The influence of gauge field smearing on discretisation effects

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Smearing in lattice QCD Monte Carlo simulations

4D gauge field smearing:

- Smearing transformation $\mathcal{S} : U \mapsto \mathcal{S}[U]$
  (e.g. HYP[1], Stout[2], HEX[3], gradient flow[4])
- Observable smearing:
$$\langle O_{\mathcal{S}}[U] \rangle := \langle O[\mathcal{S}[U]] \rangle$$
- Smearing in lattice fermion action:
$$S[U] = S_{\mathrm{g}}[U] + \overline{\Psi}\, D[\mathcal{S}[U]]\, \Psi$$
- Motivation: noise reduction, increased algorithmic stability (fermion determinant/exceptional configurations)

Questions to be asked:

- How does the smearing strength influence lattice artefacts?
- What smearing strengths allow for a controlled continuum extrapolation?

[1] Hasenfratz and Knechtli 2001.
[2] Morningstar and Peardon 2004.
[3] Capitani et al. 2006.
[4] Narayanan and Neuberger 2006; Lüscher 2010.

Gradient flow in the continuum and on the lattice

Yang-Mills continuum gradient flow[5]:

- Introduce gauge field $B_\mu(x, t_{\text{fl}})$ defined on $\mathbb{R}^4 \times [0, \infty)$ by:
$$\frac{\partial}{\partial t_{\text{fl}}} B_\mu(x, t_{\text{fl}}) = -\frac{\delta S_{\text{YM}}[B]}{\delta B_\mu(x, t_{\text{fl}})} = D_\nu G_{\nu\mu}(x, t_{\text{fl}}) \qquad B_\mu(x, 0) = A_\mu(x)$$
$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \qquad D_\mu = \partial_\mu + [B_\mu, \cdot]$$
- Gauge fields are spherically smoothed with radius $r_{\text{sm}} = \sqrt{8 t_{\text{fl}}}$
- No additional renormalisation required[6]:
$$O(x, 0) \text{ finite } \Rightarrow O(x, t_{\text{fl}}) \text{ finite } \forall t_{\text{fl}} \geq 0$$

Lattice discretisation:

- Wilson gradient flow:
$$\frac{\partial}{\partial t_{\text{fl}}} V_\mu(x, t_{\text{fl}}) = -g_0^2 (\partial_{x,\mu} S[V]) V_\mu(x, t_{\text{fl}}) \qquad V_\mu(x, 0) = U_\mu(x)$$
- Numerical integration of flow equation:
  Forward 3rd-order Runge-Kutta integration scheme, step size $\varepsilon < 0.01$

[5] Lüscher 2010.

[6] Lüscher and Weisz 2011.

Gradient flow smearing and physical gradient flow

Gradient flow smearing:

$$\frac{8t_{\mathrm{fl}}}{a^2} = \mathrm{const}$$

- Flow time shrinks with shrinking lattice spacing $8t_{\mathrm{fl}} \propto a^2$
  $\Rightarrow$ Smearing vanishes in the continuum limit
- Continuum theory is unaltered (assuming controlled continuum extrapolation)
- Smearing strengths up to $\frac{8t_{\mathrm{fl}}}{a^2} = 8$ have been used in practice

Physical gradient flow:

$$8t_{\mathrm{fl}} = \mathrm{const}$$

- Dimensionless flow time grows with shrinking lattice spacing $\frac{8t_{\mathrm{fl}}}{a^2} \propto \frac{1}{a^2}$
- Continuum theory is altered (assuming controlled continuum extrapolation)
- New observables become accessible

SU(3) gauge ensembles

SU(3) Yang Mills theory gauge ensembles:

- Wilson plaquette action
- Temporal open boundary conditions[7] (alleviate topology freezing)
- Scale setting via reference flow time[8] t_0
- Lattice spacings between 0.08 and 0.02 fm
- Constant spatial extent $L = 2\,\text{fm}$

ensemble	β	T/a	L/a	a [fm]	L [fm]
sft1	6.0662	80	24	0.0834(4)	2.00(1)
sft2	6.2556	96	32	0.0624(4)	2.00(1)
sft3	6.5619	96	48	0.0411(2)	1.97(1)
sft4	6.7859	192	64	0.0312(2)	2.00(1)
sft5	7.1146	320	96	0.0206(2)	1.98(2)

SU(3) gauge ensembles[9].

[7] Lüscher and Schaefer 2011.
[8] Lüscher 2010.
[9] Husung et al. 2018.

Reference flow time t_0 as reference scale[10]:

- Action density $E(x, t_{\text{fl}})$ in clover discretisation[11]:

$$E(x,t_{\text{fl}}) = -\frac{1}{2}\sum_{\mu,\nu} \text{tr}\left(G^{\text{clv}}_{\mu\nu}(x,t_{\text{fl}})\,G^{\text{clv}}_{\mu\nu}(x,t_{\text{fl}})\right)$$

- Reference flow time t_0:

$$t_{\text{fl}}^2 \left\langle E(x,t_{\text{fl}})\right\rangle\Big|_{t_{\text{fl}}=t_0} = 0.3$$

- t_0^{phys} via Sommer parameter[12] r_0^{phys}:

$$r_0^{\text{phys}} = 0.5\,\text{fm} \quad \Leftrightarrow \quad t_0^{\text{phys}} = 0.0268(3)\,\text{fm}^2$$

ensemble	t_0/a^2
sft1	3.990(9)
sft2	7.070(17)
sft3	16.52(6)
sft4	29.60(10)
sft5	67.94(23)

Reference flow time t_0.

[10] Lüscher 2010.
[11] Sheikholeslami and Wohlert 1985.
[12] Sommer 1994.

Creutz ratios in the continuum:

- Planar rectangular Wilson loop of size $r \times t$:

$$W(r,t) = \left\langle \operatorname{tr}\left(P \exp\left(\mathrm{i} \oint_{\gamma(r,t)} \mathrm{d}x_\mu A_\mu(x)\right)\right)\right\rangle$$

- Creutz ratio: $\chi(r,t) = -\frac{\partial}{\partial t}\frac{\partial}{\partial r} \ln\left(W(r,t)\right)$
- Static quark anti-quark force can be extracted from Creutz ratios:

$$\chi(r,t) \to F_{\overline{\mathrm{q}}\mathrm{q}}(r) \text{ for } t \to \infty$$

Creutz ratios on the lattice[13]:

- Planar rectangular Wilson loop from gauge links:

$$W(r,t) = \left\langle \operatorname{tr}\left(\prod_{(x,\mu)\in\gamma(r,t)} U_\mu(x)\right)\right\rangle$$

- Use central differences to obtain $O(a^2)$ lattice artefacts:

$$\chi\left(t+\frac{a}{2}, r+\frac{a}{2}\right) = \frac{1}{a^2} \ln\left(\frac{W(t+a,r)\cdot W(t,r+a)}{W(t,r)\cdot W(t+a,r+a)}\right)$$

- $\chi(r,t)$ renormalises trivially

[13] Creutz 1980.

Computation of Creutz ratios

From Monte Carlo simulation:

- Focus on diagonal Creutz ratios $\chi(r) := \chi(r, r)$
- Compute dimensionless quantities on the lattice:

$$(\chi \cdot a^2)\left(\frac{r}{a}\right) \quad \text{for } \frac{r}{a} = 1.5, 2.5, \ldots \qquad\qquad \frac{t_0}{a^2}$$

- Combine observables to eliminate a-factors:

$$\frac{r}{a} \cdot \left(\frac{t_0}{a^2}\right)^{-\frac{1}{2}} = \frac{r}{\sqrt{8t_0}} \qquad\qquad (\chi \cdot a^2)\left(\frac{r}{a}\right) \cdot \frac{t_0}{a^2} = (\chi \cdot t_0)\left(\frac{r}{\sqrt{8t_0}}\right)$$

- Analyse $\chi \cdot t_0$ as a function of $\frac{r}{\sqrt{8t_0}}$

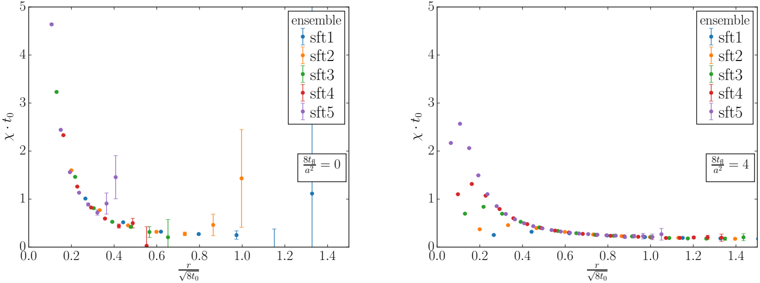
Investigation of gradient flow smearing:

- Measure $\chi \cdot t_0$ on flowed gauge configurations at gradient flow time $\frac{8t_{\text{fl}}}{a^2} = 0, 0.25, 0.5, \ldots$

Investigation of physical gradient flow:

- Measure $\chi \cdot t_0$ on flowed gauge configurations at gradient flow time $\frac{t_{\text{fl}}}{t_0^{\text{phys}}} = 0, 0.0146, 0.0292, \ldots$

Creutz ratios and gradient flow smearing



Dimensionless Creutz ratios $\chi \cdot t_0$ as functions of the distance $\frac{r}{\sqrt{8t_0}}$ on different ensembles and gradient flow times $\frac{8t_{\mathrm{fl}}}{a^2}$.

Influence of gradient flow smearing $\frac{t_{\mathrm{fl}}}{a^2} = \mathrm{const}$:

- Reduces statistical errors
- Removes $\frac{1}{r^2}$ divergence at small distances
- Alters path to continuum and hence lattice artefacts

Interpolation models for $(\chi \cdot a^2)(\frac{r}{a})$

Goal: Continuum extrapolation of $(\chi \cdot t_0)(\frac{r}{\sqrt{8t_0}})$ at fixed $\frac{r}{\sqrt{8t_0}}$

- Requires $(\chi \cdot a^2)(\frac{r}{a})$ also for $\frac{r}{a} \neq 0.5, 1.5, 2.5, \ldots$ as nodes are not at the same physical distance r on different ensembles

$$\Rightarrow \text{ Interpolate } (\chi \cdot a^2)\left(\frac{r}{a}\right) \text{ with nodes at } \frac{r}{a} = 1.5, 2.5, \ldots$$

- Piecewise polynomial $\mathrm{Pol}(n_1, \ldots, n_m)(\frac{r}{a}) = \sum_{j=1}^{m} c_{n_j} (\frac{r}{a})^{n_j}$:

$$\mathrm{Pol}(2, 1, 0) \qquad \mathrm{Pol}(0, -2, -4)$$

  (for $m > 2$ smoothing of overlapping regions by averaging)

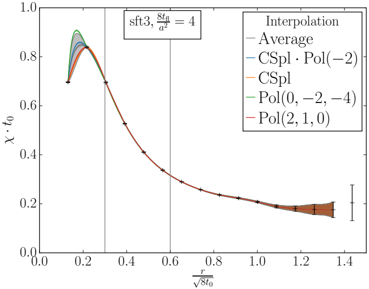
- Cubic natural spline (piecewise cubic polynomial with continuous second derivative):

$$\mathrm{CSpl}$$

- Combinations:

$$\mathrm{CSpl} \cdot \mathrm{Pol}(-2)$$

Interpolation model averaging for $(\chi \cdot a^2)(\frac{r}{a})$



Dimensionless Creutz ratio $\chi \cdot t_0$ as a function of the distance $\frac{r}{\sqrt{8t_0}}$ on sft3 with gradient flow time $\frac{8t_{fl}}{a^2} = 4$ for various interpolations.

- Average over interpolation models: $(\chi \cdot a^2)_{av}\left(\frac{r}{a}\right) = \frac{1}{n}\sum_i (\chi \cdot a^2)_i\left(\frac{r}{a}\right)$
- Add systematic error related to interpolation:
$$\Delta_{sys}(\chi \cdot a^2)_{av}\left(\frac{r}{a}\right) = \frac{1}{2}\left(\max_i \left\{(\chi \cdot a^2)_i\left(\frac{r}{a}\right)\right\} - \min_i \left\{(\chi \cdot a^2)_i\left(\frac{r}{a}\right)\right\}\right)$$
- Focus in region $0.3 \leq \frac{r}{\sqrt{8t_0}} \leq 0.6$

Combined continuum extrapolation and small flow time expansion

Continuum extrapolation of $(\chi \cdot t_0)(\frac{r}{\sqrt{8t_0}})$ at fixed distance $\frac{r}{\sqrt{8t_0}}$:

- Lattice spacing parameter $x = \frac{a}{\sqrt{8t_0}}$
- Symanzik asymptotic expansion: $\chi \cdot t_0 = \sum_{i=0}^{n} c_i x^i + O(x^{n+1})$

Combine with small flow time expansion (physical flow):

- Small flow time parameter $y = \frac{t_{\text{fl}}}{t_0}$
- Expansion of coefficients: $c_i = \sum_{i=0}^{m} c_{ij} y^j + O(y^{m+1})$

Overall fit ansatz:

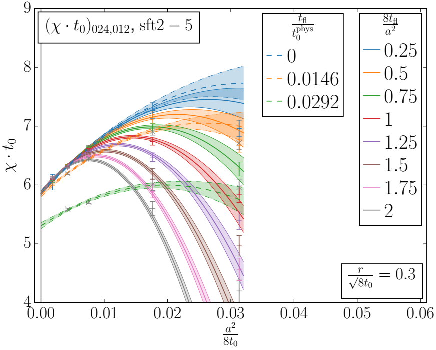
$$(\chi \cdot t_0)_{024,012}(x,y) = c_{00} + c_{20}x^2 + c_{40}x^4 + c_{01}y + c_{21}x^2 y + c_{02}y^2$$

How to describe gradient flow smearing?

- Smearing strength parametrised by $\frac{y}{x^2} = \frac{8t_{\text{fl}}}{a^2}$
- Reorder terms to describe smearing:

$$\begin{aligned}(\chi \cdot t_0)_{024,012}(x,y) = c_{00} &+ c_{20}\left(1 + \frac{c_{01}}{c_{20}}\frac{y}{x^2}\right)x^2 \\ &+ c_{40}\left(1 + \frac{c_{21}}{c_{40}}\frac{y}{x^2} + \frac{c_{02}}{c_{40}}\frac{y^2}{x^4}\right)x^4\end{aligned}$$

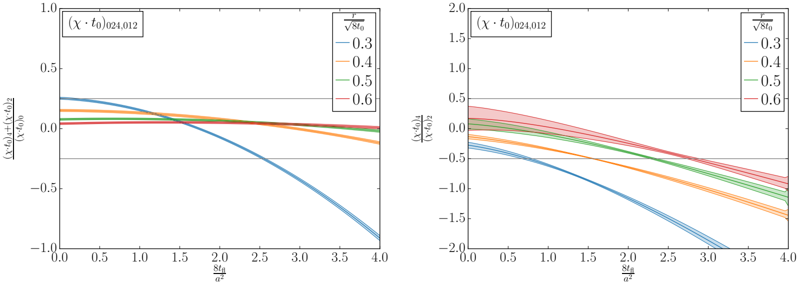
Continuum extrapolations of $(\chi \cdot t_0)\left(\frac{r}{\sqrt{8t_0}}\right)$



Dimensionless Creutz ratio as a function of the lattice spacing $\frac{a^2}{8t_0}$ at a distance of $\frac{r}{\sqrt{8t_0}} = 0.3$. Extrapolations for several gradient flow smearing strengths $\frac{8t_{fl}}{a^2}$ (solid) and for several physical gradient flows $\frac{t_{fl}}{t_0^{phys}}$ (dashed).

- Continuum limit is by construction independent of the smearing strength $\frac{8t_{fl}}{a^2}$ of the fit
- Physical gradient flow $\frac{t_{fl}}{t_0^{phys}}$ leads to an altered continuum limit
- Inclusion of data from larger $\frac{t_0}{t_{fl}}$ measurements not possible because small flow time expansion breaks down
- $\left(\chi \cdot t_0, \frac{a^2}{8t_0}\right)$-plane can be divided into smearing/physical flow regions when demanding a controlled continuum extrapolation

Influence of gradient flow smearing on lattice artefacts

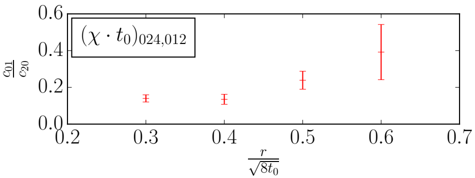


Relative contributions to the Symanzik expansion of $\chi \cdot t_0$ evaluated at $a = 0.0624(4)\,\mathrm{fm}$ (sft2) as a function of the smearing strength $\frac{8t_{\mathrm{fl}}}{a^2}$ at various distances $\frac{r}{\sqrt{8t_0}}$.

- Smaller distances: larger overall & smearing dependent lattice artefacts
- Larger distances: smaller overall lattice artefacts
- Demand $\left|\frac{(\chi\cdot t_0)_4+(\chi\cdot t_0)_2}{(\chi\cdot t_0)_0}\right| \leq 0.25$ and $\left|\frac{(\chi\cdot t_0)_4}{(\chi\cdot t_0)_2}\right| \leq 0.5$:

$$\left(\frac{8t_{\mathrm{fl}}}{a^2}\right)_{\max} \approx 1\ldots3 \qquad \text{for } 0.3 \leq \frac{r}{\sqrt{8t_0}} \leq 0.6$$

Interpretation of smearing



- Extrapolation model at fixed $\frac{r}{\sqrt{8t_0}}$ with $x = \frac{a}{\sqrt{8t_0}}$ and $\frac{y}{x^2} = \frac{8t_{\text{fl}}}{a^2}$:

$$(\chi \cdot t_0)_{024,012}(x,y) = c_{00} + c_{20}\left(1 + \frac{c_{01}}{c_{20}}\frac{y}{x^2}\right)x^2 + c_{40}\left(1 + \frac{c_{21}}{c_{40}}\frac{y}{x^2} + \frac{c_{02}}{c_{40}}\frac{y^2}{x^4}\right)x^4$$

- In the limit of small lattice spacings $\frac{a^2}{8t_0} \ll 1$:

$$\frac{a^2}{8t_0} \mapsto \frac{a^2_{\text{eff}}}{8t_0} = \left(1 + \frac{c_{01}}{c_{20}}\frac{8t_{\text{fl}}}{a^2}\right)\frac{a^2}{8t_0} \overset{!}{\ll} 1$$

$\Rightarrow$ Interpret smearing as a shift to coarser effective lattice spacings (in principle observable dependent)

Conclusion and Outlook

- Maximum tolerable smearing with controlled continuum limit is observable dependent
- For short distance observables less smearing is tolerable
- For the given set of lattice spacings between 0.08 and 0.02 fm gradient flow smearing strength should be $\frac{8t_{\mathrm{fl}}}{a^2} < 1$
- If we want QCD to be described correctly at $r \approx 0.2\,\mathrm{fm}$, we better use
$$\frac{a_{\mathrm{eff}}^2}{8t_0} = \left(1 + 0.2\frac{8t_{\mathrm{fl}}}{a^2}\right)\frac{a^2}{8t_0} \ll 1$$
- Refinements of analysis are still to be done

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