University of Zurich[UZH]

Institute for Computational Science, Institute of Mathematics

High order numerical schemes for CFD in astrophysics

Carving through the Codes: Challenges in Computational Astrophysics

Speaker: Maria Han Veiga
Supervised by: Romain Teyssier & Rémi Abgrall

Outline

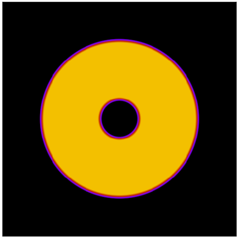
Introduction

- What are high order methods?
  - Solution error e of a smooth solution $\propto \mathcal{O}(h^k), k > 2$ [Persson2012].
  - E.g: High order reconstruction in Finite Volume methods (ENO/WENO), Finite element methods (FEM)

Introduction

- What are high order methods?
  - Solution error e of a smooth solution $\propto \mathcal{O}(h^k), k > 2$ [Persson2012].
  - E.g: High order reconstruction in Finite Volume methods (ENO/WENO), Finite element methods (FEM)
- Why are they appealing?
  - Higher fidelity predictions in computational methods
  - High-order gives superior performance for equal resolution
  - Schemes can be designed to exploit computational resources

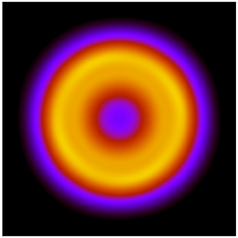
Motivation



Density profile at T=0
$N = 256^2$.

Protoplanetary disk evolution.
Modeled by 2-D inviscid Euler equation + gravity source term.

Motivation



Density profile, 1 rotation
N = 256^2

Balance law:

$$\partial_t U + \nabla \cdot F(U) = S(U) \qquad (1)$$

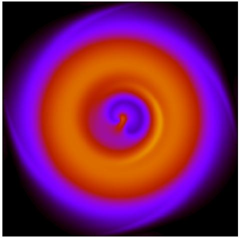
where

$$U = \left[\rho, \rho v_x, \rho v_y, \epsilon\right]^T$$

$$F(U) = \begin{bmatrix} \rho v_x & \rho v_y \\ \rho v_x^2 + p & \rho v_x v_y \\ \rho v_x v_y & \rho v_y^2 + p \\ v_x(\epsilon + p) & v_y(\epsilon + p) \end{bmatrix}$$

$$S(U) = \begin{bmatrix} 0 \\ -\rho \partial_x \phi \\ -\rho \partial_y \phi \\ -(\rho u \partial_x \phi + \rho v \partial_x \phi) \end{bmatrix}$$

Motivation



Density profile, 2 rotations
$N = 256^2$

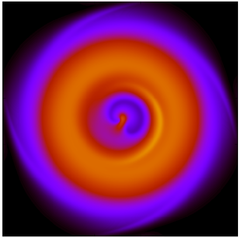
Looking at our system of PDEs:

$$\partial_t U + \nabla \cdot F(U) = S(U)$$

We can improve the quality of the solution by:

- More accurate description of U;
- For steady states, fulfill the flux-source balance $\nabla \cdot F(U) = S(U)$.

Motivation



Density profile, 2 rotations
N = 256^2

Looking at our system of PDEs:

$$\partial_t U + \nabla \cdot F(U) = S(U)$$

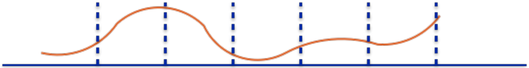
We can improve the quality of the solution by:

- More accurate description of U;
- For steady states, fulfill the flux-source balance $\nabla \cdot F(U) = S(U)$.

Improving accuracy of U

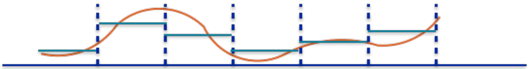
General idea: We look for a weak solution to (1) $U \in \mathcal{L}^{\infty}_{loc}(\mathbb{R}^2 \times [0, +\infty[)^4$, a locally bounded measurable function.
We further assume that $U_0 \in \mathcal{L}^{\infty}_{loc}(\mathbb{R}^2)^4$, meaning can be either continuous or discontinuous.

Improving accuracy of U



A simple example on approximating functions in 1-D.
Let us discretize $\mathbb{R} = \bigcup I_j,\ I_j = [x_i, x_{i+1}[$.

Improving accuracy of U



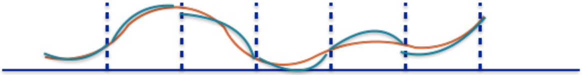
A simple example on approximating functions in 1-D.
Let us discretize $\mathbb{R} = \bigcup I_j,\ I_j = [x_i, x_{i+1}[$.
1st order Finite Volume Scheme: $u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}(F(u_{i+1/2}^n) - F(u_{i-1/2}^n))$.
$F(u_{i+1/2}^n) \approx \hat{F}(a, b)$ a suitable numerical flux.

Improving accuracy of U

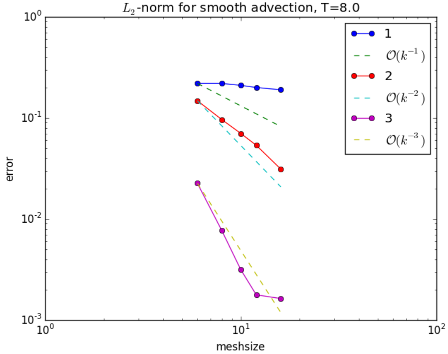
Discontinuous Galerkin method[2]

We look for $u^h \in V_k^h := \{u^h \in L^1_{loc}(\mathbb{R}) \cap BV(\mathbb{R}), u\,|^h_{I_j} \in \mathbb{P}^k(I_j)\forall I_j\}$ s.t. $\forall v^h \in V_k^h$:

$$\int_{I_j} v^h(x)\partial_t u^h dx + [v^h(x)\hat{f}(u(x,t))]_{x_{j-1/2}}^{x_{j+1/2}} - \int_{I_j} \partial_x v^h f(u^h)dx = 0$$

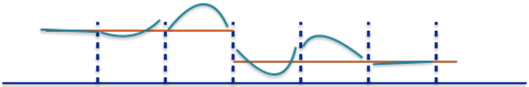


Improving accuracy of U



$\mathcal{L}_2$-error of density after 8 boundary crossings.

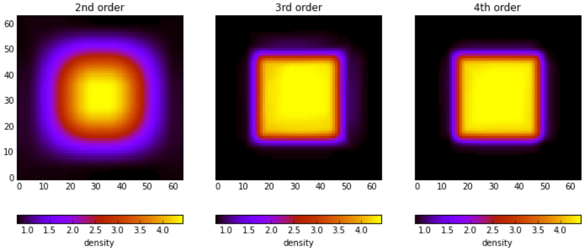
What if solution is not smooth?



- High order approximation leads to oscillations (Gibbs phenomena);
- We can't apply Weierstrass approximation theorem anymore.
- Limiters in our code:
  - TVD limiter: 2nd order [2]
  - Positivity preserving limiter [5], ideally Maximum principle preserving limiters[1]
  - High order limiter [3]

[1] If you are interested, ask me about what we are working on after the talk!

Results: Supersonic advection of a discontinuous density profile[4]



Density, $(v_x, v_y) = (100, 50)$ at $\mathrm{T} = 10$.

Results: 2D Riemann problem case 3 [1]

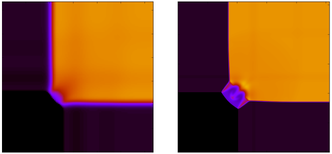


Figure: Density at T = 0.25. 1st order, $N = 128^2$ and 1024^2.

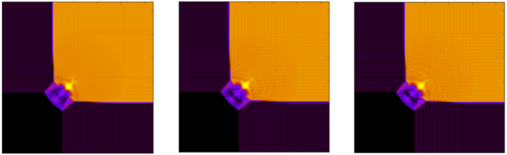
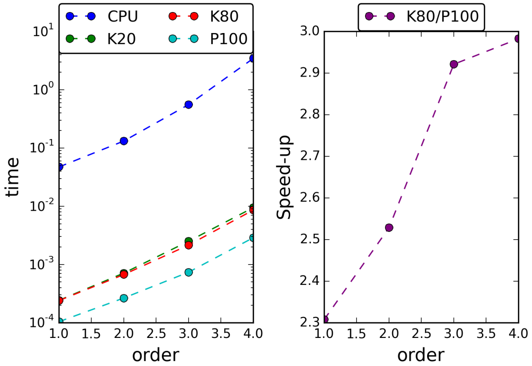


Figure: Density at T = 0.25. 2nd, 3rd, 4th order with $N = 128^2$.

Computational cost



CPU and GPU timing for advection of discontinuous density at $T = 10$ $\mathrm{N} = 64^2$.

Disks

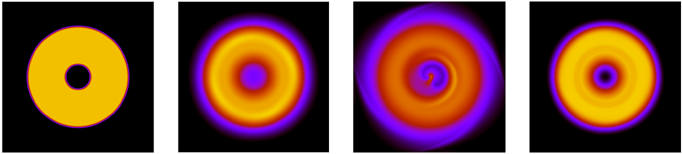


Figure: Density, 1^{st} order, rotation = 0, 1, 2 at $N = 512^2$, 1 at $N = 1600^2$

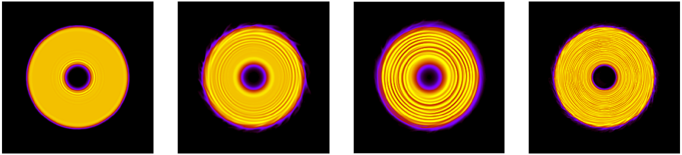


Figure: $N = 256^2$: 2^{nd} order, rotation = 1, 10, 40. 3^{rd} order, rotation = 10

Steady states: Preliminary work

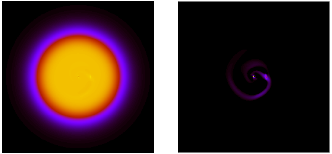


Figure: Density. Well balanced scheme, $\eta = 1x10^{-4}$, 1 rotation, 1st order

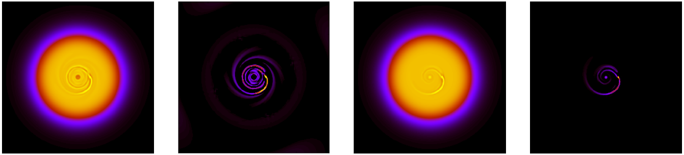


Figure: Non vs well balanced scheme, $\eta = 1x10^{-4}$, 1 rotation, 2nd order

Conclusions & Outlooks

- DG is a good scheme for parallel implementations
- Better resolution power for the same resolution
- Time integration order must be at least as high as space integration
- Going to high order can lead to less taylor made solutions (by reducing error from e.g. mesh alignment, specific geometry)
- Finding appropriate limiters is important
  - Limiting conservative variables is generally bad
  - Primitives yield better results
  - Characteristics yield the best results but unclear how to do it for cross terms in high order modes
  - Maximum preserving limiters are desirable - discretized solution mimics the solution to the original PDE
- Well balanced schemes for general equilibria states is an open question

Appendix: Test cases

Riemann problem: case 3

Configuration 3.

$$\begin{array}{ccc} & \overleftarrow{S}_{21} & \\ \overleftarrow{S}_{32} & & \overleftarrow{S}_{41} \\ & \overleftarrow{S}_{34} & \end{array}$$

The initial data are

$$\begin{array}{llll} p_2 = 0.3 & \rho_2 = 0.5323 & p_1 = 1.5 & \rho_1 = 1.5 \\ u_2 = 1.206 & v_2 = 0 & u_1 = 0 & v_1 = 0 \\ & & & \\ p_3 = 0.029 & \rho_3 = 0.138 & p_4 = 0.3 & \rho_4 = 0.5323 \\ u_3 = 1.206 & v_3 = 1.206 & u_4 = 0 & v_4 = 1.206 \end{array}$$

Appendix: Cold keplerian disk

Based on [Cullen & Dehnen 2010].

$$p = p_0$$

$$\rho(r) = \begin{cases} \rho_0 & r < 0.5 - \frac{\Delta r}{2} \\ (\rho_D - \rho_0)(r - (0.5 - \frac{\Delta r}{2})) + \rho_0 & r - 0.5 \leq |\frac{\Delta r}{2}| \\ \rho_D & 0.5 + \frac{\Delta r}{2} \leq r < 2 - \frac{\Delta r}{2} \\ -(\rho_D - \rho_0)(r - (2.0 - \frac{\Delta r}{2})) + \rho_D & r - 2 \leq |\frac{\Delta r}{2}| \\ \rho_0 & \textit{elsewhere} \end{cases}$$

$$v_x(r) = \begin{cases} -y/r^{3/2} & r - 2 \leq 2|\frac{\Delta r}{2}| \\ 0 & \textit{else} \end{cases}$$

$$v_y(r) = \begin{cases} x/r^{3/2} & r - 2 \leq 2|\frac{\Delta r}{2}| \\ 0 & \textit{else} \end{cases}$$

Appendix: Cold keplerian disk

x,y are centered at (3,3).
Aceleration is given:

$$a_x(r) = \begin{cases} -x/r^3 & r > r_c \\ -\frac{x}{r(r^2+\epsilon^2)} \frac{(r_c^2+\epsilon^2)}{r_c^3} & r \leq r_c \end{cases}$$

$$a_y(r) = \begin{cases} -y/r^3 & r > r_c \\ -\frac{y}{r(r^2+\epsilon^2)} \frac{(r_c^2+\epsilon^2)}{r_c^3} & r \leq r_c \end{cases}$$

$\epsilon = 0.25$, $r_c = 0.5 - 0.5\Delta r$, $\nabla\Phi = -a$.

Appendix: Flux-Source balance

General idea: For problems where a steady state solution exists, a solution *close by* the steady state can be seen as:

$$U = U_e + \delta U$$

For a steady state solution U_e of (1), we have the following equality:

$$\nabla \cdot F(U_e) = S(U_e) \quad (1)$$

The idea is to develop numerical schemes which can preserve a discrete steady state of interest up to machine precision.
This is called a "well-balanced scheme" [LeVeque1998].

Appendix: Flux-Source balance

General idea: For problems where a steady state solution exists, a solution *close by* the steady state can be seen as:

$$U = U_e + \delta U$$

For a steady state solution U_e of (1), we have the following equality:

$$\nabla \cdot F(U_e) = S(U_e) \tag{1}$$

The idea is to develop numerical schemes which can preserve a discrete steady state of interest up to machine precision.
This is called a "well-balanced scheme" [LeVeque1998].

Appendix: Flux-Source balance

General idea: For problems where a steady state solution exists, a solution *close by* the steady state can be seen as:

$$U = U_e + \delta U$$

For a steady state solution U_e of (1), we have the following equality:

$$\nabla \cdot F(U_e) = S(U_e) \tag{1}$$

The idea is to develop numerical schemes which can preserve a discrete steady state of interest up to machine precision.
This is called a "well-balanced scheme" [LeVeque1998].

Steady state

$\partial_t \cdot \equiv 0$
Hydrostatic equilibrium: $u, v \equiv (0,0)$
Euler system simplifies to:

$$\partial_x(p) = -\rho\Phi_x \tag{2}$$

$$\partial_y(p) = -\rho\Phi_y \tag{3}$$

Dynamic equilibrium: $v_\theta = \sqrt{(-\frac{1}{\rho}\frac{dP}{dr} + \nabla\Phi)}$ Taking a simplified solution:

$$\rho = const \tag{4}$$

$$v_x = -\frac{v_t}{r}y \tag{5}$$

$$v_y = \frac{v_t}{r}x \tag{6}$$

$$p = cs^2\rho \tag{7}$$

with $\nabla\Phi = \frac{r}{(r^2+\epsilon^2)^{\frac{3}{2}}}$ and $v_t = \sqrt{-\frac{1}{rho}(1 + 2h^2 - \frac{3h^2r^2}{r^2+\epsilon^2})r^2\Omega_k + r\nabla\Phi}$

References I

- Tung Chang, Gui-Qiang Chen, and Shuli Yang. "On the 2-D Riemann problem for the compressible Euler equations I. Interaction of shocks and rarefaction waves". In: *Discrete and Continuous Dynamical Systems* 1.4 (1995), pp. 555–584. ISSN: 1078-0947. DOI: 10.3934/dcds.1995.1.555. URL: http://aimsciences.org/journals/displayArticlesnew.jsp?paperID=748.
- Bernardo Cockburn and Chi-Wang Shu. "The Runge-Kutta Discontinuous Galerkin Method for Conservation Laws V". In: *J. Comput. Phys.* 141.2 (Apr. 1998), pp. 199–224. ISSN: 0021-9991. DOI: 10.1006/jcph.1998.5892. URL: http://dx.doi.org/10.1006/jcph.1998.5892.

References II

- Lilia Krivodonova. "Limiters for high-order discontinuous Galerkin methods". In: *Journal of Computational Physics* 226.1 (2007), pp. 879–896. ISSN: 0021-9991. DOI: http://dx.doi.org/10.1016/j.jcp.2007.05.011. URL: http://www.sciencedirect.com/science/article/pii/S0021999107002136.
- Kevin Schaal et al. "Astrophysical hydrodynamics with a high-order discontinuous Galerkin scheme and adaptive mesh refinement". In: *Monthly Notices of the Royal Astronomical Society* 453.4 (2015), p. 4278. DOI: 10.1093/mnras/stv1859. eprint: /oup/backfile/Content_public/Journal/mnras/453/4/10.1093_mnras_stv1859/3/stv1859.pdf. URL: +%20http://dx.doi.org/10.1093/mnras/stv1859.

References III

- Xiangxiong Zhang and Chi-Wang Shu. "On Positivity-preserving High Order Discontinuous Galerkin Schemes for Compressible Euler Equations on Rectangular Meshes". In: *J. Comput. Phys.* 229.23 (Nov. 2010), pp. 8918–8934. ISSN: 0021-9991. DOI: 10.1016/j.jcp.2010.08.016. URL: http://dx.doi.org/10.1016/j.jcp.2010.08.016.