Low-rank approximation for nonlinear kinetic problems
Part 3: Structure preserving dynamical low-rank algorithms

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Link to slides: `http://www.einkemmer.net/training.html`

Physical structure of the Vlasov equation

Hamiltonian systems

Reminder: In a Hamiltonian system the time evolution of a quantity $F(p, q)$ can be written as

$$\partial_t F = \{F, H\}$$

with Hamiltonian H and the symplectic Poisson bracket

$$\{F, G\} = \nabla_q F \cdot \nabla_p G - \nabla_p F \cdot \nabla_q G.$$

Since $\partial_t H = \{H, H\} = 0$ we follow that the Hamiltonian, i.e. **the energy of the system, is conserved**.

Every quantity C such that $\{C, H\} = 0$ is conserved.

A **non-canonical Hamiltonian** system admits a Poisson bracket $[\cdot, \cdot]$ (not necessarily the symplectic bracket above) that satisfies Anticommutativity, Bilinearity, Leibniz's rule, and the Jacobi identity.

Non-canonical Hamiltonian systems

Example: The generalized Lotka–Volterra model

$$\dot{u} = u(v + w), \qquad \dot{v} = v(u - w + 1), \qquad \dot{w} = w(u + v + 1)$$

is a non-canonical Hamiltonian system with

$$H(u, v) = -u + v + w + \ln v - \ln w \quad \text{and} \quad [F, G] = (\nabla_{uvw} F)^T \underbrace{\begin{bmatrix} 0 & uv & uw \\ -uv & 0 & -vw \\ -uw & vw & 0 \end{bmatrix}}_{B} \nabla_{uvw} G$$

C is a **Casimir invariant** if $\{C, F\} = 0$ holds for all F.

- We call the Poisson bracket degenerate.

Example: For the Lotka–Volterra model $C(u, v) = -\ln u - \ln v + \ln w$ is a Casimir invariant as $(\nabla_{uvw} C)^T B = 0$.

Vlasov–Maxwell equations

Vlasov equation

$$\partial_t f + v \cdot \nabla_x f - (E + v \times B) \cdot \nabla_v f = 0$$

coupled to Maxwell's equations

$$\partial_t E = c^2 \nabla_x \times B - j, \qquad \partial_t B = -\nabla_x \times E,$$

where $j = \int v f \, \mathrm{d}v$.

There are also **constraints** (automatically satisfied in the continuous case)

$$\nabla \cdot B = 0, \qquad \nabla \cdot E = 1 - \rho$$

Hamiltonian structure

The **Vlasov–Maxwell equations** have a **non-canonical Hamiltonian** structure.

$$\begin{aligned} H &= \frac{1}{2}\int |E|^2 \,\mathrm{d}x + \frac{c^2}{2}\int |B|^2 \,\mathrm{d}x + \frac{1}{2}\int v^2 f \,\mathrm{d}(x,v) \\ &=: H_E + H_B + H_f. \end{aligned}$$

Evolution of F

$$\partial_t F = [F, H] = [F, H_E] + [F, H_B] + [F, H_f]$$

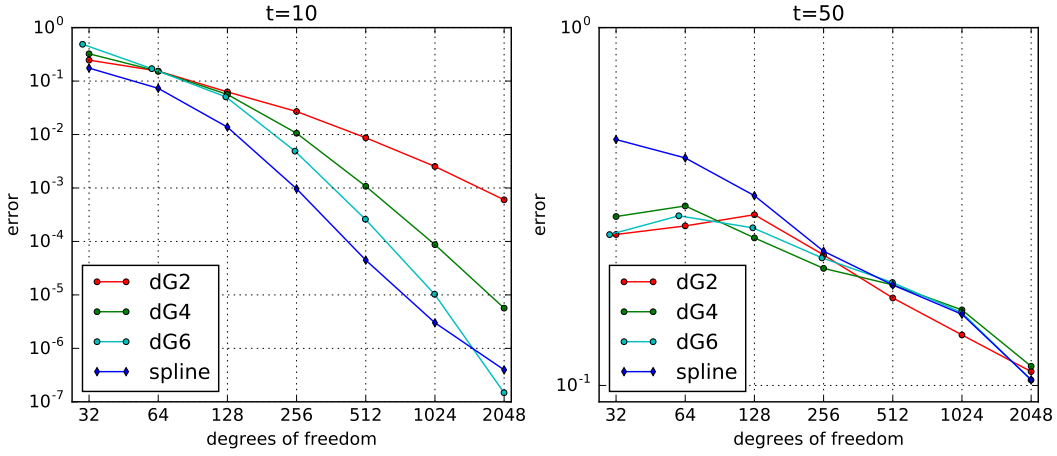
with a highly non-canonical Poisson bracket.

We have an **infinite number of Casimir invariants** as any $C(f)$ satisfies $[C, G] = 0$ for arbitrary G.

- $\|f\|_2$ (in fact, any L^p norm)
- Entropy $-\int_\Omega f \log f \,\mathrm{d}(x,v)$.

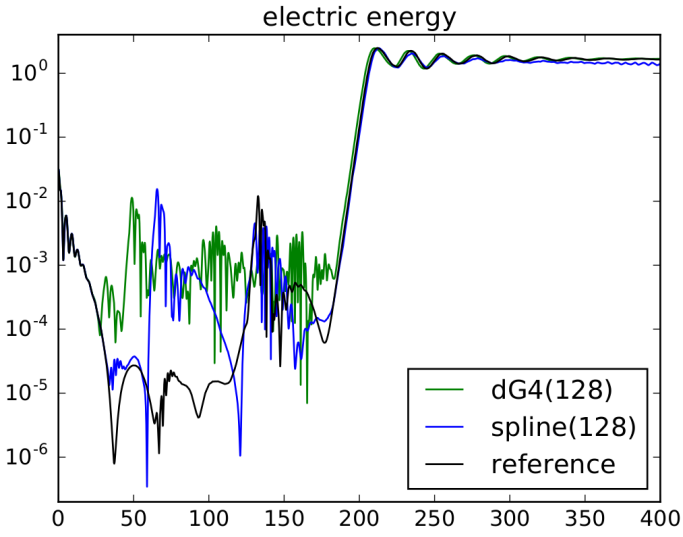
Accuracy of Vlasov simulation

Performance is often checked by using a work-precision diagram.



Two-stream instability

Vlasov–Poisson equation with 128^4 degrees of freedom.



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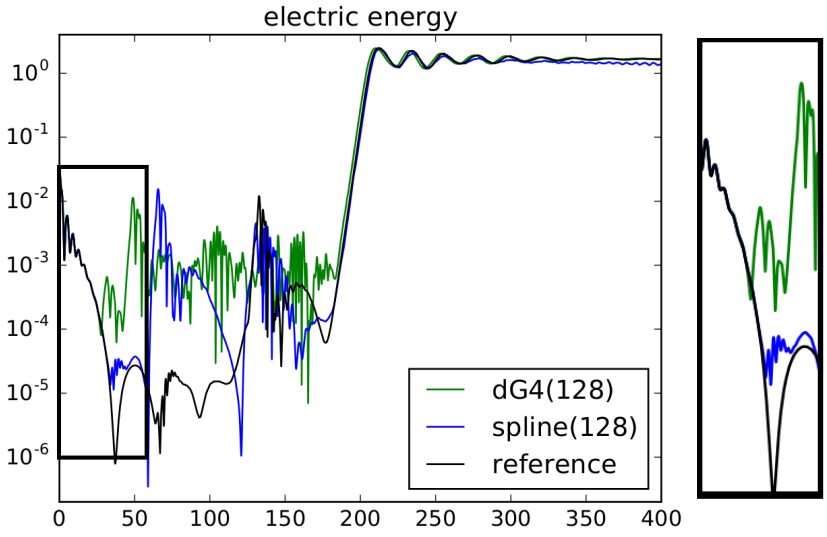
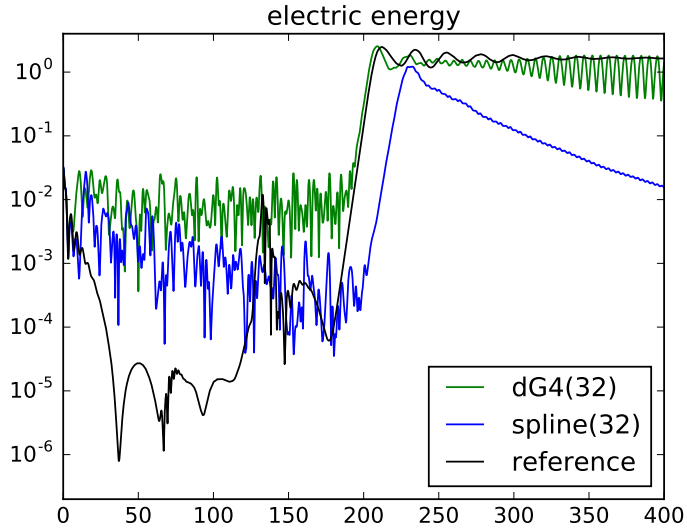


Two-stream instability

Vlasov–Poisson equation with 32^4 degrees of freedom.



Discussion

We are in the **asymptotic regime** if classic convergence theory applies. That is,

$$\text{error} \leq C\left((\Delta t)^p + (\Delta x)^q\right).$$

gives a tight bound of the error.

Why is this not the case here? Consider

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) = 0, \qquad f(0,x,v) = \mathrm{e}^{ikx}\mathrm{e}^{-v^2/2}$$

which has the solution

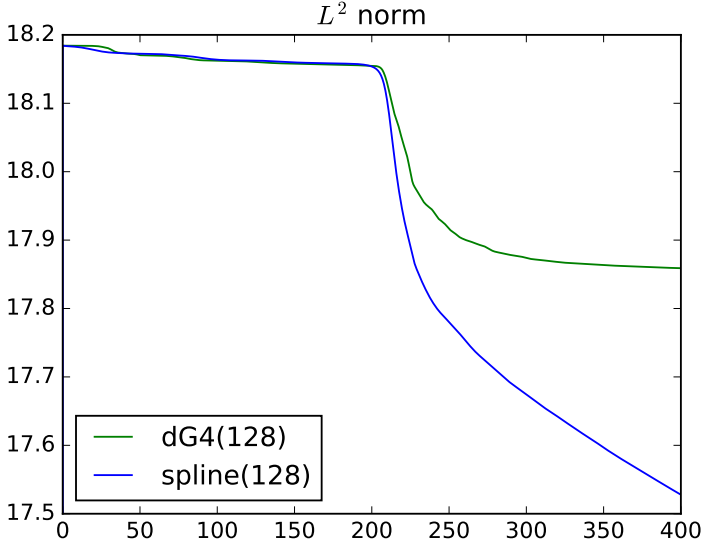
$$f(t,x,v) = \mathrm{e}^{ikt v}\mathrm{e}^{ikx}\mathrm{e}^{-v^2/2}.$$

Small scale structures (e.g. filamentation, turbulence, ...) can not be resolved.

- **All methods are necessarily inaccurate.**
- Often we can still get good physics out of those methods.

Two-stream instability

L^2 **norm** as a measure of **numerical diffusion**.



Dynamical low-rank

Galerkin condition

Orthogonal projection

$$\text{Find} \quad \partial_t f = g \in T_f\mathcal{M} \quad \text{such that} \quad \|g - \text{RHS}\| \text{ is minimal.}$$

That is, $g = P(f)\text{RHS}$.

Galerkin condition

$$\text{Find} \quad \partial_t f \quad \text{such that} \quad \langle \nu, \partial_t f \rangle = \langle \nu, \text{RHS} \rangle \quad \forall \nu \in T_f\mathcal{M}.$$

For the Schrödinger equation implies symplecticity, energy, and norm conservation.

- But the situation here is very different.

L^2 conservation

Galerkin condition implies **$\mathbf{L^2}$ norm conservation**

$$\partial_t \|f\|^2 = 2\langle f, \partial_t f\rangle_{xv} = 2\langle f, RHS\rangle_{xv} = 0$$

since $f \in T_f\mathcal{M}$.

But wait, why do we have $\langle f, RHS\rangle_{xv} = 0$?

This is how we (directly) prove L^2 conservation for the underlying model

$$\partial_t \|f\|^2 = 2\langle f, RHS\rangle_{xv} = \int \nabla_x \cdot (vf^2) - \nabla_v \cdot (Ef^2)\,\mathrm{d}(x, v) = 0.$$

The analytic argument carries over. **This will be an important technique!**

Mass conservation

From

$$\partial_t f + \nabla_x \cdot (vf) - \nabla_v \cdot (Ef) = 0$$

we follow by integrating in v

$$\partial_t \int f \, \mathrm{d}x + \nabla_x \cdot \int vf \, \mathrm{d}v = 0,$$

which is more commonly written as

$$\partial_t \rho + \nabla \cdot j = 0, \qquad \rho = \int f \, \mathrm{d}v, \qquad j = \int vf \, \mathrm{d}v.$$

Integrating in x we get

$$M = \int f \mathrm{d}(x, v) = \text{const.}$$

That is, **conservation of mass**.

Momentum or charge conservation

From

$$\partial_t(vf) + \nabla_x \cdot ((v \otimes v)f) - v\nabla_v \cdot (Ef) = 0$$

we follow by integrating in v

$$\partial_t j + \nabla_x \cdot \sigma = -\int Ef \, \mathrm{d}v = E\rho, \qquad \sigma = \int (v \otimes v) f \, \mathrm{d}v.$$

Since

$$E(1-\rho) = \nabla \cdot (E \otimes E - \tfrac{1}{2}E^2)$$

and $\int E \, \mathrm{d}x = 0$ we obtain

$$P = \int vf \, \mathrm{d}(x, v) = \text{const},$$

That is, **conservation of momentum**.

Energy conservation

We already know that **energy (i.e. the Hamiltonian) is conserved**

$$H = \frac{1}{2}\int v^2 f \,\mathrm{d}(x,v) + \frac{1}{2}\int E^2 \,\mathrm{d}x.$$

Similar to mass and momentum there is also an associated **local conservation law**

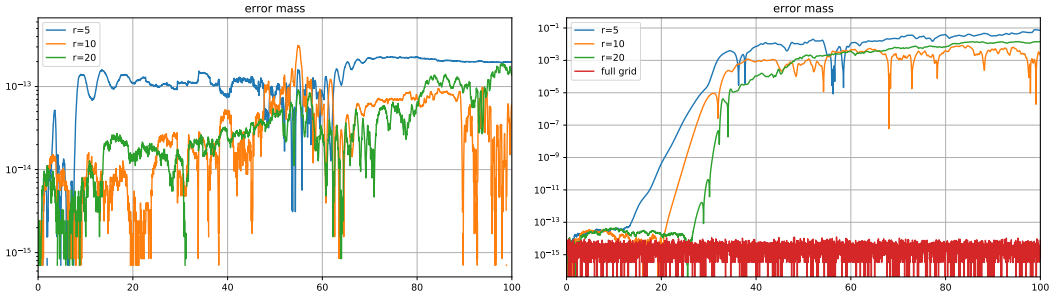
$$\partial_t e + \nabla_x \cdot Q = E \cdot (\partial_t E - j), \qquad e = \frac{1}{2}\int v^2 f \, dv + \frac{1}{2}E^2, \quad Q = \frac{1}{2}\int v v^2 f \, dv.$$

Dynamical low-rank approximation

The dynamical low-rank approximation finds the, in some sense, best L^2 approximation.

- No guarantee that mass, momentum, or energy is conserved.

Linear Landau damping (left) and two-stream instability (right).



This **failure is in stark contrast to Eulerian and particle methods**.

Literature

[Z. Peng, R. McClarren, M. Frank, J. Comput. Phys., 421 (2020)]

- Rescale solution to obtain mass conservation.
- Global mass conservation only.
- Not extensible to other invariants.

[Z. Peng, and R.G. McClarren. arXiv:2011.06072]

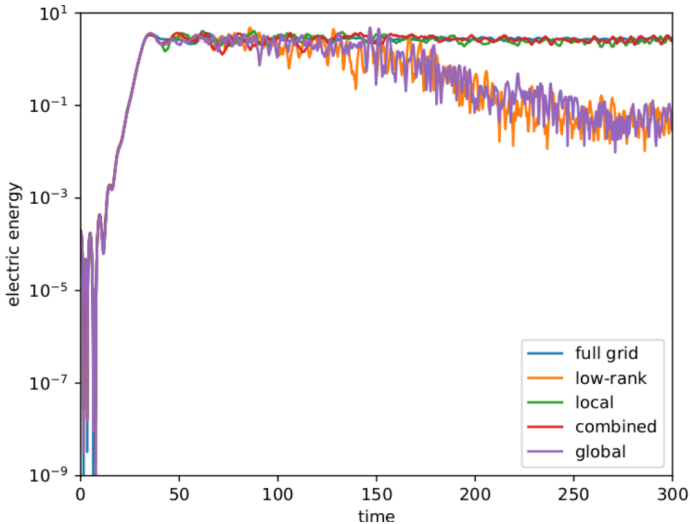
- Couple moments with low-rank approximation of g, where $f = M + g$.
- Needs to enforce $\int g \, \mathrm{d}(x, v) = 0$.
- Global invariants only.

[L. Einkemmer, C. Lubich. SIAM J. Sci. Comput., 40(5) (2018)]

- Add correction $\lambda_{ij} X_i V_j$ to enforce conservation (Lagrange multiplier).
- Conserves either global invariants or (a projected version of) conservation laws.
- Not able to simultaneously conserve both.

Global vs local conservation

We should not forget the **local conservation law!**



Conservative dynamical low-rank approximation

Conservative dynamical low-rank approximation

Fundamental observation: If $v \mapsto 1/v \mapsto v/v \mapsto v^2$ is part of the approximation space $\overline{V} = \text{span}\{V_1, \dots, V_r\}$ then we obtain the conservation laws also in the DLRA.

For $K_j = \sum_i X_i S_{ij}$ we have

$$f = \sum_j K_j V_j, \qquad \text{and thus} \qquad \rho = \int f \, \mathrm{d}v = \sum_j K_j \langle 1, V_j \rangle_v.$$

Now we assume that $V_1 \propto 1$. Then

$$\rho = \frac{1}{V_1} K_1$$

and thus

$$\partial_t \rho = \frac{1}{V_1} \langle V_1, \text{RHS} \rangle_v = \int_{\Omega_v} \text{RHS} \, dv = -\nabla \cdot j.$$

Argument from the continuous system carries over.

Problems

These functions do not lie in $L^2(\mathbb{R}^3)$.

- We use an $\mathbf{L^2}$ **space weighted by** f_{0v}.
- For kinetic equations $f_{0v}(v) = exp(-v^2/2)$ is usually a reasonable choice.

Low-rank approximation

$$f = f_{0v} \sum_{ij} X_i S_{ij} V_j$$

with $X_i \in L^2(\Omega_x)$ and

$$V_j \in L^2(\Omega_v, f_{0v}) = \left\{ g : \int f_{0v} g^2 \, \mathrm{d}x < \infty \right\}.$$

The basis functions are chosen by the algorithm to satisfy a Galerkin condition.

- Basis functions **change as time evolves in order to adapt to the problem**.

Conservative dynamical low-rank algorithm

Some of the v dependent basis functions V_j are held fixed

$$U_a(v) = V_a(t, v), \quad 1 \le a \le m \qquad \text{and} \qquad W_p(t, v) = V_p(t, v), \quad m < p \le r.$$

But orthogonality between U_a and W_p still **needs to be enforced.**

Petrov–Galerkin condition

$$\left(\frac{\nu}{f_{0v}}, \partial_t f - RHS \right)_{xv} = 0 \qquad \forall \nu \in T_f \mathcal{M}$$

with $(f, g) = \int_{\Omega_v} fg \, \mathrm{d}v$.

Equations of motion for $\mathbf{S}_{ij}$: We test with $\nu_{kl} = f_{0v} X_k V_l$

Equations of motion for X

We test with $\nu_k = f_{0v}\chi V_k$, χ is arbitrary.

- Since $\nu_k = f_{0v}\sum_{ij}\dot{X}_i S_{ij} V_j$ with $\dot{X}_i = \chi(x) S_{ki}^{-1}$ it holds that $\nu_k \in T_f\mathcal{M}$.

The Petrov–Galerkin condition becomes

$$\left(V_k\chi, f_{0v}\sum_{ij}\left(\dot{X}_i S_{ij} V_j + X_i \dot{S}_{ij} V_j\right) + f_{0v}\sum_{ip} X_i S_{ip}\dot{W}_p\right)_{xv} = (V_k\chi, \mathrm{RHS})_{xv}\,.$$

which we can rewrite as

$$\left\langle V_k\chi, \sum_{ij}\left(\dot{X}_i S_{ij} V_j + X_i \dot{S}_{ij} V_j\right) + \sum_{ip} X_i S_{ip}\dot{W}_p\right\rangle_{xv} = (V_k\chi, \mathrm{RHS})_{xv}$$

Using orthogonality/gauge cond. and χ arbitrary, we obtain the **equations of motion**

$$\sum_i \dot{X}_i S_{ik} = (V_k, \mathrm{RHS})_v - \sum_i X_i \dot{S}_{ik}.$$

Equations of motion for W

We test with $\nu_q = f_{0v}\zeta \sum_i X_i S_{iq}$, ζ is arbitrary.

- Since $\nu_q = f_{0v} \sum_{ip} X_i S_{ip} \dot{W}_p$ with $\dot{W}_p = \delta_{pq}\zeta(v)$ it holds that $\nu_q \in T_f\mathcal{M}$.

The Petrov–Galerkin condition becomes

$$\sum_i \left(\zeta X_i S_{iq}, f_{0v} \sum_{kl} \left(\dot{X}_k S_{kl} V_l + X_k \dot{S}_{kl} V_l \right) + f_{0v} \sum_{kp} X_k S_{kp} \dot{W}_p \right)_{xv} = \sum_i (\zeta X_i S_{iq}, \mathrm{RHS})_{xv}$$

Using orthogonality/gauge cond. and ζ arbitrary, we obtain the **equations of motion**

$$\sum_{ip} S_{iq} S_{ip} (\partial_t W_p) + \sum_{il} S_{iq} (\partial_t S_{il}) V_l = \frac{1}{f_{0v}} \sum_i S_{iq} (X_i, \mathrm{RHS})_x.$$

Coefficients

The **coefficients are slightly different** due to the weighted approximation space.

For example

$$\begin{aligned}
\frac{1}{f_{0v}}(X_i, \mathrm{RHS})_x &= \frac{1}{f_{0v}}\left(X_i, -v\cdot\nabla_x f + E\cdot\nabla_v f\right)_x \\
&= -\frac{1}{f_{0v}}\sum_{kl} f_{0v}\langle X_i, \nabla_x X_k\rangle_x \cdot v S_{kl} V_l + \frac{1}{f_{0v}}\sum_{kl} S_{kl}\nabla_v(f_{0v}V_l)\cdot\langle X_i, EX_k\rangle_x \\
&= -\sum_{kl}(v\cdot d^2_{ik})S_{kl}V_l + \frac{1}{f_{0v}}\sum_{kl} d^1_{ik}[E]\cdot\nabla_v(f_{0v}S_{kl}V_l) \\
&= -\sum_{kl}(v\cdot d^2_{ik})S_{kl}V_l + \sum_{kl} d^1_{ik}[E]\cdot\left[\nabla_v(S_{kl}V_l) + \nabla_v(\log f_{0v})S_{kl}V_l\right],
\end{aligned}$$

where

$$d^1_{ik}[E] = \langle X_i E X_k\rangle_x, \qquad d^2_{ik} = \langle X_i, \nabla_x X_k\rangle_x.$$

Conservative dynamical low-rank algorithm

We have

- $U_1 \propto 1$, $U_2 \propto v$, $U_3 \propto v^2$ lie in the approximation space span$\{V_1, \dots, V_r\}$ by construction;
- The dynamics determined W_p are orthogonal to the U_a as

$$\begin{aligned}\partial_t \langle U_a, W_p \rangle_v &= \sum_{iq} T^{-1}_{pq} S_{iq} \langle \tfrac{1}{f_{0v}} U_a X_i, \mathrm{RHS} \rangle_{xv} - \sum_{il} T^{-1}_{pq} S_{iq} \partial_t S_{il} \langle U_a, V_l \rangle_v \\ &= \sum_{iq} T^{-1}_{pq} S_{iq} \langle \tfrac{1}{f_{0v}} U_a X_i, \mathrm{RHS} \rangle_{xv} - \sum_{il} T^{-1}_{pq} S_{iq} (X_i U_a, \mathrm{RHS})_{xv} = 0.\end{aligned}$$

Results in a **mass, momentum, and energy conservative** DLR approximation.

Momentum conservation

We choose U_2 such that $v = \|v\| U_2$, i.e. $U_2 \propto v$.

Our **dynamical low-rank approximation is conservative** because we can use the **argument for the original problem**.

For example, for the **momentum density** we have

$$j = \int vf \,\mathrm{d}v = \sum_j K_j \int f_{0v} v V_j \,\mathrm{d}v = \|v\| \sum_j K_j \langle U_2, V_j \rangle = \|v\| K_2.$$

Conservation of momentum

$$\partial_t j = \|v\| \partial_t K_2 = \|v\| (U_2, \mathrm{RHS})_v = \int v \mathrm{RHS}\, dv = -\nabla_x \cdot \sigma - E\rho.$$

Integration in x then gives the global invariant.

Conservative time and space discretization

Time discretization

Explicit Euler scheme applied to the equations of motion

$$S_{kl}^{n+1} = S_{kl}^{n} + \Delta t \, (X_k^n V_l^n, \mathrm{RHS}^n)_{xv} \, ,$$

$$X_i^{n+1} = X_i^n + \Delta t \sum_k (S^n)_{ik}^{-1} \left[(V_k^n, \mathrm{RHS}^n)_v - \sum_l X_l^n \, (X_l^n V_k^n, \mathrm{RHS}^n)_{xv} \right],$$

$$W_p^{n+1} = W_p^n + \Delta t \sum_q ((S^n)^T S^n)_{pq}^{-1} \left[\frac{1}{f_{0v}} \sum_i S_{iq}^n (X_i^n, \mathrm{RHS}^n)_x - \sum_{il} S_{iq}^n \, (X_i^n V_l^n, \mathrm{RHS}^n)_{xv} \, V_l^n \right],$$

is **not** conservative.

Uses S^n, i.e. S at time t^n, to compute X^{n+1}.

- There is no well defined K^n and K^{n+1} and thus the argument applied before does not carry over.

Conservative time discretization

We can rewrite the equation for K in conservative form

$$\partial_t \left(\sum_i X_i S_{ik} \right) = \left(V_k, \mathrm{RHS} \right)_v .$$

Discretization yields the **conservative Euler** scheme

$$\begin{aligned}
S_{kl}^{n+1} &= S_{kl}^n + \Delta t \left(X_k^n V_l^n, \mathrm{RHS}^n \right)_{xv} , \\
X_i^{n+1} &= \sum_k (S^{n+1})_{ik}^{-1} \left[\sum_j X_j^n S_{jk}^n + \Delta t \left(V_k^n, \mathrm{RHS}^n \right)_v \right], \\
W_p^{n+1} &= W_p^n + \Delta t \sum_{qi} ((S^n)^T S^n)_{pq}^{-1} S_{iq}^n \left[\frac{1}{f_{0v}} (X_i^n, \mathrm{RHS}^n)_x - \sum_l \left(X_i^n V_l^n, \mathrm{RHS}^n \right)_{xv} V_l^n \right].
\end{aligned}$$

Method is **fully explicit** and **mass and momentum conservative up to machine precision**.

Conservation laws

The **conservative Euler scheme** also satisfies the **discretized versions of the local conservation laws**.

Mass:

$$\frac{\rho^{n+1}-\rho^n}{\Delta t} = \frac{1}{U_1}\frac{K_1^{n+1}-K_1^n}{\Delta t} = \int_{\Omega_v} \mathrm{RHS}^n \, dv = -\nabla_x \cdot j^n.$$

Momentum:

$$\frac{j^{n+1}-j^n}{\Delta t} = \|v\|\frac{K_2^{n+1}-K_2^n}{\Delta t} = \int_{\Omega_v} v\mathrm{RHS}^n \, dv = -\nabla_x \cdot \sigma^n - E^n\rho^n.$$

Failure of energy conservation

We choose U_3 such that $v^2 - 1 = \|v^2 - 1\| U_3$, i.e. $U_3 \propto v^2 - 1$.

We have

$$\begin{aligned}\frac{e^{n+1} - e^n}{\Delta t} &= \|v^2 - 1\| \frac{K_3^{n+1} - K_3^n}{2\Delta t} + \|1\| \frac{K_1^{n+1} - K_1^n}{2\Delta t} + \frac{(E^{n+1})^2 - (E^n)^2}{2\Delta t} \\ &= \frac{1}{2} \int_{\Omega_v} v^2 \mathrm{RHS}^n \, dv + E^n \frac{E^{n+1} - E^n}{\Delta t} + \frac{(E^{n+1} - E^n)^2}{2\Delta t} \\ &= \nabla_x \cdot Q^n + E^n \cdot \left(\frac{E^{n+1} - E^n}{\Delta t} - j^n \right) + \frac{(E^{n+1} - E^n)^2}{2\Delta t}.\end{aligned}$$

Integrating in x yields

$$H^{n+1} - H^n = \Delta t \int_{\Omega_x} E^n \cdot \left(\frac{E^{n+1} - E^n}{\Delta t} - j^n \right) dx + \frac{1}{2} \int_{\Omega_x} (E^{n+1} - E^n)^2 \, \mathrm{d}x = \mathcal{O}(\Delta t^2).$$

Energy conservation

Can be remedied by solving

$$\partial_t f + v\nabla_x f - E^{n+1/2}\nabla_v f = 0, \qquad E^{n+1/2} = (E^{n+1} + E^n)/2.$$

Resulting scheme is energy conservative

$$\begin{aligned}\frac{e^{n+1} - e^n}{\Delta t} &= \nabla_x \cdot Q^n - E^{n+1/2} \cdot j^n + \frac{(E^{n+1} - E^n)(E^{n+1} + E^n)}{2\Delta t} \\ &= \nabla_x \cdot Q^n + E^{n+1/2} \cdot \left(\frac{E^{n+1} - E^n}{\tau} - j^n \right)\end{aligned}$$

but **implicit**.

Conservative space discretization

Obtaining a **conservative space discretization is straightforward**.

- Assumption on the method is that discrete integration by parts is exact.

Examples

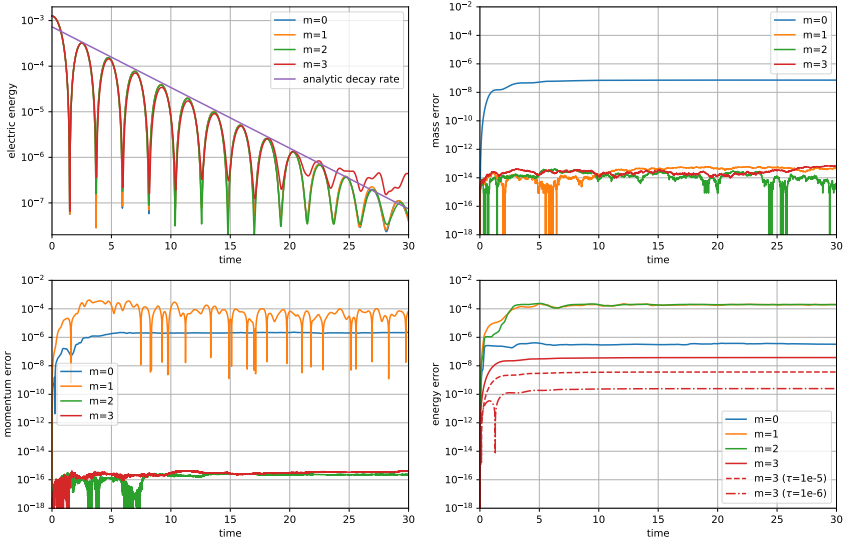
- FFT based methods
- Standard second-order centered finite differences
- discontinuous Galerkin schemes with centered flux

Discrete integration by parts for centered differences and periodic boundary conditions

$$\sum_{i=0}^{n-1}(g_{i+1} - g_{i-1}) = \sum_{i=1}^{n} g_i - \sum_{i=-1}^{n-2} g_i = g_n - g_0 + g_{n-1} - g_{-1} = 0.$$

Numerical results

Conservative DLR and (fully explicit) conservative Euler scheme.



Dynamical low-rank in uncertainty quantification

Low-rank and uncertainty quantification

Nonlinear hyperbolic conservation law with uncertainty

$$\partial_t u(t,x,\xi) + \nabla \cdot f(u(t,x,\xi)) = 0.$$

Dynamical low-rank approximation

$$u(t,x,\xi) = \sum_{ij} X_i(t,x) S_{ij}(t) V_j(t,\xi)$$

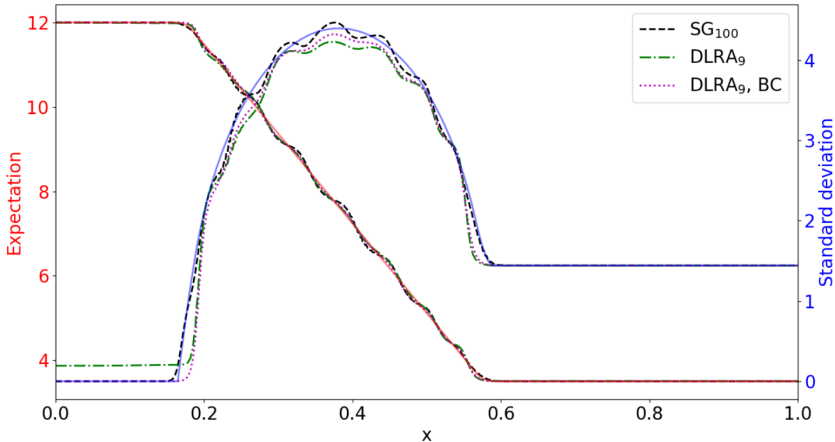
DLR approximation separates deterministic from stochastic dynamics.

- Captures **time dependent phenomena not well resolved by polynomial chaos**.

K equations maintain hyperbolicity (compare with moments in Stochastic Galerkin).

Shock with uncertainty

Initial shock with uncertainty in shock position and right state.



Boundary conditions

Dirichlet **boundary conditions**

$$u(t, x_L, \xi) = u_L(\xi), \qquad u(t, x_R, \xi) = u_R(\xi).$$

The low-rank basis is **not able to represent the boundary condition** as

$$u_L(\xi) \neq \sum_j \mathbb{E}[u(t, x_L, \cdot) V_j(t, \cdot)] V_j(t, \xi).$$

We seek an approximation of the form

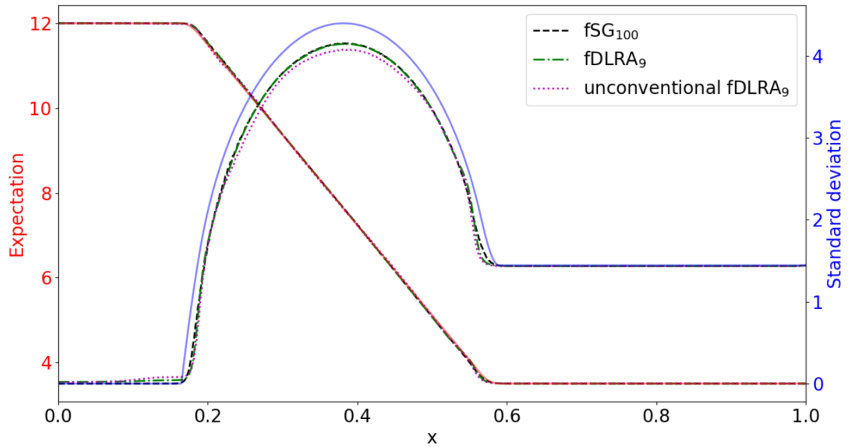
$$u(t, x, \xi) = \sum_i \hat{u}_i(t, x) U_i(\xi) + \sum_{ij} X_i(t, x) S_{ij}(t) V_j(t, \xi).$$

Once again, **exerting more control over the approximation space is required**.

J. Kusch, G. Ceruti, L.E., M. Frank, arXiv:2105.04358.

Shock with uncertainty

Initial shock with uncertainty in shock position and right state.



Literature

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[L.E., I. Joseph. J. Comput. Phys. 443, 2021]

- The conservative dynamical low-rank method described in this talk.

[J. Kusch, G. Ceruti, L.E., M. Frank, arXiv:2105.04358]

- Related ideas for enforcing boundary conditions in uncertainty quantification.

[L.E. J. Comput. Phys. 376, 2019]

- Role of conservative methods for integrating the Vlasov equation.
- Accurate solution despite large phase space error.

[N. Crouseilles, L.E., E. Faou. J. Comput. Phys. 283, 2015.]

- Hamiltonian splitting for the Vlasov–Maxwell equations.