Entropy-dissipation/stability and local linear stability

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Robustness and Entropy-Dissipation/Stability

- Many (all?) practical/interesting applications are multi-scale in nature and thus under-resolved due to insufficient compute hardware
- Per definition, high-order methods are designed for well resolved problems
- High-order schemes such as the DG method are prone to stability issues when grid resolution is insufficient
- Additional robustness enhancements are necessary, to make high-order DG methods fit for real life applications

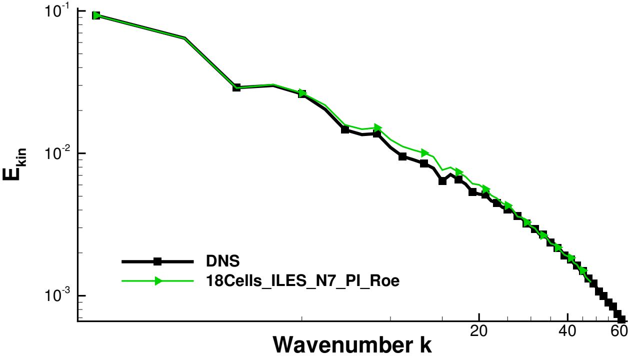
  $\Rightarrow$ Preserving the second law of thermodynamics (entropy) is linked to non-linear stability

  $\Rightarrow$ Entropy evolution is dissipative

  $\Rightarrow$ Entropy-dissipation/stability

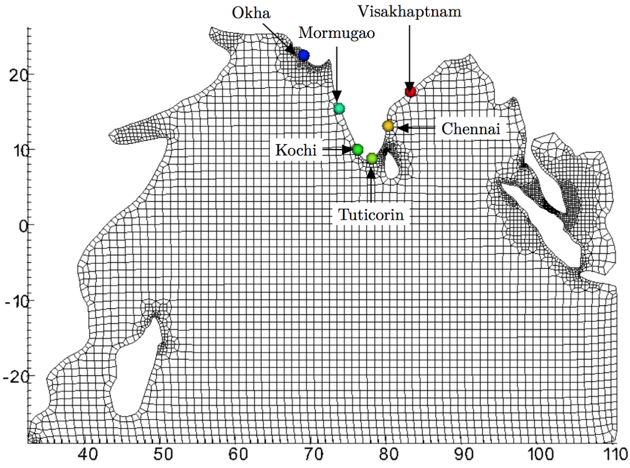
Provably Entropy-Dissipative Discontinuous Galerkin Methods

- Decaying homogeneous isotropic turbulence (Flad and Gassner, JCP, 2017)
- Non-linear diffusion terms as in the compressible Navier-Stokes (Gassner et al., JSC, 2018)
- Mach number $Ma = 0.1$ and Reynolds number based on Taylor micro scale $Re_\lambda = 97 - 162$
- 18^3 grid cells with $N = 7$
- Plot of the spectrum of kinetic energy



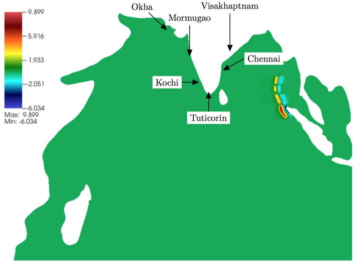
Provably Entropy-Dissipative Discontinuous Galerkin Methods

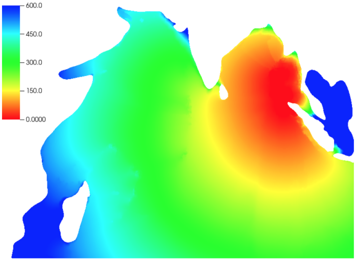
- Tsunami simulation (Indian Ocean, December 2004)
- Shallow water equations including positivity preservation and shock capturing (Wintermeyer et al., PHD, 2019)
- Simulation with $N = 7$ and $60,000$ grid cells



Provably Entropy-Dissipative Discontinuous Galerkin Methods

- Tsunami simulation (Indian Ocean, December 2004)
- Visualisation of the arrival times in minutes (right plot)



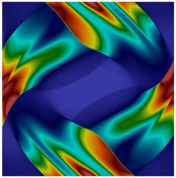


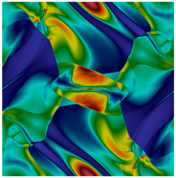
- Comparison to real world data of arrival times in minutes

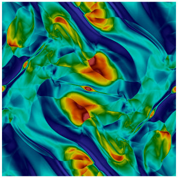
Place	measured	simulation	error in %
Kochi	280	270	3,6
Mormugao	355	375	5,6
Chennai	150	148	1,3
Tuticorin	200	212	6,0
Okha	485	507	4,5
Visakhaptnam	160	158	1,3

Provably Entropy-Dissipative Discontinuous Galerkin Methods

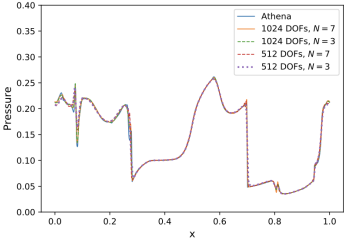
- Orzag Tang Vortex
- GLM-MHD with shock capturing (Rueda et al., in preparation)
- 256^2 grid cells with $N = 3$
- Plot of the pressure at times $t = 0.25;\ 0.50;\ 0.75$





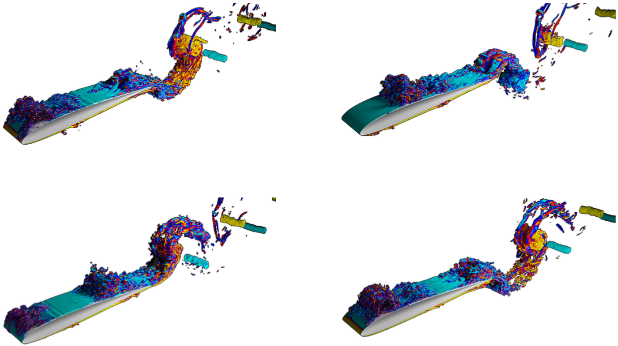


- Slice through the domain at $y = 0.3125$ and comparison with Athena



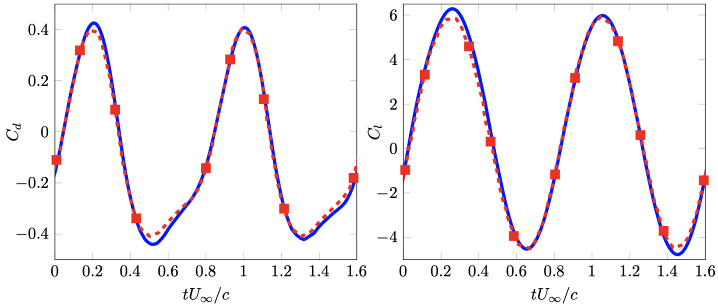
Provably Entropy-Dissipative Discontinuous Galerkin Methods

- Flow past a plunging SD7003 airfoil
- Moving meshes (Krais et al., JCP, 2020)
- Mach number $Ma = 0.1$ and $Re_c = 40,000$
- $58,490$ grid cells with $N = 7$ (about 150 mill. DOF)
- Iso-contour plot of vorticity magnitude at different times throughout the plunging movement



Provably Entropy-Dissipative Discontinuous Galerkin Methods

- Flow past a plunging SD7003 airfoil
- Moving meshes (Krais et al., JCP, 2020)
- Mach number $Ma = 0.1$ and $Re_c = 40,000$
- $58,490$ grid cells with $N = 7$ (about 150 mill. DOF)
- Plot of temporal evolution of drag and lift coefficient (Comparison with Visbal, AIAA, 2009 - red square-line)



Robustness of DG is drastically enhanced with great results

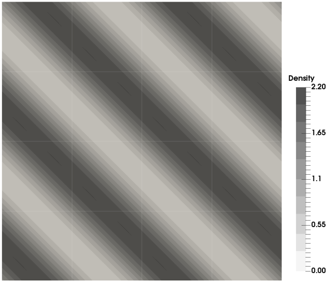
- Many researchers in the high-order community working on entropy stability, e.g.
  - My research group :-)
  - Magnus Svärd, Florian Hindenlang, Hendrik Ranocha
  - David C. Del Rey Fernandez, Matteo Parsani
  - David Flad, Scott Murman
  - David Kopriva, Claus-Dieter Munz
  - Rodrigo Moura, Gianmarco Mengaldo, Joaquim Peiro, Spencer J. Sherwin
  - David W. Zingg, Jason Hicken, Jan Nordström, Tim Warburton
  - Travis Fisher, Mark Carpenter
  - ...

A simple test case

- Consider the compressible Euler equations in 2D
- Density wave initial conditions with periodic boundary conditions

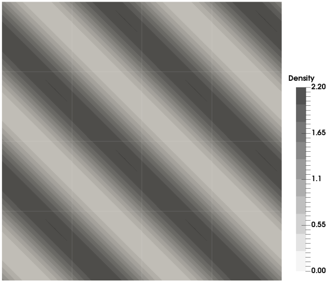
$$\begin{aligned} \rho &= 1 + 0.98\,\sin(2\,\pi\,(x+y)) \\ v_1 &= 0.1 \\ v_2 &= 0.2 \\ p &= 20 \end{aligned} \tag{1}$$

- Well resolved with 4^2 grid cells and $N = 5$
- Exact solution is the traveling density wave



A simple test case

- Standard DG scheme with central flux at $t = 5$ (no problem)



A simple test case

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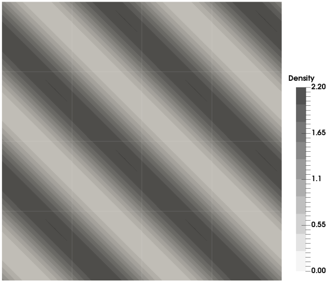
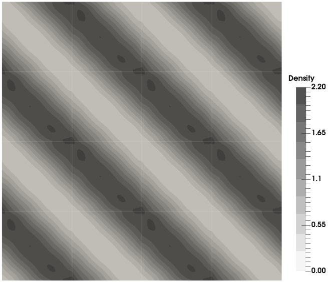


- Entropy-dissipative/stable DG scheme with LxF at $t = 0.65$ (crashes!?)



Content of the Talk

- Entropy-dissipation/stability
- Local linear stability
- Burgers equation
- Compressible Euler equations

Acknowledgments & References

- Magnus Svärd
- Florian Hindenlang

  G.J. Gassner, M. Svärd and F. Hindenlang. Stability issues of entropy-stable and/or split-form high-order schemes. arXiv:2007.09026v1.

- Hendrik Ranocha

  H. Ranocha and G.J. Gassner. Preventing pressure oscillations does not fix local linear stability issues of entropy-based split-form high-order schemes. arXiv:2009.13139v1.

Entropy

- We consider the 1D hyperbolic PDE

$$u_t + f(u)_x = 0 \tag{2}$$

- We further consider an entropy function $U(u)$ with
  - $U(u)$ is convex
  - entropy variables $w := U_u$
  - contraction property $w^T f_u = F_u$
  - entropy flux $F(u)$
  - entropy potential $\Psi := w^T f - F$
- Entropy evolution is dissipative

$$U(u)_t + F(u)_x \leq 0, \tag{3}$$

which is an incarnation of the second law of thermodynamics

Discrete Entropy

- We consider the 1D standard FV discretization

$$(u_i(t))_t + \frac{f_{i+1/2} - f_{i-1/2}}{h} = 0 \tag{4}$$

- Discrete entropy analysis of Tadmor
  - multiply FV scheme by $w_i^T = U_u(u_i)^T$
  - discrete contraction property $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) = 0$
  - discrete entropy flux $F_{i+1/2} = \frac{1}{2}(w_{i+1}^T + w_i^T) f_{i+1/2} - \frac{1}{2}(\Psi_{i+1} + \Psi_i)$
- Semi-discrete entropy evolution

$$(U_i)_t + \frac{F_{i+1/2} - F_{i-1/2}}{h} = 0 \tag{5}$$

- Semi-discrete entropy evolution is dissipative

$$(U_i)_t + \frac{F_{i+1/2} - F_{i-1/2}}{h} \leq 0, \tag{6}$$

if the numerical flux $f_{i+1/2}$ satisfies

$$(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) \leq 0 \tag{7}$$

Entropy-Conservation/Stability/Dissipation

- A numerical scheme is

  (i) *Entropy-conservative:* if $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) = 0$ is satisfied for **one** entropy at all i

  (ii) *Entropy-stable:* if $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) \leq 0$ is satisfied for **all** admissible entropies at all i

  (iii) *Entropy-dissipative:* if $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) \leq 0$ is satisfied, but the scheme is neither entropy-stable or entropy-conservative

Entropy-Conservation/Stability/Dissipation

- A numerical scheme is

  (i) *Entropy-conservative:* if $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) = 0$ is satisfied for **one** entropy at all i

  (ii) *Entropy-stable:* if $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) \leq 0$ is satisfied for **all** admissible entropies at all i

  (iii) *Entropy-dissipative:* if $(w_{i+1}^T - w_i^T)\, f_{i+1/2} - (\Psi_{i+1} - \Psi_i) \leq 0$ is satisfied, but the scheme is neither entropy-stable or entropy-conservative

- **Most so-called entropy-stable high-order schemes, e.g. DG, are indeed entropy-dissipative. It is important to note, that the entropy-conservative numerical flux with**

$$(\boldsymbol{w}_{\boldsymbol{i}+1}^{\boldsymbol{T}} - \boldsymbol{w}_{\boldsymbol{i}}^{\boldsymbol{T}})\, \boldsymbol{f}_{\boldsymbol{i}+1/2} - (\Psi_{\boldsymbol{i}+1} - \Psi_{\boldsymbol{i}}) = 0 \tag{8}$$

  is a key-building block in the construction of high-order accuracy.

Linear Stability

- In linear stability analysis, we consider linear PDEs

$$u_t = P\,u \tag{9}$$

with initial data u_0 and periodic BC

- We are looking for L_2-estimates of the form

$$\|u(\cdot, T)\|_2 = K\, \exp(\alpha\, T)\, \|u_0\|_2 \tag{10}$$

- A well known example is the constant coefficient linear advection

$$u_t + a\, u_x = 0, \tag{11}$$

with the L_2-estimate

$$\|u(\cdot, T)\|_2 = \|u_0\|_2, \tag{12}$$

i.e. growth rate $\alpha = 0$ and $K = 1$

- **The zero growth rate corresponds to a spectrum of the PDE operator that is purely imaginary**

Discrete Linear Stability

- We consider the FV discretization

$$(u_i(t))_t + \frac{f_{i+1/2} - f_{i-1/2}}{h} = 0 \tag{13}$$

- We are looking for discrete L_2-estimates of the form

$$\|u^h(\cdot, T)\|_{2,h} = K_h \exp(\alpha_h T) \|u_0^h\|_{2,h} \tag{14}$$

  with the discrete growth rate α_h

- The scheme is energy stable (linearly stable), if the discrete growth rate is less or equal than the continuous growth

$$\alpha_h \leq \alpha \tag{15}$$

- For linear advection, the central numerical flux

$$f_{i+1/2}^{CN} = \frac{f(u_{i+1}) + f(u_i)}{2} = \frac{au_{i+1} + au_i}{2} \tag{16}$$

  gives $K_h = 1$ and

$$\alpha_h = 0 = \alpha \tag{17}$$

- **The operator of the central FV scheme has a purely imaginary spectrum**

Linear Stability for Non-linear PDEs

- **We are interested in non-linear PDEs**
- 'Non-linear stability' analysis
  - Non-linear PDE $\rightarrow$ discretization $\rightarrow$ entropy analysis
- How to analyze the linear stability in case of non-linear PDEs?
- The order matters!

  (i) Non-linear PDE $\rightarrow$ linearization $\rightarrow$ discretization $\rightarrow$ L_2-analysis

  (ii) Non-linear PDE $\rightarrow$ discretization $\rightarrow$ linearization $\rightarrow$ L_2-analysis

- It is important to realize that $(\boldsymbol{i}) \neq (\boldsymbol{ii})$!

Local Linear Stability

- Discrete entropy bound gives an estimate for the global behaviour of the solution
- What about the local solution behaviour?
  - The idea is to consider a steady state solution $\widetilde{u}(x)$
  - In fluid dynamics, this is often referred to as a 'baseflow'
  - We add small fluctuations $u'(x,t)$ to this baseflow

$$u(x,t) = \widetilde{u}(x) + u'(x,t), \tag{18}$$

    where $|u'(x,t)| << |\widetilde{u}(x,t)|$

- Analysis of the evolution of the small scale fluctuations.

Local Linear Stability

- Example: Burgers' equation

$$u_t + \frac{1}{2}\,(u^2)_x = 0 \tag{19}$$

- We plug in our perturbation ansatz

$$(\widetilde{u}(x,t) + u'(x,t))_t + \frac{1}{2}\left((\widetilde{u}(x,t) + u'(x,t))(\widetilde{u}(x,t) + u'(x,t))\right)_x = 0, \tag{20}$$

- The baseflow solves the equation; neglect all but the leading order terms

$$(u')_t + (\widetilde{u}(x,t)\,u')_x = 0, \tag{21}$$

  gives a linear variable coefficient PDE

- Classic linear stability analysis

$$\|u'(\cdot,T)\|^2 \leq \exp\left(T\,\alpha_h\right)\,\|u'(\cdot,0)\|^2 \tag{22}$$

  with $\alpha_h = \frac{1}{2}\sup_{x,t}|\,(\widetilde{u}(x,t))_x\,|$

- Depending on $\widetilde{u}(x,t)$, there might be growth/decay or stagnation

Entropy-conservation and local linear stability I

- Example: Burgers' equation

$$u_t + \frac{1}{2}(u^2)_x = 0 \tag{23}$$

- Entropy $U(u) = u^2/2$ with entropy variable $w = U_u = u$
- We consider the FV discretization

$$(u_i(t))_t + \frac{f_{i+1/2} - f_{i-1/2}}{h} = 0 \tag{24}$$

- Tadmor's condition for entropy-conservation gives

$$f^{EC}_{i+1/2} = \frac{1}{6}(u_i^2 + u_i\, u_{i+1} + u_{i+1}^2) \tag{25}$$

- We get entropy-conservation (non-linear stability)

$$\frac{d}{dt}(\|u\|_h^2) = 0. \tag{26}$$

Entropy-conservation and local linear stability II

- We can re-write the EC-flux to

$$f_{i+1/2}^{EC} = \frac{1}{2}\left(f(u_i) + f(u_{i+1})\right) - \frac{1}{2}\lambda_{i+1/2}^{EC}(u_{i+1} - u_i), \tag{27}$$

where we get the non-linear diffusion coefficient

$$\lambda_{i+1/2}^{EC} = \left(\frac{u_{i+1} - u_i}{6}\right) \tag{28}$$

- Note, that this diffusion coefficient can be positive, but also negative!

  - For solutions with negative gradients

$$\lambda_{i+1/2}^{EC} < 0 \tag{29}$$

$\Rightarrow$ The scheme can be anti-dissipative!

Entropy-conservation and local linear stability III

- Discrete local linear stability analysis

$$u_i = \widetilde{u}_i + u_i', \qquad (30)$$

- Perturbation analysis; neglect higher order terms gives the linearized flux

$$\widetilde{f}^{EC}_{i+1/2} = \frac{(\widetilde{u}_{i+1}\, u_{i+1}') + (\widetilde{u}_i\, u_i')}{2} - \frac{1}{2}\,\widetilde{\lambda}^{EC}_{i+1/2}\,(u_{i+1}' - u_i'), \qquad (31)$$

with the diffusion coefficient

$$\widetilde{\lambda}^{EC}_{i+1/2} = \left(\frac{\widetilde{u}_{i+1} - \widetilde{u}_i}{3}\right) \qquad (32)$$

- Recall, that the central flux $\widetilde{f}^{CN}_{i+1/2} = \frac{(\widetilde{u}_{i+1}\, u_{i+1}') + (\widetilde{u}_i\, u_i')}{2}$ is neutral stable for linear problems

- Note again, that this diffusion coefficient can be positive, but also negative!
  - For baseflows with negative gradients

$$\widetilde{\lambda}^{EC}_{i+1/2} < 0 \qquad (33)$$

$\Rightarrow$ The scheme is not (locally) linearly stable!

Numerical Investigation Ia

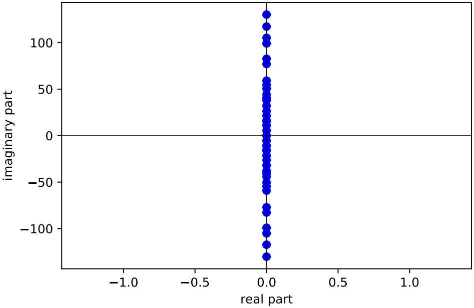
- High-order DG for non-linear Burgers' equation with forcing term
- Baseflow

$$\widetilde{u}(x) = 2 + \sin(\pi\, x - 0.7) \tag{34}$$

- Linearization of the non-linear scheme with $\epsilon = 10^{-8}$

$$A\underline{e}_j \approx \frac{\underline{rhs}(\widetilde{\underline{u}} + \underline{e}_j\,\epsilon) - \underline{rhs}(\widetilde{\underline{u}} - \underline{e}_j\,\epsilon)}{2\,\epsilon} \tag{35}$$

- Spectra of standard DG with $f^{CN}_{i+1/2}$ with $N = 3$ and 10 elements



$\Rightarrow$ no growth

Numerical Investigation Ib

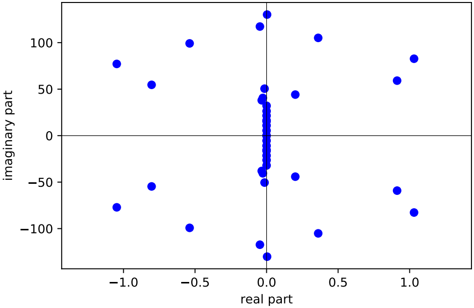
- High-order DG for non-linear Burgers' equation with forcing
- Baseflow

$$\widetilde{u}(x) = 2 + \sin(\pi\, x - 0.7) \tag{36}$$

- Linearization of the non-linear scheme with $\epsilon = 10^{-8}$

$$A\underline{e}_j \approx \frac{\underline{rhs}(\underline{\widetilde{u}} + \underline{e}_j\, \epsilon) - \underline{rhs}(\underline{\widetilde{u}} - \underline{e}_j\, \epsilon)}{2\, \epsilon} \tag{37}$$

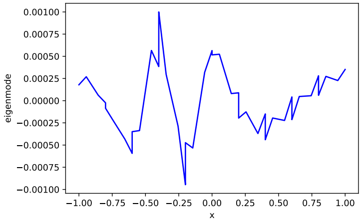
- Spectra of entropy-conserving DG with $f^{EC}_{i+1/2}$ with $N = 3$ and 10 elements



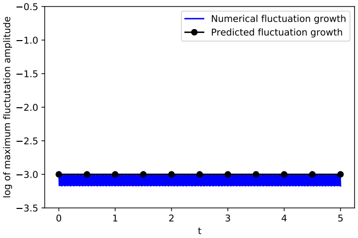
$\Rightarrow$ artificial growth of eigenmodes with positive real part

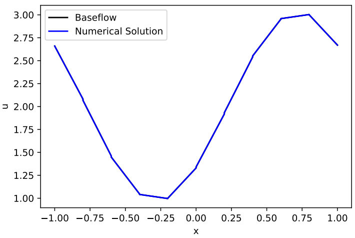
Numerical Investigation IIa

- Standard DG with $f^{CN}_{i+1/2}$ with $N = 3$ and 10 elements
- Eigenmode with the largest positive real part



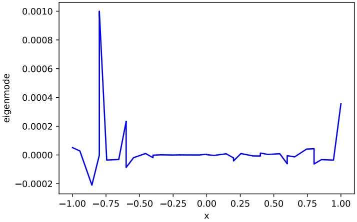
- Perform simulation and add fluctuations in form of eigenmode scaled at 10^{-3} to baseflow



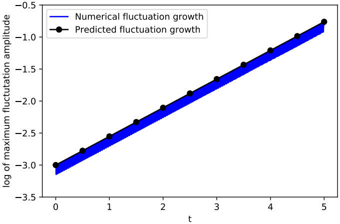


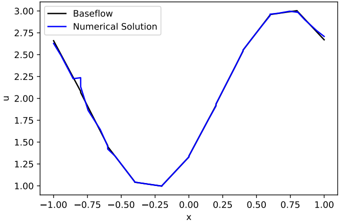
Numerical Investigation IIb

- Entropy-conserving DG with $f_{i+1/2}^{EC}$ with $N = 3$ and 10 elements
- Eigenmode with the largest positive real part (active where baseflow gradient is negative!)



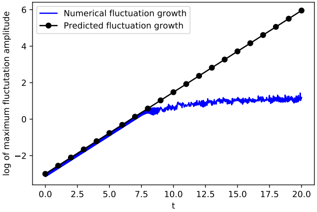
- Perform simulation and add fluctuations in form of eigenmode scaled at 10^{-3} to baseflow



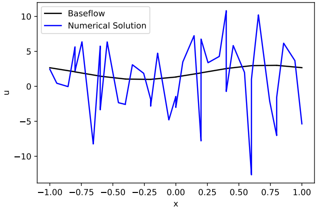


Numerical Investigation IIc

- Entropy-conserving DG with $f^{EC}_{i+1/2}$ with $N = 3$ and 10 elements
- **Long time behaviour:** Perform simulation and add fluctuations in form of eigenmode scaled as 10^{-3} to baseflow

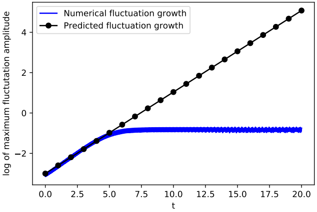


- **Recall: by construction, the scheme is non-linearly stable!**
- Scheme is non-linearly stable, but final numerical solution is crazy

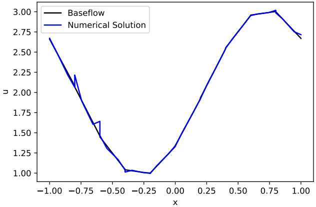


Numerical Investigation IId

- Entropy-dissipative DG with $N = 3$ and 10 elements
- **Long time behaviour:** Perform simulation and add fluctuations in form of eigenmode scaled at 10^{-3} to baseflow

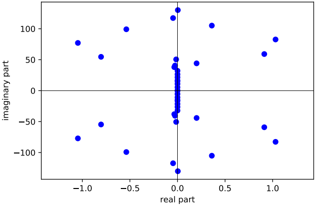


- **Recall: by construction, the scheme is non-linearly stable!**
- Wrong local behaviour; dissipation in equilibrium with artificial growth?

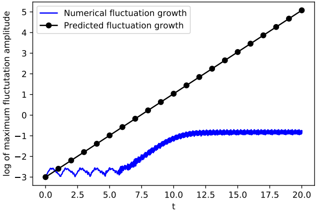


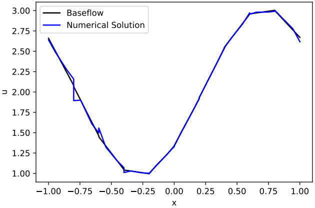
Numerical Investigation IIIa

- Influence of grid resolution ($N = 3$ with 10 elements)
- Smooth initial fluctuations $u'(x) = 0.001\,cos(\pi\,x)$



note that the imaginary values correspond to eigenmode frequency

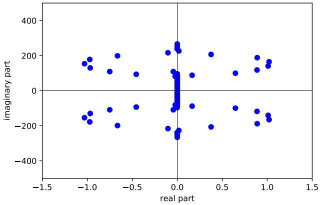




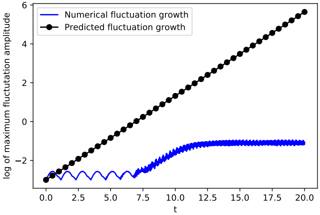
solution ok for small times, until erroneous eigenmode grows and dominate

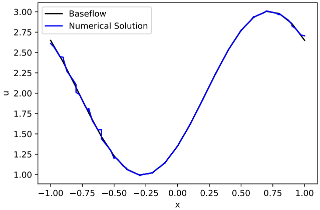
Numerical Investigation IIIb

- Influence of grid resolution ($N = 3$ with 20 elements)
- Smooth initial fluctuations $u'(x) = 0.001\, cos(\pi\, x)$



higher resolution shifts erroneous eigenmodes to higher frequencies





smooth high frequency content takes longer time to grow and dominate

Compressible Euler Equations I

- Unfortunately, all issues carry over to the compressible Euler equations
- To get a numerical flux that satisfies Tadmor's entropy condition, we need to use the logarithmic mean, e.g., in the mass flux

$$(f_\rho)^{EC}_{i+1/2} = \{\rho\}^{\ln}_{i+1/2} \, \{\!\{v\}\!\}_{i+1/2} \tag{38}$$

where

$$\{\rho\}^{\ln}_{i+1/2} := \frac{\rho_{i+1} - \rho_i}{\ln(\rho_{i+1}) - \ln(\rho_i)} \tag{39}$$

- Again, this flux can be recast into

$$(f_\rho)^{EC}_{i+1/2} = (f_\rho)^{CN}_{i+1/2} - \frac{1}{2}\,(\lambda_\rho)^{EC}_{i+1/2}\,(\rho_{i+1} - \rho_i), \tag{40}$$

with diffusion coefficient

$$(\lambda_\rho)^{EC}_{i+1/2} = (\{\!\{\rho\}\!\}_{i+1/2} - \{\rho\}^{\ln}_{i+1/2})\frac{2\,\{\!\{v\}\!\}_{i+1/2}}{\rho_{i+1} - \rho_i} + \frac{(v_{i+1} - v_i)}{2}, \tag{41}$$

which can get negative (anti-diffusion) for

$$\rho_x < 0 \tag{42}$$

Compressible Euler Equations II

- **Theorem:** The numerical flux of Ranocha

$$
\begin{aligned}
(f_\rho)^{EC}_{i+1/2} &= \{\rho\}^{ln} \{\!\{v\}\!\}, \\
(f_{\rho v})^{EC}_{i+1/2} &= \{\rho\}^{ln} \{\!\{v\}\!\}^2 + \{\!\{p\}\!\}, \\
(f_{\rho e})^{EC}_{i+1/2} &= \frac{1}{2}\{\rho\}^{ln} \{\!\{v\}\!\} \{v \cdot v\}^{zip} + \frac{1}{\gamma - 1}\{\rho\}^{ln}(\{\frac{\rho}{p}\}^{ln})^{-1} \{\!\{v\}\!\} + \{p \cdot v\}^{zip},
\end{aligned}
\tag{43}
$$

  with product mean

$$
\{a \cdot b\}^{zip}_{i+1/2} := \frac{a_{i+1}b_i + a_i b_{i+1}}{2} = 2\,\{\!\{a\}\!\}_{i+1/2}\{\!\{b\}\!\}_{i+1/2} - \{\!\{ab\}\!\}_{i+1/2}, \tag{44}
$$

  for the compressible Euler equations is EC, KEP, PEP, and has a density flux $(f_\rho)^{EC}_{i+1/2}$ that does not depend on the pressure. Moreover, it is the only numerical flux with these properties for constant v.

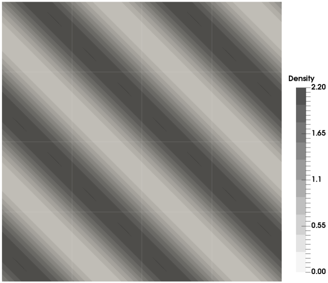
- This numerical flux function preserves three structural properties
  - EC: entropy-conserving
  - KEP: kinetic-energy-preserving
  - PEP: pressure-equilibrium-preserving

Recall: A simple test case

- Consider the compressible Euler equations in 2D
- Density wave initial conditions with periodic boundary conditions

$$
\begin{aligned}
\rho &= 1 + 0.98\,\sin(2\,\pi\,(x+y)) \\
v_1 &= 0.1 \\
v_2 &= 0.2 \\
p &= 20
\end{aligned}
\tag{45}
$$

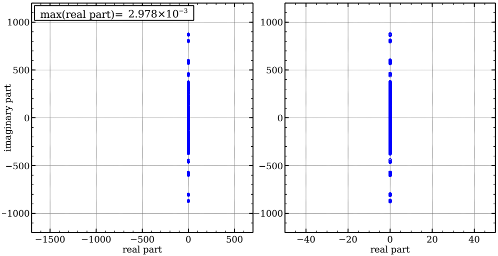
- Exact solution is the traveling density wave

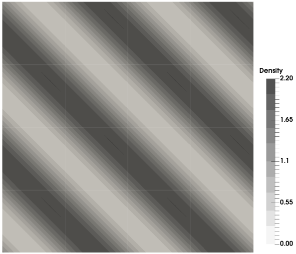


- PEP: temporal change of pressure (and velocity) is exactly zero

Numerical investigation

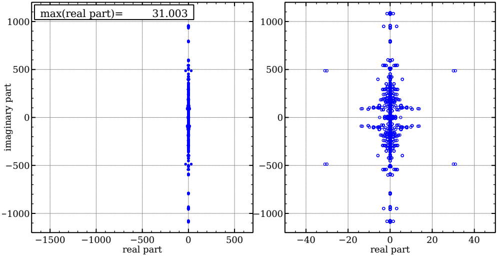
- Standard DG scheme with central flux
- Spectra with $N = 5$ with 4^2 elements and solution at $t = 5$

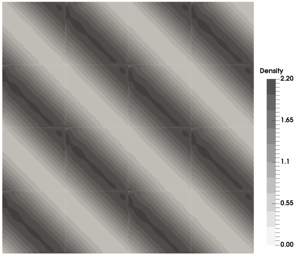




Numerical investigation

- Entropy-conserving DG (fluxes by Ismail&Roe, Chadrashekar, Ranocha)
- Spectra with $N = 5$ with 4^2 elements and solution at $t = 0.55$

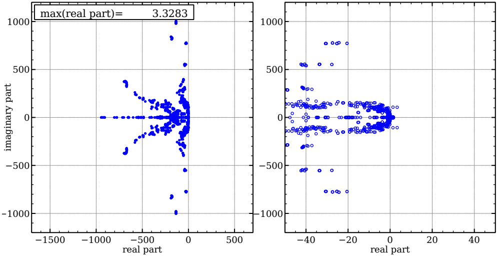


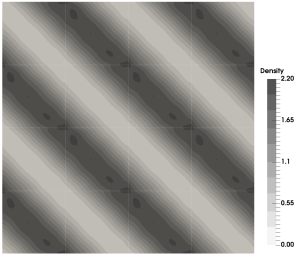


crash

Numerical investigation

- Entropy-dissipative DG (Rusanov/LxF flux at element surface)
- Spectra with $N = 5$ with 4^2 elements and solution at $t = 0.65$





crash!

Conclusion

- High-order structure preserving FV/DG/SBP-FD
  - Entropy-conservative/dissipative
  - Kinetic-Energy-preserving/dissipative
  - Pressure-equilibrium-preserving
- *Many complex applications, (e.g. turbulent flow in complex geometries on moving meshes) work well!?*
- The schemes are not locally linearly stable
  - *Small scale fluctuations can grow and can turn into artificial solution features!?*
- Wrong entropy-analysis?
  - We can prove that there are no Harten entropies for the compressible Euler equations such that the associated entropy-conserving numerical flux is locally linearly stable.
- **So far, we do not have a well working fix...**