KW} = m + \not{D}$ has the following properties

$$\not{D}^\dagger = \gamma_5 \not{D} \gamma_5 \qquad \gamma_5 - \text{hermiticity}$$

$$D^{KW\dagger}\gamma_5 = \gamma_5 D^{KW}$$

$$\gamma_5 \not{D} \gamma_5 = -\not{D} \qquad \text{chiral symmetry}$$

$$D^{KW\dagger} = m - \not{D}$$

$$D^{KW\dagger} D^{KW} = (m - \not{D})(m + \not{D}) = m^2 - \not{D}^2 = D^{KW} D^{KW\dagger} \qquad \mathrm{D}^{\mathrm{KW}} \text{ is normal}$$

$$D^{KW\dagger} D^{KW} \gamma_5 = D^{KW\dagger} \gamma_5 D^{KW\dagger} = \gamma_5 D^{KW} D^{KW\dagger} = \gamma_5 D^{KW\dagger} D^{KW}$$

Consequences:
The eigenvalues of $\not{D}$ consist of complex conjugate pairs $\pm i\lambda$.
$D^{KW\dagger} D^{KW}$ is positive definite with eigenvalues $m^2 + \lambda^2$ and its eigenvectors are left(L)- or right(R)-handed.

Simulating with HMC

Properties of D^{KW} makes it possible to use Hybrid Monte Carlo simulations without the rational approximation.

$$M = \begin{pmatrix} M_{LL} & M_{LR} \\ M_{RL} & M_{RR} \end{pmatrix} = \left(\begin{array}{c|c} m\mathbb{1} & \not{D}_{LR} \\ \hline \not{D}_{RL} & m\mathbb{1} \end{array}\right)$$

$$M^+M = \begin{pmatrix} m^2 - \not{D}_{LR}\not{D}_{RL} & 0 \\ 0 & m^2 - \not{D}_{RL}\not{D}_{LR} \end{pmatrix}$$

Then the action takes the form $S_f^{KW} = \chi_L^+[(M^+M)_{LL}]^{-N_f/2}\chi_L$ $(N_f = 2)$ with $\chi_L = P_L D^{KW}\eta$, where $P_L = \frac{1}{2}(1+\gamma_5)$ and η is a random Gaussian field.

Dynamical simulations with KW action

We produced gauge configurations dynamically for the first time with Karsten-Wilczek action. We tuned the three coefficients of the counter-terms c, ξ, ξ_β were tuned non-perturbatively.
The setup of the simulations was:

HMC and Rational HMC algorithm was used with Hasenbusch preconditioning.
For the preconditioned field we used a Multishift Conjugate Gradient (MCG) solver, for the preconditioner CG solver was used on $\mathrm{D}^{\mathrm{KW}\dagger}\mathrm{D}^{\mathrm{KW}}$.
Temporal and spatial size of the lattices : $N_t = 64,\ N_s = 16$
Inverse gauge coupling : $\beta = 3.5$ corresponding to $a_s = 0.180(3)\ \mathtt{fm}$
For each different setup of c, ξ and ξ_β the number of configurations : $\mathrm{n_{cf}} \approx 200$

Tuning the parameter c

For a non-perturbatve tuning of the c parameter we measured the mesonic correlation function in the γ_0 channel

$$C_0(x,y) \sim \langle \bar{\psi}(x)\gamma_0\psi(x)\bar{\psi}(y)\gamma_0\psi(y)\rangle$$

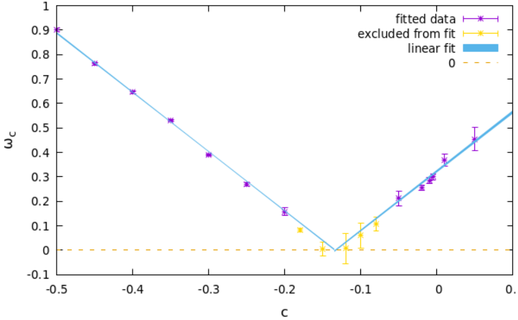
For the correlator parallel to the KW direction oscillation happens if c is not tuned properly [J. Weber (2017)]

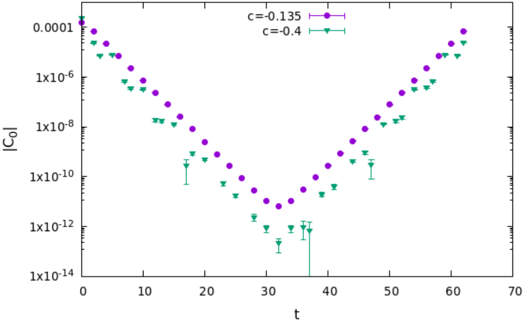
$$C_0(t) \approx A\left[\cos(t\omega+\phi)\exp(-mt)+\cos((N_t-t)\omega+\phi)\exp(-m(N_t-t))\right]$$

We have to set c such that $\omega_c \equiv \omega - \pi = 0$.

We fitted the correlation functions measured on tiled configurations.
(For more details about tiling and the tuning of c see the next talk presented by D. Godzieba.)

We fixed $\xi = \xi_\beta = 1$ and did a scan in the c parameter. By fitting $C_0(t)$ (right plot) at each c we extracted the oscillation frequency ω_c (left plot). We performed a linear fit on the data and interpolated the point where $\omega_c = 0$: $c = -0.1336(13)$.





Tuning the parameters ξ and ξ_β

Fortunately ω_c remained small by keeping c at its previously tuned value even for different settings of ξ and ξ_β. Thus we could perform a 2D scan in the ξ-ξ_β plane by keeping c fixed.

To find the tuned values we checked two criteria for lattice isotropy:

A1 We measured the parallel and perpendicular components of γ_5 channel of meson (pion) correlation function

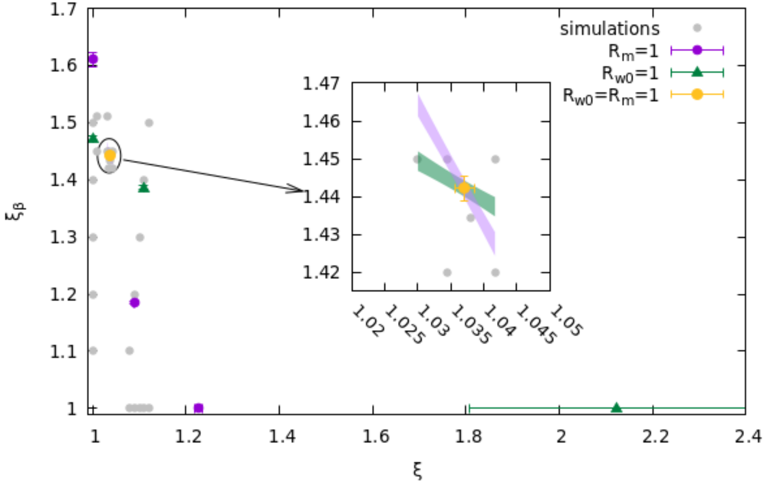
$$C_5(x,y) \sim \langle \bar{\psi}(x)\gamma_5\psi(x)\bar{\psi}(y)\gamma_5\psi(y)\rangle$$

After a fit was performed on $C_{5||}$ and $C_{5\perp}$ we searched for parameter setups where the mass ratio $R_m = \frac{m_{||}}{m_\perp} = 1$.

A2 We measured the lattice spacing in the parallel (a_t) and perpendicular (a_s) directions using the w_0 scale [S.Borsanyi et.al.(2012)]. Then we searched for setups where $R_a = \frac{w_0 a_t}{w_0 a_s} = 1$.

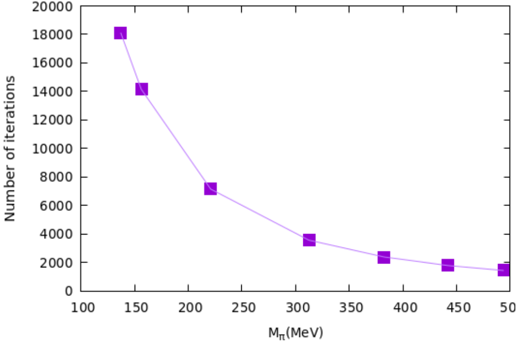
2D scan in ξ and β_ξ

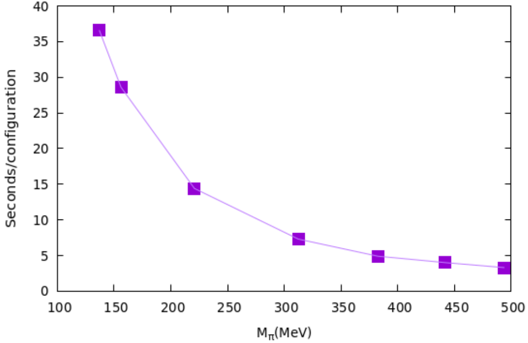
Scanning the 2D plane at different points we could interpolate points where the criteria A_1 and A_2 are satisfied. This defined two lines in the parameter plane. They cross each other at $\xi_\beta = 1.442(3)$, $\xi = 1.0370(15)$.



Cost at the physical point

A mass scan was done starting from pion mass $M_\pi = 486(8)$MeV to $M_\pi = 135(2)$MeV with larger volumes $N_s = 24$, $N_t = 48$ at $\xi_\beta = 1.4345$, $\xi = 1.0381$ for which R_a and R_{w_0} are both 0.1% away from ratio 1.



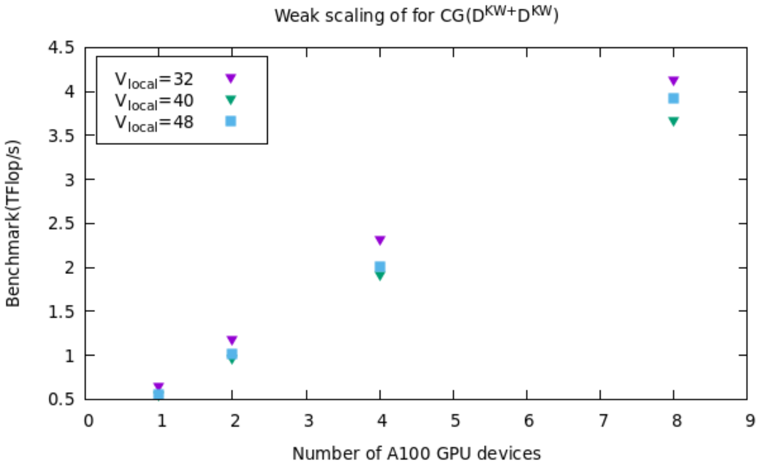


Summary

- We did dynamical simulations with Karsten-Wilczek fermions for the first time.
- We eliminated the $\mathcal{O}(a)$ errors by introducing an improvement of the Laplacian.
- We tuned the coefficients of the counter terms c, ξ and β_ξ at $a = 0.180(3)\mathrm{fm}$ nonperturbatively.
- We checked the computational cost going toward the physical pont.

- Outlook: With S. Capitani we are working on the construction of a renormalized action with beyond tree level improvement by using perturbation theory. For this we need to determine values of $c_1 = 9/8 + g_0^2 c_1^{(1)}$ and $c_3 = -1/8 + g_0^2 c_3^{(1)}$.

Backup



Weak scaling of for CG(D^KW+D^KW)
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Benchmark(TFlop/s)
V_local=32
V_local=40
V_local=48
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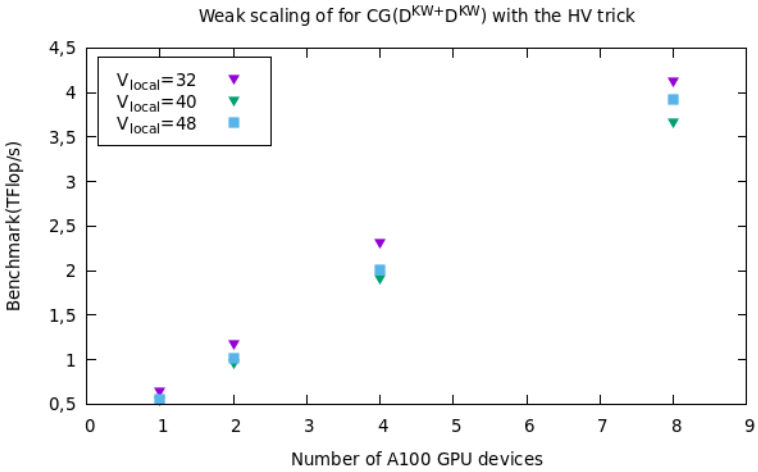
Number of A100 GPU devices


Weak scaling of for CG(D^KW+D^KW) with the HV trick
Benchmark(TFlop/s)
Number of A100 GPU devices
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V_local=48
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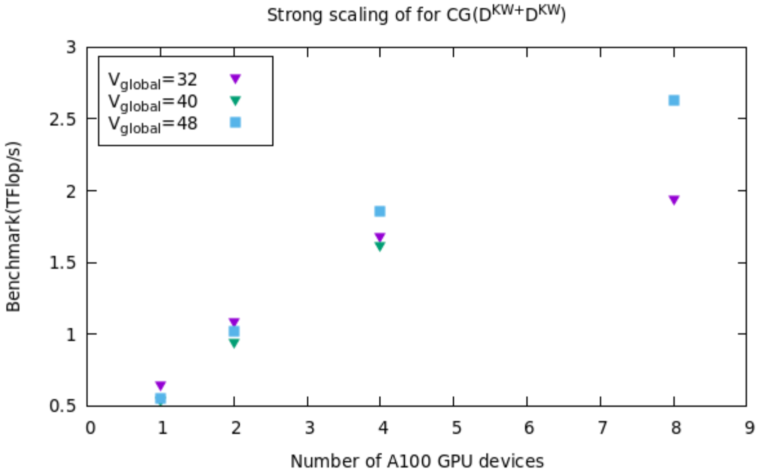

Strong scaling of for CG(D^KW+D^KW)
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Benchmark(TFlop/s)
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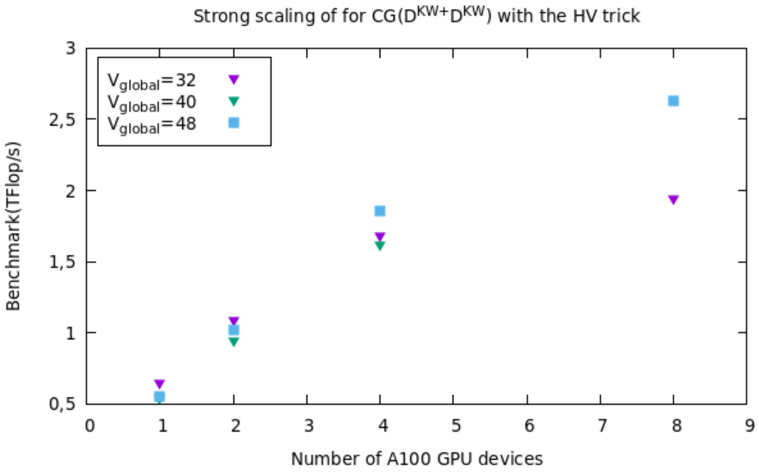

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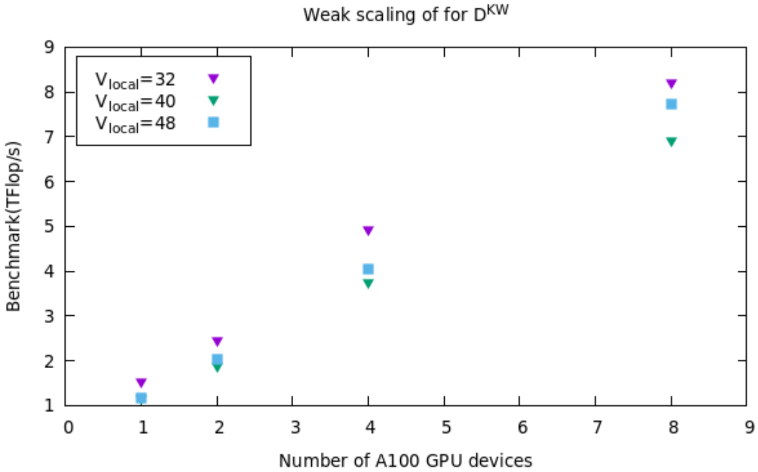
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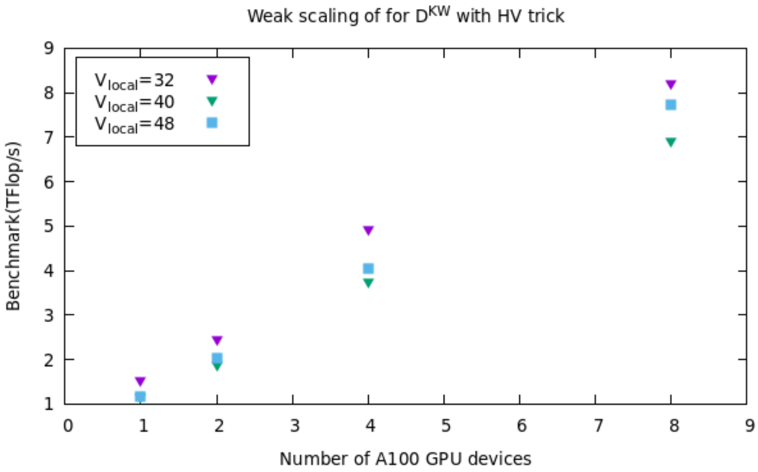
Weak scaling of for D^KW with HV trick
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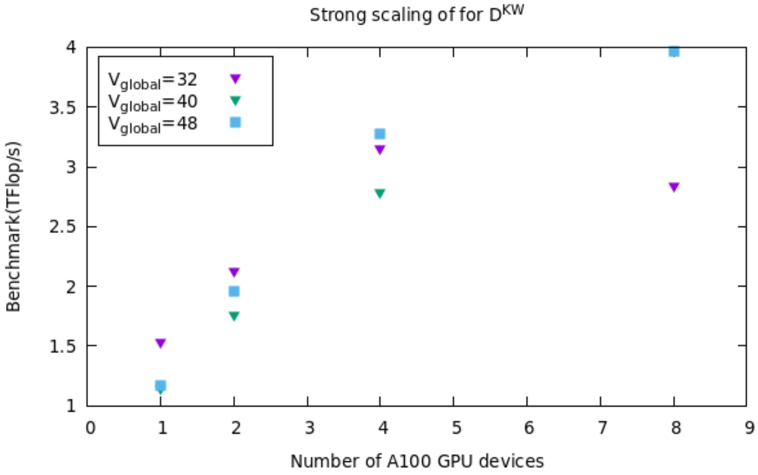

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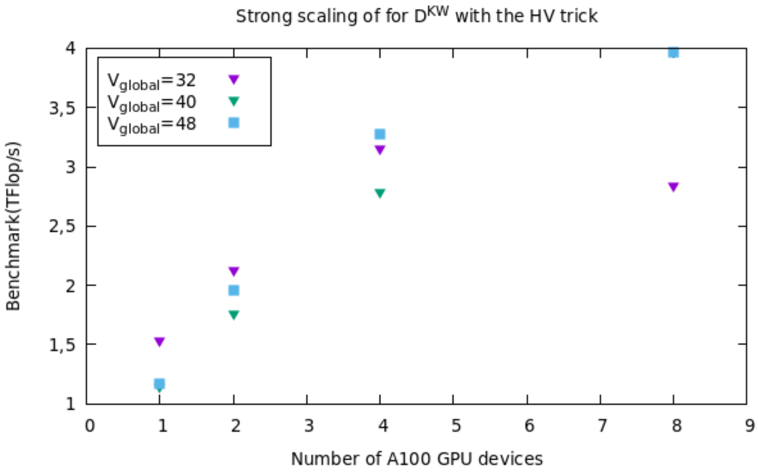

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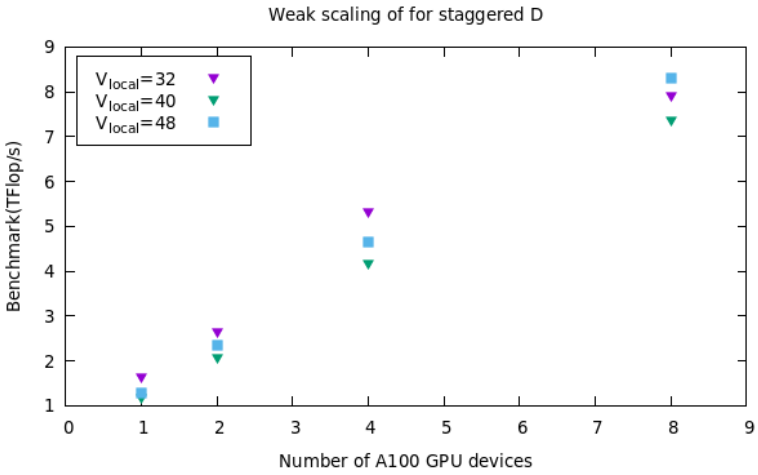
Weak scaling of for staggered D
Benchmark(TFlop/s)
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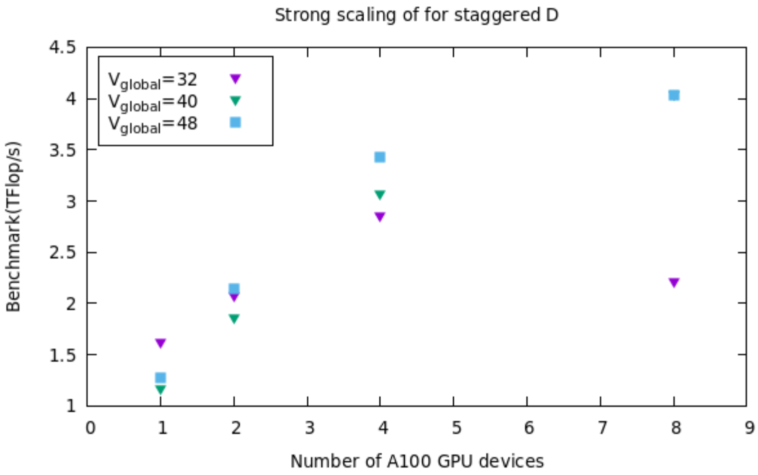

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