Accuracy and Numerical Stability Investigations of Hessian-Free Force-Gradient Integrators

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References


Kevin Schäfers, Jacob Finkenrath, Michael Günther, and Francesco Knechtli. "Hessian-free force-gradient integrators". In: *Computer Physics Communications* 309 (2025), p. 109478. arXiv: 2403.10370


Kevin Schäfers, Jacob Finkenrath, Michael Günther, and Francesco Knechtli. "Hessian-free force-gradient integrators and their application to lattice QCD simulations". In: *PoS* LATTICE2024 (2025), p. 025. arXiv: 2501.17632


Kevin Schäfers, Jacob Finkenrath, Michael Günther, and Francesco Knechtli. *Numerical stability of force-gradient integrators and their Hessian-free variants in lattice QCD simulations*. 2025. arXiv: 2506.08813

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HMC algorithm and the demands on the integrator [Duane et al. 1987]

HMC algorithm

1. Start with a gauge field of links $[U]_i$.
2. Draw a field of random and fictitious momenta $[P]_i$.
3. Perform a molecular dynamics step
$$([U]_i, [P]_i) \to ([U]_{i+1}, [P]_{i+1}) = \Phi_h([U]_i, [P]_i)$$
using a numerical integration scheme Φ_h.
4. Accept the new configuration with probability $\min(1, \exp(-\Delta\mathcal{H}))$, where $\Delta\mathcal{H} = \mathcal{H}([U]_{i+1}, [P]_{i+1}) - \mathcal{H}([U]_i, [P]_i)$.
5. Proceed with step 2.

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HMC algorithm and the demands on the integrator [Duane et al. 1987]

Detailed balance condition

The integrator Φ_h must satisfy

- *Volume-preservation*: $|\det \partial \Phi_h([U]_{i+1}, [P]_{i+1}) / \partial([U]_i, [P]_i)| = 1$.
- *Time-reversibility*: $\rho \circ \Phi_h \circ \rho \circ \Phi_h([U]_i, [P]_i) = ([U]_i, [P]_i)$, where $\rho([U]_i, [P]_i) = ([U]_i, [-P]_i)$.

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More demands: good *energy conservation*, efficient computational process

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Decomposition algorithms

- Hamiltonian $\mathcal{H}(U,P) = \frac{1}{2}\langle P,P\rangle + \mathcal{S}(U)$
- Equations of motion

$$\boldsymbol{e}_i(U) \coloneqq -T_i U$$

$$\begin{pmatrix}\dot{U}\\ \dot{P}\end{pmatrix} = \begin{pmatrix}0\\ \hat{\mathcal{S}}P\end{pmatrix} + \begin{pmatrix}\hat{\mathcal{T}}U\\ 0\end{pmatrix}, \quad \hat{\mathcal{T}} = p^i \boldsymbol{e}_i,\ \hat{\mathcal{S}} = -\boldsymbol{e}_i(\mathcal{S})\frac{\partial}{\partial p_i}$$

- Exact flows of subsystems
  - $\mathbf{e}^{h\hat{\mathcal{S}}}(U_0,P_0) = (U_0, P_0 - h\boldsymbol{e}_i(\mathcal{S})T^i)$ (momentum update)
  - $\mathbf{e}^{h\hat{\mathcal{T}}}(U_0,P_0) = (\exp(-P_0 h)U_0, P_0)$ (link update)

  are reversible and symplectic maps.
- Promising approaches: splitting methods [McLachlan and Quispel 2002] and force-gradient integrators [Omelyan, Mryglod, and Folk 2003]

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Splitting methods [McLachlan and Quispel 2002]

Splitting Method

$$\Phi_h = \mathbf{e}^{a_1 h\hat{\mathcal{T}}}\mathbf{e}^{b_1 h\hat{\mathcal{S}}}\cdots\mathbf{e}^{a_{s-1}h\hat{\mathcal{T}}}\mathbf{e}^{b_{s-1}h\hat{\mathcal{S}}}\mathbf{e}^{a_s h\hat{\mathcal{T}}}\mathbf{e}^{b_s h\hat{\mathcal{S}}}$$

- Consistent, if $\sum_k a_k = \sum_k b_k = 1$
- Symplectic (thus volume-preserving) as a composition of symplectic maps
- Time-reversible, if composition is self-adjoint
- A consistent self-adjoint splitting method satisfies

$$\Phi_h = \exp\left(h(\hat{\mathcal{T}}+\hat{\mathcal{S}}) + \alpha h^3[\hat{\mathcal{T}},[\hat{\mathcal{T}},\hat{\mathcal{S}}]] + \beta h^3[\hat{\mathcal{S}},[\hat{\mathcal{T}},\hat{\mathcal{S}}]] + \mathcal{O}(h^5)\right).$$

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Force-gradient integrators [Omelyan, Mryglod, and Folk 2003]

- Enhance splitting methods by including the commutator

$$\hat{\mathcal{C}} := [\hat{\mathcal{S}}, [\hat{\mathcal{T}}, \hat{\mathcal{S}}]] = 2\hat{\mathcal{S}}\hat{\mathcal{T}}\hat{\mathcal{S}} = 2\boldsymbol{e}^j(\mathcal{S})\boldsymbol{e}_j\boldsymbol{e}_i(\mathcal{S})\frac{\partial}{\partial p_i}$$

  into the computational process
- Force-gradient update

$$\mathbf{e}^{b_k h\hat{\mathcal{S}} + c_k h^3 \hat{\mathcal{C}}}(U_0, P_0) = (U_0, P_0 - b_k h \boldsymbol{e}_i(\mathcal{S})T^i + 2c_k h^3 \boldsymbol{e}^j(\mathcal{S})\boldsymbol{e}_j\boldsymbol{e}_i(\mathcal{S})T^i)$$

Force-Gradient Integrator

$$\Phi_h = \mathbf{e}^{a_1 h\hat{\mathcal{T}}}\mathbf{e}^{b_1 h\hat{\mathcal{S}} + c_1 h^3\hat{\mathcal{C}}} \cdots \mathbf{e}^{a_{s-1}h\hat{\mathcal{T}}}\mathbf{e}^{b_{s-1}h\hat{\mathcal{S}} + c_{s-1}h^3\hat{\mathcal{C}}}\mathbf{e}^{a_s h\hat{\mathcal{T}}}\mathbf{e}^{b_s h\hat{\mathcal{S}} + c_s h^3\hat{\mathcal{C}}}$$

- Same geometric properties as splitting methods, provided that weights c_k are symmetric

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Benefits and Drawbacks of the Force-Gradient Approach

Benefits	Drawbacks
Explicit integration	force-gradient term more expensive than force evaluation
Symplectic and time-reversible	requires the implementation of second-order derivatives contracted with first-order ones
Higher order with less stages	non-trivial implementation
Higher accuracy	

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Approximation of Force-Gradient Updates [Schäfers et al. 2025]

- Force-gradient update: $P_0 - b_k h \boldsymbol{e}_i(\mathcal{S}) T^i + 2c_k h^3 \boldsymbol{e}^j(\mathcal{S}) \boldsymbol{e}_j \boldsymbol{e}_i(\mathcal{S}) T^i$
- Approximation idea dates back to [Wisdom, Holman, and Touma 1996]
- Generalization to Lie groups [Yin and Mawhinney 2012]

Lie series expansion ($F^j \boldsymbol{e}_j := \boldsymbol{e}^j(\mathcal{S})(U_0)\boldsymbol{e}_j$ frozen vector field):

$$
\begin{aligned}
&P_0 - b_k h \boldsymbol{e}_i(\mathcal{S}) \left(\exp\left(-\frac{2c_k h^2}{b_k} F^j T_j \right) U_0 \right) T^i \\
&= P_0 - b_k h \boldsymbol{e}_i(\mathcal{S}) T^i + 2c_k h^3 \boldsymbol{e}^j(\mathcal{S}) \boldsymbol{e}_j \boldsymbol{e}_i(\mathcal{S}) T^i \\
&\quad - \frac{2c_k^2 h^5}{b_k} \boldsymbol{e}^i(\mathcal{S}) \boldsymbol{e}^j(\mathcal{S}) \boldsymbol{e}_i \boldsymbol{e}_j \boldsymbol{e}_k(\mathcal{S}) + \frac{4c_k^3 h^7}{3b_k^2} \boldsymbol{e}^i(\mathcal{S}) \boldsymbol{e}^j(\mathcal{S}) \boldsymbol{e}^\ell(\mathcal{S}) \boldsymbol{e}_i \boldsymbol{e}_j \boldsymbol{e}_\ell \boldsymbol{e}_k(\mathcal{S}) + \mathcal{O}(h^9)
\end{aligned}
$$

No force-gradient term required at the price of a second force evaluation

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Hessian-Free Force-Gradient Integrators [Schäfers et al. 2025]

$$\mathbf{e}^{b_k h\hat{\mathcal{D}}(b_k,c_k,h)}(U_0,P_0) \coloneqq \left(U_0, P_0 - h\boldsymbol{e}_i(\mathcal{S})\left(\exp\left(-\frac{2c_k h^2}{b_k}\boldsymbol{e}^j(\mathcal{S})(U_0)T_j\right)U_0\right)T^i\right)$$

Hessian-Free Force-Gradient Integrator

$$\Phi_h = \mathbf{e}^{a_1 h\hat{\mathcal{T}}}\mathbf{e}^{b_1 h\hat{\mathcal{D}}(b_1,c_1,h)}\cdots\mathbf{e}^{a_{s-1}h\hat{\mathcal{T}}}\mathbf{e}^{b_{s-1}h\hat{\mathcal{D}}(b_{s-1},c_{s-1},h)}\mathbf{e}^{a_s h\hat{\mathcal{T}}}\mathbf{e}^{b_s h\hat{\mathcal{D}}(b_s,c_s,h)}$$

Approximation neither affects the time-reversibility nor the volume-preservation of the integrator, but it introduces additional error terms and the approximated force-gradient updates are no longer symplectic!

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Energy Conservation of Hessian-Free Force-Gradient Integrators

- Hessian-free variants no longer preserve a shadow Hamiltonian
- In general: linear energy drift of size $\mathcal{O}(\tau h^{\max\{4,p\}})$
- For trajectory lengths of $\tau \approx 2$, the energy drift will not have a significant impact on the acceptance probability

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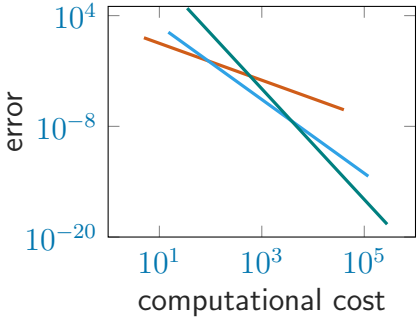
Convergence Order

- Order theory based on the Baker–Campbell–Hausdorff formula
- For force-gradient integrators, the order theory is available in [Omelyan, Mryglod, and Folk 2003] and also covers conventional splitting methods as a special case
- In [Schäfers et al. 2025], we extended the order theory to the Hessian-free framework



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Minimization of the Principal Error Term

- Consider the norm of the leading error coefficients Err_{p+1} as a measure of the accuracy (i.e., all brackets are set equal to one)
- Moreover, assume that two integrators $\Phi_h^{\{1\}}$ and $\Phi_h^{\{2\}}$ of the same order p have principal error terms $\mathrm{Err}_{p+1}^{\{1\}}$ and $\mathrm{Err}_{p+1}^{\{2\}}$, as well as computational costs $\mathrm{cost}^{\{1\}}$ and $\mathrm{cost}^{\{2\}}$, respectively.
- Applying $\Phi_h^{\{1\}}$ with step size h has the same costs as applying $\Phi_{\tilde{h}}^{\{2\}}$ with step size $\tilde{h} := \frac{\mathrm{cost}^{\{2\}}}{\mathrm{cost}^{\{1\}}} h$
- Then, $\Phi_h^{\{1\}}$ is expected to be more accurate than $\Phi_{\tilde{h}}^{\{2\}}$ at the same computational costs, provided that

$$\mathrm{Err}_{p+1}^{\{1\}} \cdot (\mathrm{cost}^{\{1\}})^p < \mathrm{Err}_{p+1}^{\{2\}} \cdot (\mathrm{cost}^{\{2\}})^p$$

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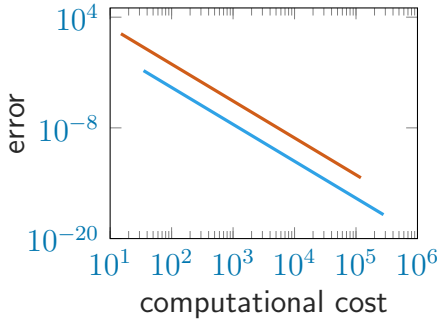
Efficiency Measure

- Efficiency measure

$$\mathrm{Eff}^{(p)} := \frac{1}{(n_f + c \cdot n_g)^p \cdot \mathrm{Err}_{p+1}}$$

  with Err_{p+1} norm of leading error coefficients [Omelyan, Mryglod, and Folk 2003]

- Principal error term has been modified for the Hessian-free framework by incorporating the additional error terms with appropriate weights [Schäfers et al. 2025]



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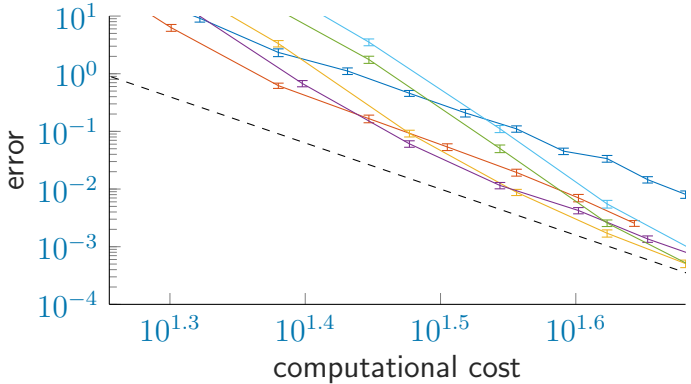
Instabilities of Decomposition Schemes



In lattice QCD simulations, the integrator with the highest efficiency value is not necessarily the most efficient integrator!

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Numerical Stability

Hypothesis for interacting field theories

[Edwards, Horváth, and A. Kennedy 1997; Joó, Pendleton, A. D. Kennedy, Irving, Sexton, Pickles, and Booth 2000]

Since the high frequency modes of an asymptotically free field theory can be considered as a collection of weakly coupled oscillator modes, the instability described in the harmonic oscillator system will also be present for interacting field theories. The onset of the instability will be caused by the mode with highest frequency $\omega_{\max}$.

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Linear Stability Analysis

- Application of (Hessian-free) force-gradient integrators to the harmonic oscillator

$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \left[\begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix} + \begin{pmatrix} 0 & -\omega \\ 0 & 0 \end{pmatrix} \right] \begin{pmatrix} p \\ q \end{pmatrix}$$

- Since the right-hand side is linear, the two frameworks are equivalent
- Exact solution

$$\begin{pmatrix} p(h) \\ q(h) \end{pmatrix} = \underbrace{\begin{pmatrix} \cos(z) & -\sin(z) \\ \sin(z) & \cos(z) \end{pmatrix}}_{=O(z)} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}, \quad z := \omega h.$$

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Linear Stability Analysis

- Applying a self-adjoint force-gradient integrator yields an approximation

$$K(z) = \prod_{k=1}^{s} \begin{pmatrix} 1 & -b_k z + 2c_k z^3 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ a_k z & 1 \end{pmatrix} = \begin{pmatrix} p(z) & K_{1,2}(z) \\ K_{2,1}(z) & p(z) \end{pmatrix}$$

  to $O(z)$ with stability polynomial $p(z)$.
- Decomposition algorithms typically will be unstable for $|h\omega| > z_*$, where the parameter z_* denotes the stability threshold of the integrator
- By adapting the linear stability analysis for splitting methods [Blanes, Casas, and Murua 2008], one can determine the stability threshold z_* so that the integrator is stable for all $z \in (-z_*, z_*)$.

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Determination of the Stability Threshold

- We denote by z^* the largest real non-negative number such that $|p(z)| \leq 1 \; \forall z \in [0, z^*]$
- Suppose that $0 = z_0 < z_1 < \ldots < z_\ell$ are the real zeros with even multiplicity of the polynomial $p(z)^2 - 1$ in the interval $[0, z^*]$. Then, $z_* = z^*$ if

$$K_{1,2}(z_k) = K_{2,1}(z_k) = 0$$

  for each $k = 1, \ldots, \ell$. Otherwise, z_* is the smallest z_k violating the condition.
- For $|p(z)| < 1$, the eigenvalues are distinct. For $|p(z)| = 1$, $K(z)$ has double eigenvalue 1 or -1 and thus is only diagonalizable if $K(z) = \pm I$, i.e., if $K_{2,1}(z) = K_{1,2}(z) = 0$.

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Relative Stability Threshold

- Consider the stability threshold z_* as a measure of the numerical stability
- Moreover, assume that two integrators $\Phi_h^{\{1\}}$ and $\Phi_h^{\{2\}}$ have stability thresholds $z_*^{\{1\}}$ and $z_*^{\{2\}}$, as well as computational costs $\mathrm{cost}^{\{1\}}$ and $\mathrm{cost}^{\{2\}}$, respectively.
- Applying $\Phi_h^{\{1\}}$ with step size h has the same costs as applying $\Phi_{\tilde{h}}^{\{2\}}$ with step size $\tilde{h} := \frac{\mathrm{cost}^{\{2\}}}{\mathrm{cost}^{\{1\}}} h$
- Then, $\Phi_h^{\{1\}}$ is expected to be stable at a lower computational cost than $\Phi_{\tilde{h}}^{\{2\}}$, provided that

$$\frac{\mathrm{cost}^{\{2\}}}{\mathrm{cost}^{\{1\}}} z_*^{\{1\}} > z_*^{\{2\}} \quad \Leftrightarrow \quad \frac{z_*^{\{1\}}}{\mathrm{cost}^{\{1\}}} > \frac{z_*^{\{2\}}}{\mathrm{cost}^{\{2\}}}$$

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$$\frac{\mathrm{cost}^{\{2\}}}{\mathrm{cost}^{\{1\}}} z_*^{\{1\}} > z_*^{\{2\}} \quad \Leftrightarrow \quad \frac{z_*^{\{1\}}}{n_f^{\{1\}} + c \cdot n_g^{\{1\}}} > \frac{z_*^{\{2\}}}{n_f^{\{2\}} + c \cdot n_g^{\{2\}}}$$

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Detection of Promising Integrators Variants

Detecting promising integrators demands the investigation of

- the convergence order p,
- the leading error term, and
- the numerical stability.

Maximizing the Stability Threshold?

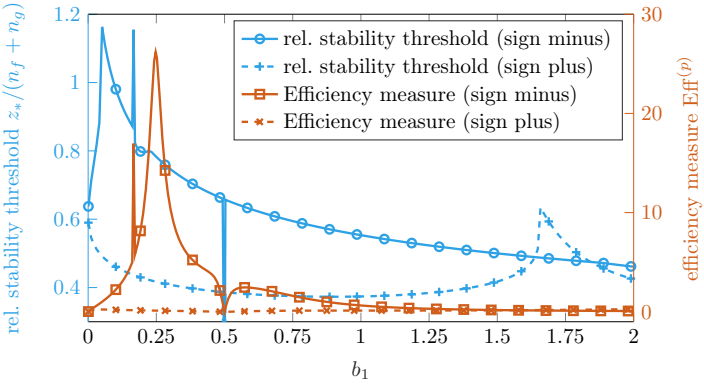

Figure: Analysis of the Hessian-free force-gradient integrator ABADADBA in terms of the efficiency measure $\mathrm{Eff}^{(p)}$ and the relative stability threshold $z_*/(n_f+n_g)$.

Example for 2 Degrees of Freedom

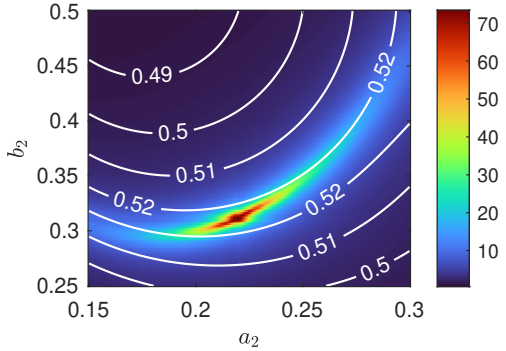

Figure: The efficiency measure $\mathrm{Eff}^{(4)}$ for the integrator BADABADAB evaluated at different values of a_2 and b_2. The white contour lines indicate the values for the relative stability threshold $z_*/(n_f + n_g)$.

Promising Integrators

Integrator ID	p	n_f	n_g	$\mathrm{Eff}^{(p)}$	$z_*/(n_f+n_g)$
BAB/ABA	2	1	0	10.73	2.0000
BABAB/ABABA	2	2	0	29.24	1.2766
BADAB	4	2	1	16.96	1.1547
ABADABA	4	3	1	26.19	0.7844
BABABABABAB	4	5	0	59.26	0.6284
BADABADAB	4	4	2	73.45	0.5243
BADABABADAB	4	5	2	80.13	0.4482
ABADABADABA	4	5	2	93.60	0.4463
BABABABABABABAB	6	7	0	1.40	0.4515

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Twisted Mass Simulations

- $N_f = 2$ twisted mass fermions with a clover term $c_{sw} = 1.57551$ and a bare mass parameter of $\kappa = 0.137322$
- one Hasenbusch mass $a\kappa\mu_1 = 0.1$
- nested integrator with three integration levels:
  - macro level: ratio operator with lower bound $\lambda_{\min} \geq (\mu_1^2 - \mu_0^2)/\mu_0^2 \approx \mu_1^2/\mu_0^2$
  - intermediate level: additional Hasenbusch term $D^\dagger D + \mu_1^2$
  - micro level: Iwasaki pure gauge action
- on all integration levels, we use the integrator

$$\Phi_h = \mathbf{e}^{\lambda h \hat{\mathcal{S}}} \mathbf{e}^{h/2 \hat{\mathcal{T}}} \mathbf{e}^{(1-2\lambda) h \hat{\mathcal{S}}} \mathbf{e}^{h/2 \hat{\mathcal{T}}} \mathbf{e}^{\lambda h \hat{\mathcal{S}}}$$

  - $\lambda = \lambda_{\texttt{err}} \approx 0.193, \quad \mathrm{Eff}^{(2)} \approx 29.24, \quad z_* \approx 2.5531$
  - $\lambda = \lambda_{\texttt{stab}} = 0.25, \quad \mathrm{Eff}^{(2)} \approx 10.73, \quad z_* = 4$

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Twisted Mass Simulations

- Stability-enhanced version allows for a $z_*(\lambda_{\texttt{stab}})/z_*(\lambda_{\texttt{err}}) \approx 1.5667$ times larger step size when employed to the harmonic oscillator
- For varying number of time steps N on the macro level, we compute 30 trajectories of length $\tau = 1.0$
- As a criterion for instability, we choose

$$\sigma^2(\Delta\mathcal{H}(N)) + 1.5 \cdot \mathrm{std}\left(\sigma^2(\Delta\mathcal{H}(N))\right) > f(N)$$

  where $\sigma^2(\Delta\mathcal{H}(N))$ denotes the variance of $\Delta\mathcal{H}$ when computing N time steps per trajectory, $\mathrm{std}(\sigma^2(\Delta\mathcal{H}(N)))$ its standard deviation, and $f(N) = c_0 + \frac{c_1}{N^{2p}}$ is a least squares fitting function of the data $(N, \sigma^2(\Delta\mathcal{H}(N)))$
- We denote the onset of instability as $N_{\texttt{min}}$.

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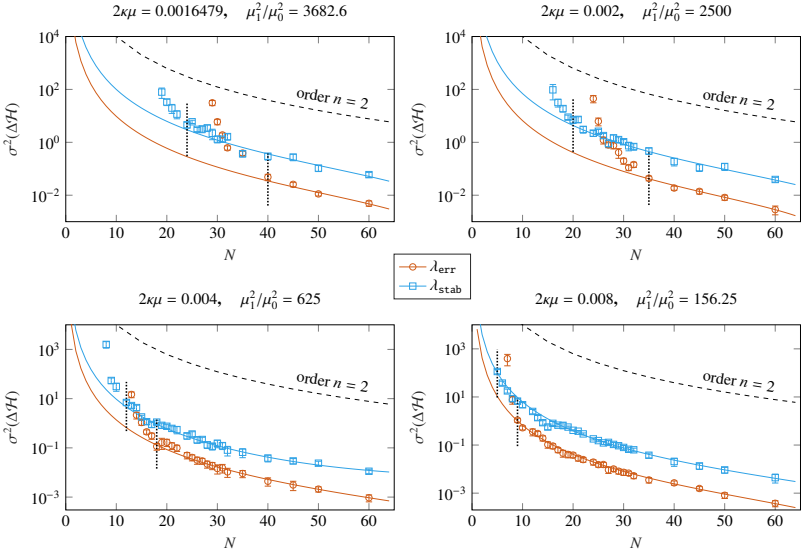
$2\kappa\mu = 0.0016479, \quad \mu_1^2/\mu_0^2 = 3682.6$
$2\kappa\mu = 0.002, \quad \mu_1^2/\mu_0^2 = 2500$
$2\kappa\mu = 0.004, \quad \mu_1^2/\mu_0^2 = 625$
$2\kappa\mu = 0.008, \quad \mu_1^2/\mu_0^2 = 156.25$
order $n = 2$
$\sigma^2(\Delta H)$
N
λ_{err}
λ_{stab}

Twisted Mass Simulations

μ_1^2/μ_0^2	$N_{\mathtt{min}}(\lambda_{\mathtt{err}})$	$N_{\mathtt{min}}(\lambda_{\mathtt{stab}})$	$N_{\mathtt{min}}(\lambda_{\mathtt{err}})/N_{\mathtt{min}}(\lambda_{\mathtt{stab}})$
156.25	9	5	1.8000
625.00	18	12	1.5000
2500.00	35	20	1.7500
3682.60	40	24	1.6667

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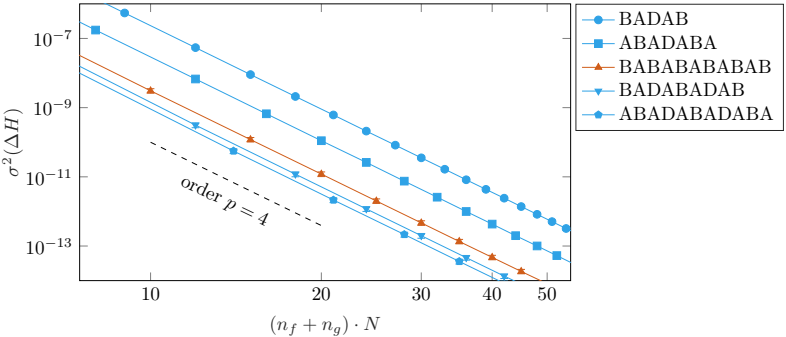
4D Gauge Field Simulations in Lattice QCD with Wilson Fermions

Ensemble with a 48×24^3 lattice generated with two dynamical nonperturbatively $O(a)$ improved Wilson quarks with a mass equal to half of the physical charm

[Knechtli, Korzec, Peardon, and Urrea-Niño 2022]

$\beta = 5.3$, $\kappa = 0.1327$, trajectory length $\tau = 0.1$, varying step size h



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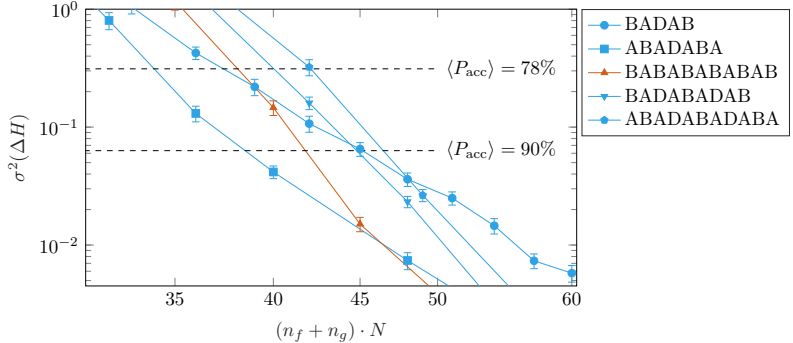
$\beta = 5.3$, $\kappa = 0.1327$, trajectory length $\tau = 2.0$, varying step size h



4D Gauge Field Simulations in Lattice QCD with Wilson Fermions

ID	$(n_f + n_g) \cdot N$ for $\langle P_{\text{acc}} \rangle_{\text{opt}}$
BADAB	37.3751
ABADABA	34.0219
BABABABABAB	38.1049
BADABADAB	40.0282
BADABABADAB	46.1456
ABADABADABA	42.0871

Table: Comparison of the required computational cost $(n_f + n_g) \cdot N$ to achieve the optimal acceptance rate $\langle P_{\text{acc}} \rangle_{\text{opt}} = \exp(-1/p) \approx 78\%$ for fourth-order integrators. The results are obtained by performing a linear interpolation in logarithmic space of the two data points that are closest to the optimal acceptance rate.

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Conclusion and Outlook

- Refined analysis of Hessian-free force-gradient integrators (order theory, geometric properties, minimum-error variants) available
- Hessian-free force-gradient integrators allow for a more efficient computational process and are straightforward to implement into existing software
- Numerical stability is crucial for the performance in lattice QCD simulations
- Next steps:
  - Extension of the order theory and the linear stability analysis to multiple time scales (nested integration)
  - Problem-dependent integrator tuning by using a weighted norm of the leading error coefficients

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Hessian-free force-gradient integrators in openQCD

- Hessian-free force-gradient integrators have been implemented in openQCD (based on version 2.4).
- The code is publicly available on GitHub.

Thank you for your attention!

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References I

Blanes, Sergio, Fernando Casas, and Ander Murua. "On the Linear Stability of Splitting Methods". In: *Found. Comput. Math.* 8.3 (2008), pp. 357–393.

Edwards, R.G., Ivan Horváth, and A.D. Kennedy. "Instabilities and non-reversibility of molecular dynamics trajectories". In: *Nuclear Physics B* 484.1 (1997), pp. 375–399.

Joó, Bálint, Brian Pendleton, Anthony D. Kennedy, Alan C. Irving, James C. Sexton, Stephen M. Pickles, and Stephen P. Booth. "Instability in the molecular dynamics step of a hybrid Monte Carlo algorithm in dynamical fermion lattice QCD simulations". In: *Phys. Rev. D* 62 (11 Oct. 2000), p. 114501.

References II

Knechtli, Francesco, Tomasz Korzec, Michael Peardon, and Juan Andrés Urrea-Niño. "Optimizing creation operators for charmonium spectroscopy on the lattice". In: *Phys. Rev. D* 106 (3 Aug. 2022), p. 034501.

McLachlan, Robert I. and G. Reinout W. Quispel. "Splitting methods". In: *Acta Numer.* 11 (2002), pp. 341–434.

Omelyan, I.P., I.M. Mryglod, and R. Folk. "Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations". In: *Comput. Phys. Commun.* 151.3 (2003), pp. 272–314.

Schäfers, Kevin, Jacob Finkenrath, Michael Günther, and Francesco Knechtli. "Hessian-free force-gradient integrators". In: *Computer Physics Communications* 309 (2025), p. 109478. arXiv: 2403.10370.

References III

Schäfers, Kevin, Jacob Finkenrath, Michael Günther, and Francesco Knechtli. "Hessian-free force-gradient integrators and their application to lattice QCD simulations". In: *PoS* LATTICE2024 (2025), p. 025. arXiv: 2501.17632.

— .*Numerical stability of force-gradient integrators and their Hessian-free variants in lattice QCD simulations*. 2025. arXiv: 2506.08813.

Wisdom, Jack, M Holman, and J Touma. "Symplectic correctors". In: *Integration algorithms and classical mechanics*. Amer. Math. Soc., 1996, pp. 217–244.

Yin, Hantao and Robert D. Mawhinney. "Improving DWF Simulations: the Force Gradient Integrator and the Möbius Accelerated DWF Solver". In: *PoS* LATTICE2011 (2012).