Structure preserving low-rank algorithms for plasma simulations
Part 4: Conservative and asymptotic preserving low-rank methods

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Structure-Preserving Scientific Computing and Machine Learning Summer School and Hackathon, UW Seattle, 2025

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

Conservative dynamical low-rank approximation

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

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

$$\partial_t \rho = \frac{1}{V_1} \partial_t K_1 = \frac{1}{V_1} \langle V_1, \text{RHS} \rangle_v = \int_{\Omega_v} \text{RHS}\, dv = -\nabla \cdot j.$$

Argument from the continuous system carries over.

Problems

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**.

Idea: Keep some basis functions fixed (to ensure conservation) and choose the remaining by a Galerkin condition.

- Orthogonality between all these basis functions still needs to be satisfied.

Solutions

Modify the equations of motions to keep 1, v, v^2 in the approximation space.
[L.E., I. Joseph. J Comput. Phys. 443, 2021]

- Conservative on the continuous level. Requires an integrator that does not destroy this property.
- Difficult to do with projector splitting integrator.

Micro-macro decomposition
[J. Coughlin, J. Hu, U. Shumlak. J. Comput. Phys. 509, 2024]

- Solve the equations for the moments explicitly and remainder with low-rank.
- Still needs to enforce condition on low-rank solution $\Rightarrow$ Hermite spectral discretization.

I will show you an easy way to add conservation based on the **basis update & Galerkin** robust integrator.
[L.E., J. Kusch, S. Schotthöfer. arXiv:2311.06399]

- The idea of basis augmentation can be useful for a range of other problems.

Basis update & Galerkin (BUG) integrator

BUG integrator

Basis update & Galerkin (BUG) integrator (also called the unconventional integrator)

1.1 **K step** with $K_j(0) = \sum_i X_i^n S_{ij}^n$ to obtain $X^{n+1} = \text{orth}(K(\Delta t))$.

1.2 **L step** with $L_i(0) = \sum_j V_j^n S_{ij}^n$ to obtain $V^{n+1} = \text{orth}(L(\Delta t))$.

2 Compute $M_{ij} = \langle X_i^{n+1}, X_j^n \rangle_x$ and $N_{ij} = \langle V_i^{n+1}, V_j^n \rangle_v$ and set

$$S(0) = MSN^T.$$

Note that

$$\sum_{ij} X_i^{n+1} S_{ij}(0) V_j^{n+1} = P_{X^{n+1}} P_{V^{n+1}} \sum_{ij} X_i^n S_{ij}^n V_j^n.$$

3 **S step** to get $S^{n+1} = S(\Delta t)$.

G. Ceruti, C. Lubich. BIT Numer. Math. 62, 2022.

BUG integrator

Note that

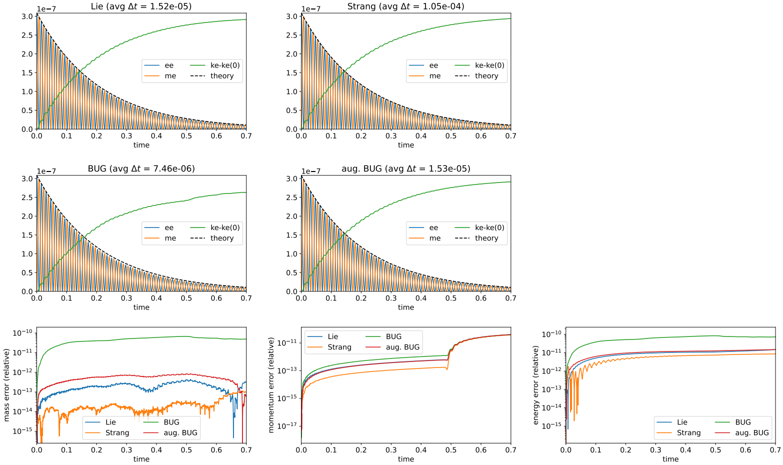
- S step is forward in time.
- S step is a Galerkin projection on the basis X^{n+1} and V^{n+1}.

We only use the basis information from the K and L step (S is not changed).

- In the QR decomposition, e.g. $K(\Delta t) = X^{n+1}R$, we throw away the R.

Problems with the BUG integrator

The **initial value can not be exactly represented**, i.e. $f^n \neq P_{X^{n+1}} P_{V^{n+1}} f^n$.



Results in issues with stability, step size, conservation, etc.

Augmented BUG integrator

To fix this we consider the **augmented BUG integrator**

1.1 **K step** to get $K(\Delta t)$.

1.2 **L step** to get $L(\Delta t)$.

2 Construct augmented basis $\overline{X} = \mathrm{orth}([X^n, K(\Delta t)])$ and $\overline{V} = \mathrm{orth}([V^n, L(\Delta t)])$.

3 **S step** is a Galerkin projection on $\overline{X}$ and $\overline{V}$.

4 Truncate to rank r (or a given tolerance) by SVD of S.

We require truncation because otherwise the rank doubles in each time step.

We require low-rank factors of size $2r \Rightarrow$ added computational cost.

- Gain flexibility with respect to augmenting the basis (conservation, AP, ...).
- Natural rank adaptivity.

This is a first order scheme, but has recently been extended to higher order.

G. Ceruti. J. Kusch. C. Lubich. BIT Numer. Math. 62, 2022.
G. Ceruti, L.E., J. Kusch, C. Lubich. BIT Numer. Math. 64:30, 2024.

Implementation details

To compute X^{n+1} we do a QR decomposition

$$\overline{X}, \_ = qr([X^n, K(\Delta t)]).$$

We know that X^n is already orthogonal, so we set

$$\widehat{X} = [X^n, \overline{X}(\cdot, r:2r)].$$

Same for V^{n+1}.
Then the initial condition for the S step is

$$S(0) = \begin{bmatrix} S^n & 0 \\ 0 & 0 \end{bmatrix}.$$

We have an exact representation of the initial value in the new basis

$$X^n S^n V^n = \widehat{X} S(0) \widehat{V}$$

Rank truncation

We need to truncate after each time step.

Compute SVD of S

$$S(\Delta t) = U\Sigma W^T$$

Computational effort is low as $S \in \mathbb{R}^{2r\times 2r}$.

Set

$$X^{n+1} = (\widehat{X}U)(\cdot, 1:r), \qquad V^{n+1} = (\widehat{V}W)(\cdot, 1:r), \qquad S^{n+1} = \Sigma(1:r, 1:r)$$

which can be done in $\mathcal{O}(n^d r^2)$.

Can also be done adaptively (only drop singular values that are small enough).

Mass conservative BUG integrator

Problem

We consider

$$\partial_t f = \text{RHS}(f).$$

For a velocity-dependent function $U(v)$ assume that we have a **moment equation**

$$\phi(t,x) = \langle f, U \rangle_v, \qquad \partial_t \phi(t,x) = \langle \text{RHS}(f), U \rangle_v$$

such that

$$\partial_t \langle \phi(t,x) \rangle_x = \langle \text{RHS}(f), U \rangle_{xv} = 0.$$

For $U(v) = 1$ we get **mass conservation**.

Mass conservation

We want to preserve the moment equation moment

$$\partial_t \phi = \langle \mathrm{RHS}\,(f)\,, U \rangle_v \,.$$

S step can be written as (Galerkin projection)

$$\partial_t f_r(t,x,v) = P_{\widehat{V}} P_{\widehat{X}} \mathrm{RHS}(f_r)$$

which for the moment gives

$$\begin{aligned}
\partial_t \phi_r(t,x) &= \langle P_{\widehat{V}} P_{\widehat{X}} \mathrm{RHS}(f_r), U \rangle_v \\
&= \langle P_{\widehat{X}} \mathrm{RHS}(f_r), P_{\widehat{V}} U \rangle_v \\
&= \langle P_{\widehat{X}} \mathrm{RHS}(f_r), U \rangle_v .
\end{aligned}$$

since we have constructed our basis such that $U \in \operatorname{span} \widehat{V}$.

Mass conservation

We have

$$\partial_t \phi_r = P_{\widehat{X}} \langle \mathrm{RHS}(f_r), U \rangle_v .$$

For

$$\langle \mathrm{RHS}(f_r), U \rangle_v \in \mathrm{span}(\widehat{X}).$$

we have

$$\partial_t \phi_r = \langle \mathrm{RHS}(f_r), U \rangle_v$$

which is **exactly the mass continuity equation**.

Integrating in x would give **mass conservation**.

But, we can not augment $\langle \mathrm{RHS}(f_r), U \rangle_v(t, x)$ for each t.

Special case: Explicit Euler

K step:

$$K^\star = K^n + \Delta t P_{\widehat{V}} \mathrm{RHS}(K^n \widehat{V}^\mathsf{T}).$$

By augmentation we have $\mathrm{span}(\widehat{X}) = \mathrm{span}([X^n, P_{\widehat{V}} \mathrm{RHS}(K^n \widehat{V}^\mathsf{T})])$.

S step:

$$\begin{aligned} \widehat{S}^{n+1} &= \widehat{S}^n + \Delta t P_{\widehat{X}} P_{\widehat{V}} \mathrm{RHS}(\widehat{X}\widehat{S}^n \widehat{V}^T) \\ &= \widehat{S}^n + \Delta t P_{\widehat{V}} \mathrm{RHS}(\widehat{X}\widehat{S}^n \widehat{V}^T) \end{aligned}$$

Special case: Explicit Euler

We have

$$
\begin{aligned}
\phi^{n+1} &= \phi^n + \Delta t \langle P_{\widehat{V}} \mathrm{RHS}(\widehat{X}\widehat{S}^n\widehat{V}^T), U\rangle_v \\
&= \phi^n + \Delta t \langle \mathrm{RHS}(\widehat{X}\widehat{S}^n\widehat{V}^T), P_{\widehat{V}} U\rangle_v \\
&= \phi^n + \Delta t \langle \mathrm{RHS}(\widehat{X}\widehat{S}^n\widehat{V}^T), U\rangle_v \\
&= \phi^n + \partial_x j^n.
\end{aligned}
$$

which is the **explicit Euler approximation of the mass continuity equation**.

Integrating in x

$$
\text{mass} = \langle \phi^{n+1} \rangle_x = \langle \phi^n \rangle_x + \cancel{\langle \partial_x j^n \rangle_x}.
$$

Mass conservation!

General Runge–Kutta methods

For $i = 1, \dots, s$

$$\widehat{S}^{(i)} = \left\langle \mathrm{RHS}^{(i)}, \widehat{X}\widehat{V} \right\rangle_{xv},$$

$$\mathrm{RHS}^{(i)} = \mathrm{RHS}\left(\widehat{X}\widehat{S}^n\widehat{V}^T + \Delta t \sum_{j=1}^{i-1} a_{ij}\widehat{X}\widehat{S}^{(j)}\widehat{V}^T \right).$$

$$\begin{array}{c|ccccc}
0 & & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & & \ddots & & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}$$

Without low-rank (RK methods conserve all linear invariants)

$$\phi^{n+1}(x) = \phi^n(x) + \Delta t \sum_{i=1}^{s} b_i \langle \mathrm{RHS}^{(i)}, U \rangle_v .$$

For the **low-rank scheme** we get

$$\phi_r^{n+1}(x) = \phi_r^n(x) + \Delta t P_{\widehat{X}} \sum_{i=1}^{s} b_i \langle \mathrm{RHS}^{(i)}, U \rangle_v .$$

General Runge–Kutta methods

We can satisfy

$$\sum_{i=1}^{s} b_i \langle \mathrm{RHS}^{(i)}, U \rangle_v \in \mathrm{span}(\widehat{X})$$

easily by augmenting a single basis

$$\overline{X} = \mathrm{ortho}\left(\left[\widehat{X}, \sum_{i=1}^{s} b_i \langle \mathrm{RHS}^{(i)}, U \rangle_v\right]\right) = [\widehat{X}, X^\star].$$

RK approximation of the mass continuity equation and **mass conservative**.

Details

The K and L step has no bearing on conservation.

1. For $i = 1, \cdots, s$ compute

$$\widehat{S}^{(i)} = \left\langle \mathrm{RHS}_K^{(i)}, \widehat{X} \right\rangle_x \quad \text{with} \qquad \mathrm{RHS}_K^{(i)} = \langle \mathrm{RHS}^{(i)}, \widehat{V} \rangle_v.$$

   Note that RHS_K is the rhs of the K step.

2. Augment (see last slide)
3. Compute

$$\overline{S}^{(i)} = [\widehat{S}^{(i),\top}, S^{\star,\top}]^\top \in \mathbb{R}^{(2r+1)\times 2r} \quad \text{with} \quad S^\star = \langle \mathrm{RHS}_K^{(i)}, X^\star \rangle_x$$

   and

$$\overline{S}^{n+1} = \overline{S}^n + \Delta t \sum_{i=1}^{s} b_i \overline{S}^{(i)} .$$

Conservative truncation

We have to truncate.

- SVD minimizes the L^2 error $\Rightarrow$ destroys conservation.

Idea

- First project onto U (guarantees conservation)
- Truncate the remainder by performing an SVD.
- More details later

Momentum and energy conservation

In principle, works in the same way.

But, the growth of $U(v) = v$ becomes an issue at the (artificial) boundary.

We reformulate the method in a weighted space $L^2(\Omega_v, f_{0v})$ with

$$f(t,x,v) = f_{0v}(v) \sum_{ij} X_i(t,x) S_{ij}(t,x) V_j(t,v),$$

where $V_j \in L^2(\Omega_v, f_{0v})$.

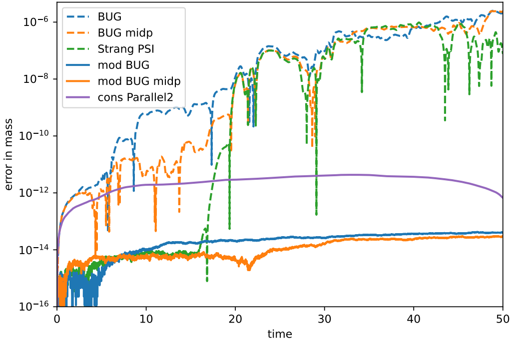
Caution: V needs to the orthogonalized with respect to the weighted norm.

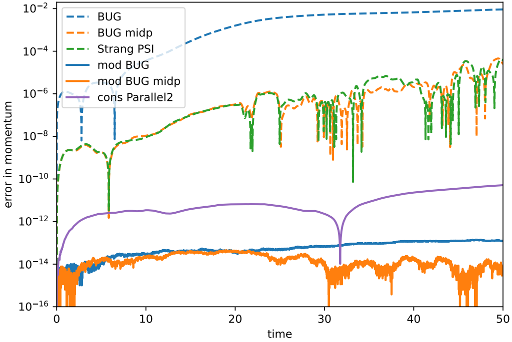
Same for $U(v) = v^2$ and **energy conservation**

- Exact for DLR, but error of the time integrator needs to be taken into account.

Numerical example

Conservative (full lines) and standard (dashed lines) integrators for a bump-on-tail instability.





Conservative truncation algorithm: Part 1

1. Compute $\widetilde{K} = \widetilde{X}^{n+1}\widetilde{S}^{n+1}$ and distribute it into two parts
$$\widetilde{K} = [\widetilde{K}^{cons}\ \widetilde{K}^{rem}],$$
where $\widetilde{K}^{cons}$ consists of the first m columns of $\widetilde{K}$ and $\widetilde{K}^{rem}$ of the remaining columns.
2. Perform a QR decomposition of $\widetilde{K}^{cons}$, getting
$$\widetilde{K}^{cons} = X^{cons}S^{cons}.$$
3. Perform a QR decomposition of $\widetilde{K}^{rem}$, getting
$$\widetilde{K}^{rem} = \widetilde{X}^{rem}\widetilde{S}^{rem}.$$
4. Compute the singular value decomposition (SVD) of $\widetilde{S}^{rem}$, keep the largest $r - m$ singular values
$$\widetilde{S}^{rem} \approx \widehat{U}\widehat{S}\widehat{W}^T$$
and compute
$$X^{rem} = \widetilde{X}^{rem}\widehat{U}, \quad S^{rem} = \widehat{S}, \quad W^{n+1} = \widetilde{W}^{n+1}\widehat{W}.$$

Conservative truncation algorithm: Part 2

4 Set

$$V^{n+1} = \left[U \; W^{n+1} \right].$$

5 Set $\widehat{X} = [X^{cons} \; X^{rem}]$ and perform a QR decomposition

$$\widehat{X} = X^{n+1} R.$$

6 Set

$$S^{n+1} = R \begin{bmatrix} S^{cons} & 0 \\ 0 & S^{rem} \end{bmatrix}.$$

7 The computed approximation at time t^{n+1} is then given by

$$f^{n+1} = f_{0v} \sum_{ij} X_i^{n+1} S_{ij}^{n+1} V_j^{n+1}.$$

Outlook

One strength of DLR is that it can be easily combined with a variety of time and space discretization strategies.

- Much work on implicit, IMEX, semi-Lagrangian, spectral, etc. methods.

Collisional problems are even more suited for low-rank methods (collisions regularize the solution).

- Much work on asymptotic preserving methods and efficient schemes.

One can also further decompose the problem, i.e. **tensor decompositions**.

- Much work on different tensor formats (tree tensor networks, hierarchical Tucker, tensor trains, ...).

Interpolatory low-rank methods require only point-wise evaluations of the right-hand side.

- Allows for treatment of more general nonlinearities.

Literature

Literature

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

- The conservative dynamical low-rank equations of motions.

[L.E., A. Ostermann, C. Scalone. J. Comput. Phys. 484, 2023]
[W. Guo, J.-M. Qiu. J. Sci. Comput. 61, 2024]

- The conservative truncation.

[J. Coughlin, J. Hu, U. Shumlak. J. Comput. Phys. 509, 2024]

- Solve the equations for the moments explicitly and remainder with low-rank.

[L.E., J. Kusch, S. Schotthöfer. arXiv:2311.06399]

- The conservative method described here.

[L.E., K. Kormann, J. Kusch, R.G. McClarren, J.-M. Qiu. arXiv:2412.05912]

- Review article with comparison to other methods and survey of the literature.