Hessian-free force-gradient integrators

and their application to lattice QCD simulations

K. Schäfers, J. Finkenrath, M. Günther, F. Knechtli

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MACM
Institute of Modelling, Analysis and Computational Mathematics

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Decomposition algorithms

- Hamiltonian $\mathcal{H}(U,P) = \mathcal{T}(P) + \mathcal{V}(U)$
- equations of motion

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

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

- exact flows of subsystems
  - $\mathbf{e}^{h\hat{\mathcal{V}}}(U_0, P_0) = (U_0, P_0 - h\boldsymbol{e}_i(\mathcal{V})T^i)$ (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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Approximation of force-gradient updates [Schäfers et al. 2024]

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

Lie series expansion ($F_i := -\boldsymbol{e}_i(\mathcal{V})$):

$$
\begin{aligned}
&P_0 - b_k h \boldsymbol{e}_i\left(\mathcal{V}\right)\left(\exp\left(\frac{2c_k h^2}{b_k} F^j(Q_0) T_j\right) Q_0\right) T^i \\
=&P_0 - b_k h \boldsymbol{e}_i(\mathcal{V}) T^i + 2c_k h^3 \boldsymbol{e}^j(\mathcal{V}) \boldsymbol{e}_j \boldsymbol{e}_i(\mathcal{V}) T^i \\
&- \frac{2c_k^2 h^5}{b_k} \boldsymbol{e}^i(\mathcal{V}) \boldsymbol{e}^j(\mathcal{V}) \boldsymbol{e}_i \boldsymbol{e}_j \boldsymbol{e}_k(\mathcal{V}) + \frac{4c_k^3 h^7}{3b_k^2} \boldsymbol{e}^i(\mathcal{V}) \boldsymbol{e}^j(\mathcal{V}) \boldsymbol{e}^\ell(\mathcal{V}) \boldsymbol{e}_i \boldsymbol{e}_j \boldsymbol{e}_\ell \boldsymbol{e}_k(\mathcal{V}) + \mathcal{O}(h^9)
\end{aligned}
$$

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. 2024]

$$\mathbf{e}^{b_k h \hat{\mathcal{D}}(b_k, c_k, h)}(U_0, P_0) := \left(U_0, P_0 - h\boldsymbol{e}_i(\mathcal{V})\left(\exp\left(-\frac{2c_k h^2}{b_k}\boldsymbol{e}^j(\mathcal{V})(Q_0)T_j\right)Q_0\right)T^i\right)$$

Hessian-free force-gradient integrator

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

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

On 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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Additional order conditions

order	#order conditions FGI	#order conditions Hessian-free
2	2	2
4	2	2
6	4	5
8	10	13

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How to find efficient integrators

- 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 (i.e. Poisson brackets are set equal to one) [Omelyan, Mryglod, and Folk 2003]
- has been adapted for the Hessian-free variants by incorporating the additional error terms [Schäfers et al. 2024]
- Numerical results emphasize that

  integrator with highest efficiency value $\neq$ most efficient integrator

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Numerical stability

Hypothesis for interacting field theories

[Edwards, Horváth, and Kennedy 1997; Joó et al. 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 $p(z)$.
- 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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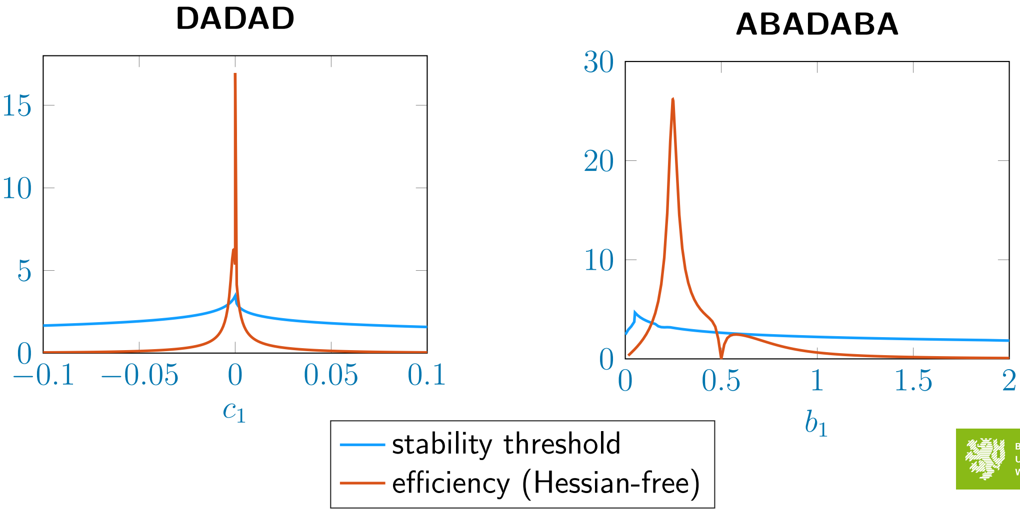
Maximizing the stability threshold?



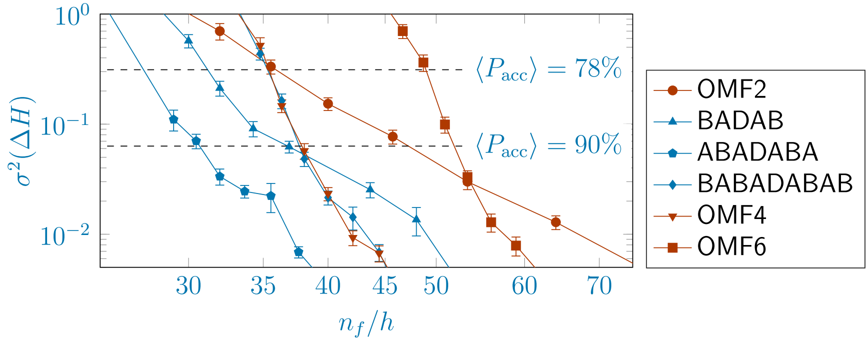
Promising integrators

integrator ID	p	n_f	n_g	$\mathrm{Eff}^{(p)}$	$z_*/(n_f+n_g)$
OMF2/2MN	2	2	0	29.2	1.2766
OMF4/4MN	4	5	0	59.3	0.6284
BADAB	4	2	1	17.0	1.1547
ABADABA	4	3	1	26.2	0.7844
BABADABAB	4	4	1	24.6	0.6225
OMF6	6	7	0	1.4	0.4515

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 et al. 2022]

$\beta = 5.3, \quad \kappa = 0.1327, \quad$ varying τ, step size $h = \tau/4$



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openQCD package

- 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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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 $K_{2,1}(z) = K_{1,2}(z) = 0$.