

On semilagrangian methods for kinetic equations

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Numerical methods for PDEs: optimal control, games and image processing
In honor of the 60th birthday of Maurizio Falcone
University of Rome, La Sapienza
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Main collaborators:
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Maria Groppi, Giuseppe Stracquadanio, Univ. of Parma

Outline

- 1 Vlasov-Poisson system
- 2 High order semilagrangian for BGK
- 3 Conservative correction

Motivation: Vlasov-Poisson system

The collisionless and non-relativistic plasma may be described by the well-known Vlasov-Poisson (VP) system,

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{E}(t, \mathbf{x}) \cdot \nabla_{\mathbf{v}} f = 0, \quad (1)$$

$$\mathbf{E}(t, \mathbf{x}) = -\nabla_{\mathbf{x}} \phi(t, \mathbf{x}), \quad -\Delta_{\mathbf{x}} \phi(t, \mathbf{x}) = \rho(t, \mathbf{x}). \quad (2)$$

$f(t, \mathbf{x}, \mathbf{v})$: probability density of finding a particle with velocity \mathbf{v} at position \mathbf{x} at time t .

$\rho(t, \mathbf{x}) = \int f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$ - 1: charge density

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e.g., finite difference method, finite volume method, disc. Galerkin

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 - with operator splitting:
easy to trace characteristics, but subject to splitting error
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Other subdivision is between

- Forward SL schemes (FSL)
- Backward SL schemes (BSL)

We only adopt Backward Semi Lagrangian (BSL) here.

Semi-Lagrangian: without splitting

How to update solution: $\{f_{i,j}^n\} \Rightarrow \{f_{i,j}^{n+1}\}$?

- 1 Tracing characteristics: locate the foot of characteristics
 $(x_{i,j}^*, v_{i,j}^*) = (x(t^n), v(t^n))$ subject to the following **final** value problem

$$\begin{cases} \frac{dx(t)}{dt} = v(t); & \frac{dv(t)}{dt} = E(x(t), t), \\ x(t^{n+1}) = x_i; & v(t^{n+1}) = v_j \end{cases} \quad (3)$$

- 2 High order interpolation:

$$f_{i,j}^{n+1} = f(x_{i,j}^*, v_{i,j}^*, t^n),$$

where the R.H.S. is approximated by high-dimensional interpolation (for example WENO).

Tracing Characteristics

- *First order accuracy:*

$$x_i^{(1)} = x_i - v_j \Delta t; \quad v_j^{(1)} = v_j - E_i^n \Delta t$$

from which one can update $f^{(1)}$, $\rho^{(1)}$ and $E^{(1)}$ at t^{n+1} . ^{1,2}

¹superscript (1) means first order approximation

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- *Second order accuracy:*

$$x_i^{(2)} = x_i - \frac{1}{2}(v_j + v_j^{(1)})\Delta t;$$

$$v_j^{(2)} = v_j - \frac{1}{2}(E(x_i^{(1)}, t^n) + E^{(1)}(x_i, t^{n+1}))\Delta t$$

from which one can update $f^{(2)}$, $\rho^{(2)}$ and $E^{(2)}$ at t^{n+1} .

¹superscript (1) means first order approximation

² $E_i^n = E(x_i, t^n)$

Tracing Characteristics (cont.)

- *Third order accuracy:*

$$x_i^{(3)} = x_i - v_j \Delta t + \frac{\Delta t^2}{2} \left(\frac{2}{3} E^{(2)}(x_i, t^{n+1}) + \frac{1}{3} E(x_i^{(2)}, t^n) \right);$$

$$v_j^{(3)} = v_j - E^{(2)}(x_i, t^{n+1}) \Delta t + \frac{\Delta t^2}{2} \left(\frac{2}{3} \frac{d}{dt} E^{(2)}(x_i, t^{n+1}) + \frac{1}{3} \frac{d}{dt} E(x_i^{(2)}, t^n) \right);$$

from which one can update $f^{(3)}$, $\rho^{(3)}$ and $E^{(3)}$ at t^{n+1} .

Simulation results: two-stream instability

Consider the symmetric two stream instability, the VP system with initial condition

$$f(x, v, t = 0) = \frac{2}{7\sqrt{2\pi}}(1 + 5v^2)(1 + \alpha(\cos(2kx) + \cos(3kx)) / 1.2 + \cos(kx)) \exp(-\frac{v^2}{2}),$$

with $\alpha = 0.01$, $k = 0.5$ and the length of domain in x -direction $L = \frac{2\pi}{k}$.

Order or accuracy

Table: Order of accuracy in time: two stream instability with sixth order WENO interpolation $Nx = Nv = 160$ and $T = 5$.

	first order		second order		third order	
CFL	L^1 error	order	L^1 error	order	L^1 error	order
6	1.17E-4	–	2.40E-6	–	1.13E-7	–
7	1.40E-4	1.13	2.80E-6	2.04	1.79E-7	3.02
8	1.63E-4	1.16	3.69E-6	2.07	2.69E-7	3.02
9	1.87E-4	1.16	4.69E-6	2.04	3.84E-7	3.03
10	2.12E-4	1.20	5.84E-6	2.08	5.31E-7	3.06

VP system: weak Landau damping $\alpha = 0.01$

Consider the VP system with initial condition,

$$f(x, v, t = 0) = \frac{1}{\sqrt{2\pi}}(1 + \alpha \cos(kx))\exp\left(-\frac{v^2}{2}\right),$$

with $\alpha = 0.01$, $k = 2$.

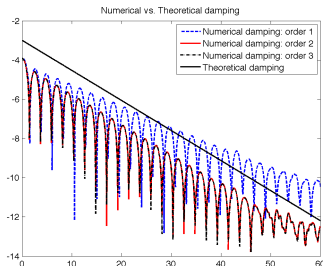


Figure: Time evolution of L^2 norm of electric field.

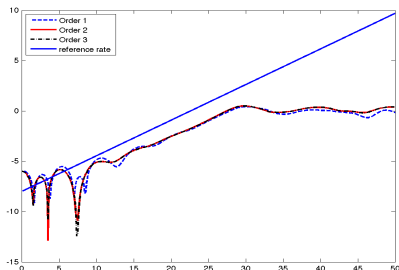
Symmetric two stream instability

Initial condition:

$$f(x, v, t = 0) = \frac{1}{\sqrt{8\pi}v_{th}} \left[\exp\left(-\frac{(v-u)^2}{2v_{th}^2}\right) + \exp\left(-\frac{(v+u)^2}{2v_{th}^2}\right) \right] (1 + 0.0005 \cos(kx)) \quad (4)$$

with $u = 5\sqrt{3}/4$, $v_{th} = 0.5$ and $k = 0.2$.

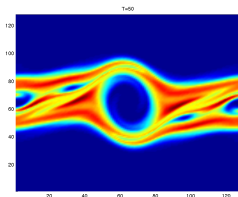
Constant background ion distribution chosen so that net charge density is zero.



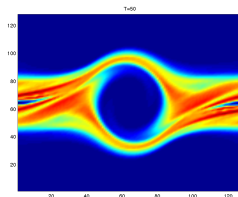
Time evolution of electric field in L^2 norm (from J. Banks and J. Hittinger, 2010)

2 stream instab.: phase space portraits

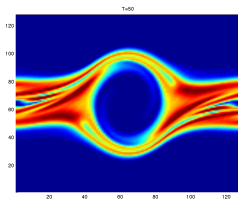
First order, CFL = 5.0



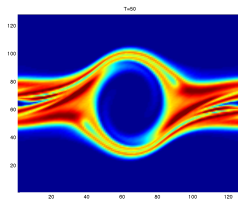
First order, CFL = 0.1



Second order, CFL = 5.0



Third order, CFL = 5.0



BGK model

The BGK model (Bhatnagar-Gross-Krook '54) approximates Boltzmann equation for the evolution of a rarefied gas.

The main variable is the distribution function f of the particles, as in the Boltzmann equation. The evolution of f is given by:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\epsilon} (M[f] - f) \quad (5)$$

with initial condition $f(x, v, 0) = f_0(x, v)$.

Here ϵ represents the non dimensional collision time. Hydrodynamic regime

$\rightarrow \epsilon \ll 1$

Rarefied regime $\rightarrow \epsilon \sim O(1)$

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Here we present a numerical method for the BGK equation based on a Semi-Lagrangian formulation using BDF (Stracquadanio, Russo, Groppi, in progress).

The method is compared with a RK-based approach (Russo, Santagati, 2008).

Semi-Lagrangian formulation

Simplified model: 1D in space and velocity:

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = \frac{1}{\epsilon} (M[f] - f). \quad (6)$$

with

$$M[f] = \frac{\rho}{(2\pi RT)^{1/2}} \exp\left(-\frac{(v-u)^2}{2RT}\right)$$

$t \geq 0, \quad x, v \in \mathbb{R}.$

Semi-Lagrangian: follow the evolution along the characteristics.

$$\begin{aligned} \frac{df(x, v, t)}{dt} &= \frac{1}{\epsilon} \left(M[f](x, v, t) - f(x, v, t) \right), \\ \frac{dx}{dt} &= v, \quad x(0) = \tilde{x}, \quad f(0, t, v) = f_0(\tilde{x}, v) \quad t \geq 0, \quad x, v \in \mathbb{R}. \end{aligned} \quad (7)$$

Note that x becomes a time dependent variable and its equation gives:

$$x(t) = \tilde{x} + vt, \quad t \geq 0, \quad x, v \in \mathbb{R}, \quad (\text{characteristic straight lines}).$$

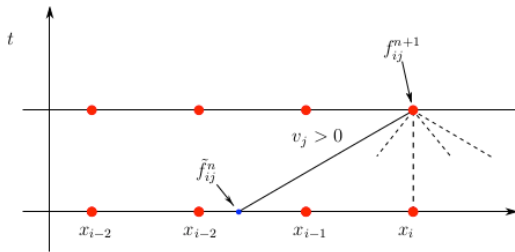
Implicit first order Semi-Lagrangian scheme

Let $f_{ij}^n \approx f(x_i, v_j, t^n)$ be approximate solution.

Possible stiffness (small ϵ) \Rightarrow implicit formulation.

$$f_{ij}^{n+1} = \tilde{f}_{ij}^n + \frac{\Delta t}{\epsilon} (M_{ij}^{n+1} - f_{ij}^{n+1}), \quad (8)$$

Here $\tilde{f}_{ij}^n = f(t^n, \tilde{x}_i = x_i - v_j \Delta t, v_j)$ can be calculated by (linear) interpolation from $\{f_j^n\}$.



Solution of the implicit step

Equation (8) is non linear.

Indeed $M[f]_{i,j}^{n+1}$ depends on f_{ij}^{n+1} through its moments.

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Let $\phi(v)$ be the vector $\phi(v) = (1, v, v^2)^T$. Compute the moments of f_{ij}^{n+1} :

$$\langle f_{ij}^{n+1} \phi \rangle = \langle \tilde{f}_{ij}^n \phi \rangle + \frac{\Delta t}{\epsilon} \langle (M_{ij}^{n+1} - f_{ij}^{n+1}) \phi \rangle.$$

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From the conservation, we have

$$\langle (M_{ij}^{n+1} - f_{ij}^{n+1}) \phi \rangle = 0 \quad \Rightarrow \quad \langle f_{ij}^{n+1} \phi \rangle = \langle \tilde{f}_{ij}^n \phi \rangle$$

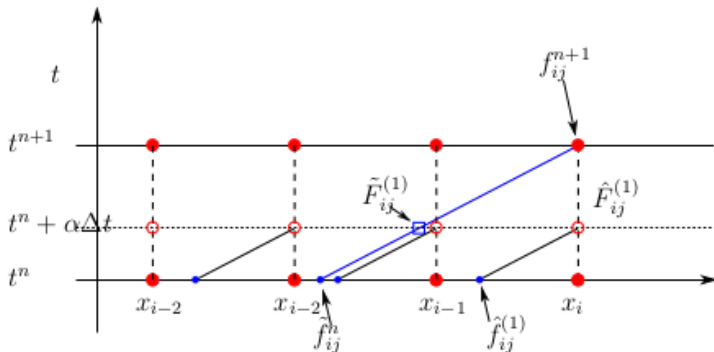
Hence we immediately find the macroscopic variables ρ_i^{n+1} , u_i^{n+1} and T_i^{n+1} corresponding to f_{ij}^{n+1} using \tilde{f}_{ij}^n and with these values the approximated Maxwellian is updated.

Higher order: Runge-Kutta

Classical RK schemes can be adopted.

Stage values are computed along the characteristics.

First they are computed at grid position x_i (empty circles) and then the value of f (or the RK flux) is interpolated on the characteristics (empty squares)



High order BDF schemes

Runge-Kutta methods may be expensive.

The BDF (Backward Difference Formula) methods allow same order of accuracy at lower cost.

We will show some numerical results concerning the BDF methods with 2 (BDF2) and 3 (BDF3) steps. Applying these methods to the Lagrangian formulation of the BGK model we obtain the following schemes:

$$f_{ij}^{n+1} = \frac{4}{3} f_{ij}^{(1)n} - \frac{1}{3} f_{ij}^{(2)n-1} + \frac{\Delta t}{\epsilon} (M_{ij}^{n+1} - f_{ij}^{n+1})$$

$$f_{ij}^{n+1} = \frac{11}{18} f_{ij}^{(1)n} - \frac{9}{11} f_{ij}^{(2)n-1} + \frac{2}{11} f_{ij}^{(3)n-2} + \frac{\Delta t}{\epsilon} (M_{ij}^{n+1} - f_{ij}^{n+1})$$

where $f_{ij}^{(s)n} = f^n(x_i - sv_j \Delta t, v_j)$, $s = 1, 2, 3$, obtained **by interpolation**.

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where $f_{ij}^{(s)n} = f^n(x_i - sv_j\Delta t, v_j)$, $s = 1, 2, 3$, obtained by interpolation. High order in space is obtained by WENO reconstruction.

Numerical test for the problem 1+1D

We have considered two numerical test:

1 Smooth initial data

$$(f_0 = M[v, \rho = 1, u = 0.1 \exp(-(10x - 1)^2) - 2 \exp(-(10x + 3)^2), T = 1])$$

- time interval $[0, 0.04]$;
- space interval $[-1, 1]$;
- velocity interval $[-10, 10]$;
- $N_v = 40$;
- $\Delta t = CFL \Delta x / |v_{max}|$;

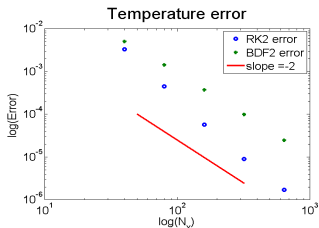
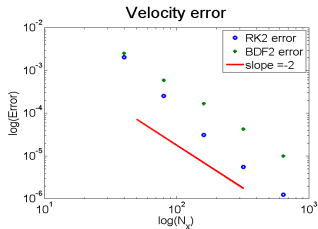
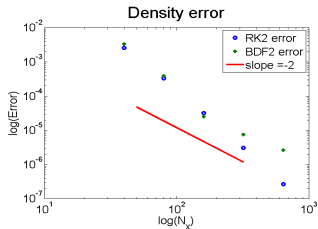
2 Riemann problem (jump in $x = 0.5$):

- $(\rho_L, u_L, T_L) = (2.25, 0, 1.125)$, $(\rho_R, u_R, T_R) = (3/7, 0, 1/6)$
- time interval $[0, 0.16]$;
- space interval $[0, 1]$;
- velocity interval $[-10, 10]$;
- $N_x = 100$;
- $N_v = 60$;
- $\Delta t = CFL \Delta x / |v_{max}|$;

For each test the cases $\epsilon = 10^{-2}$ and $\epsilon = 10^{-6}$ have been studied.

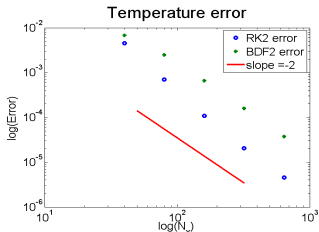
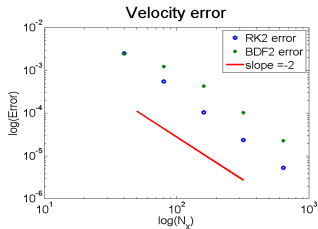
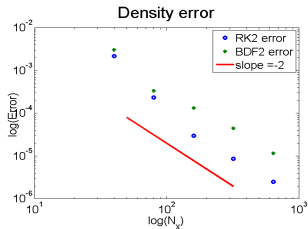
RK2 and BDF2 accuracy 1+1D in rarefied regime

($\epsilon = 10^{-2}$)



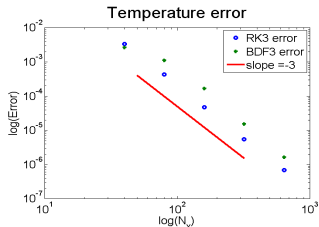
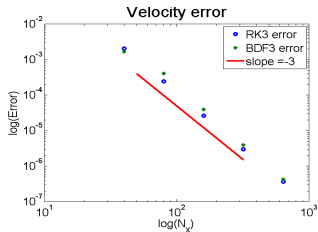
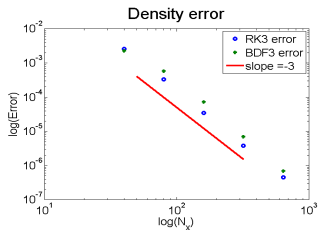
RK2 and BDF2 accuracy 1+1D in hydrodynamic regime

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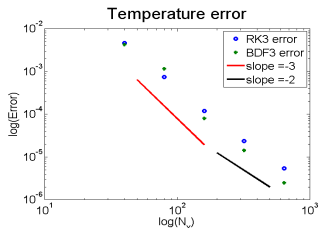
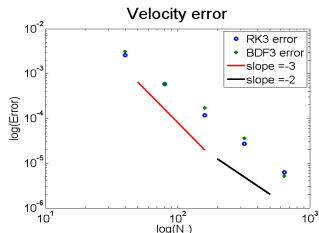
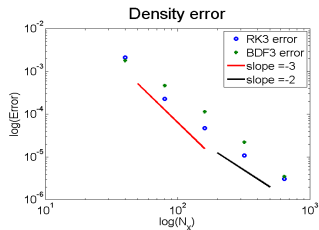
RK3 and BDF3 accuracy 1+1D in rarefied regime

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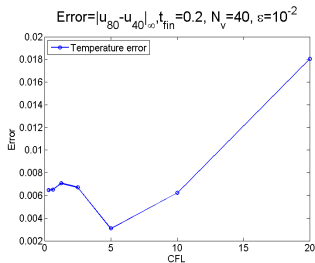
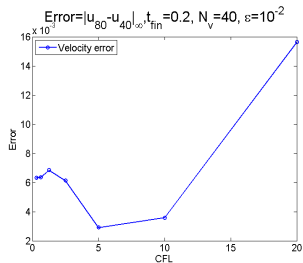
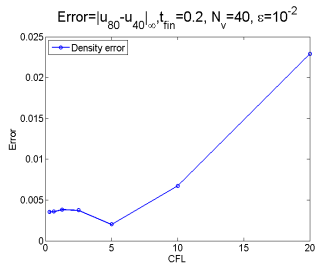


RK3 and BDF3 accuracy 1+1D in hydrodynamic regime

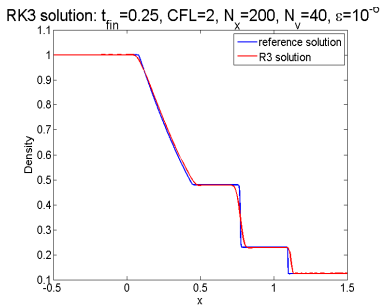
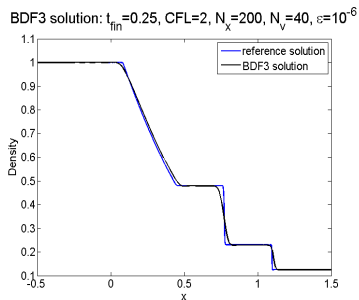
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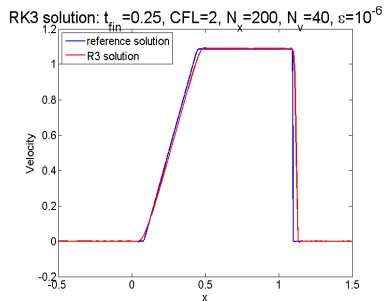
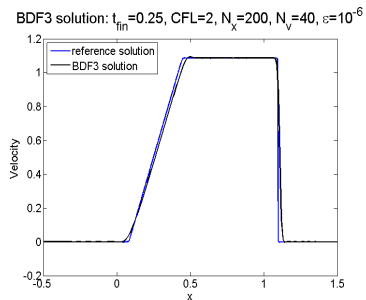
BDF3-weno3-5, CFL-Error for the problem 1D+1D



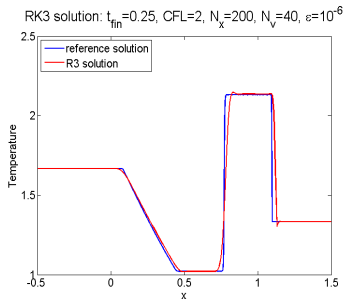
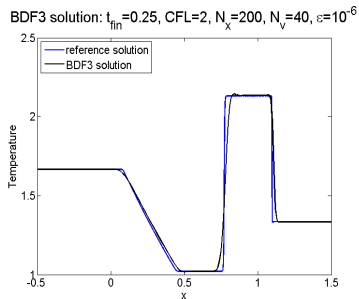
Comparison with the solution of gas dynamics: density given by BDF3 and RK3 for 1+3D



Comparison with the solution of gas dynamics: velocity given by BDF3 and RK3 for 1+3D

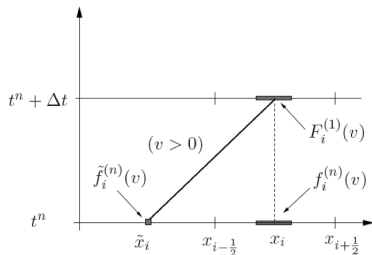


Comparison with the solution of gas dynamics: temperature given by BDF3 and RK3 for 1+3D



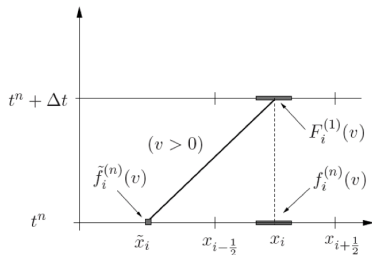
Conservative correction

Can be adopted both at *finite volume* or *conservative finite difference* level (which is what we treat here)



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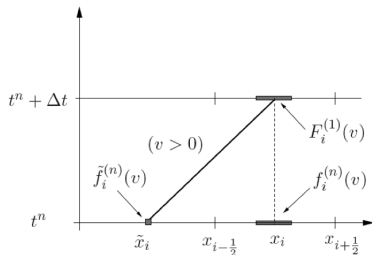
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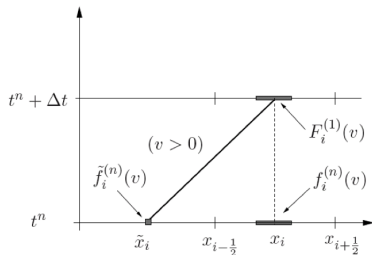
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Conservative correction

Can be adopted both at *finite volume* or *conservative finite difference* level (which is what we treat here)



- 1 compute a predictor value at the center of the cell
- 2 use such a predictor to perform reconstruction of the fluxes, at cell edges
- 3 evolve the conservative values according to the computed fluxes

Application to conservation laws

Consider a system of conservation laws

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

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$$\frac{\partial u}{\partial t} + A(u) \frac{\partial u}{\partial x} = 0$$

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Application to conservation laws

Consider a system of conservation laws

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where $u = U(v)$ is an **invertible mapping** ($v = V(u)$ is the inverse) and the formulation in v is somehow *simpler*.

Then one can apply a conservative correction using finite volume or finite difference discretization.

skip to stability

Finite volume approach

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- ③ Compute the splitter fluxes f^- and f^+ ($f^- + f^+ = f$) at cell center x_j at each stage l
- ④ Reconstruct (from cell average to pointwise) the fluxes f^+ and f^- at cell edges $f_{j+\frac{1}{2}}^{(k)} = f^-(x_{j+1/2}^+, t^n + c_k \Delta t) + f^+(x_{j+1/2}^-, t^n + c_k \Delta t)$

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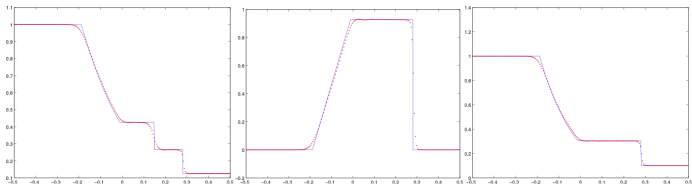
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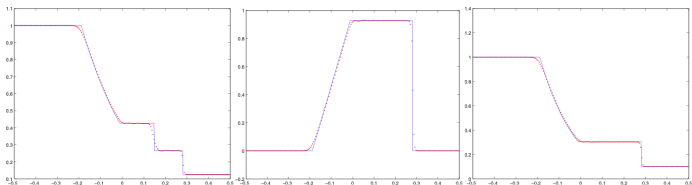
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Application to gas dynamics

Classical Sod problem solved using primitive variables as predictor



WENO 2-3



WENO 3-5

Stability analysis

Consider linear convective equation

$$u_t + (vu)_x = 0,$$

Evolve by conservative FD scheme:

$$\frac{du_j}{dt} = -\frac{1}{\Delta x} \left(\hat{f}_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} \right),$$

The numerical solution is computed as

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} \sum_{\ell=1}^s b_\ell \left(\hat{f}_{j+\frac{1}{2}}^{(\ell)} - \hat{f}_{j-\frac{1}{2}}^{(\ell)} \right).$$

$$u_j^{(\ell)} = u^n(x_j^{(\ell)}), \quad x_j^{(\ell)} = x_j - v c_\ell \Delta t$$

Look for Fourier modes

$$u_j^n[\xi] = \rho^n e^{ij\xi},$$

Stability analysis

Use Fourier interpolation for arbitrary x

$$u^n(x) = \rho^n e^{ix\xi/\Delta x}.$$

Compute the non conservative semilagrangian stages

$$u_j^{(\ell)} = u^n(x_j^{(\ell)}) = \rho^n \exp(i\xi(x_j - v\Delta t c_\ell)/\Delta x) = \rho^n e^{ij\xi} e^{-ic_\ell a \xi},$$

From this obtain the amplification factor

$$\rho = 1 - i\xi a \sum_{\ell=1}^s b_\ell \exp(-ic_\ell a \xi).$$

Analogy with A-stability

Test equation for A-stability

$$w'(t) = \lambda w(t), \quad w(0) = 1$$

Exact solution

$$w(\Delta t) = e^{\lambda \Delta t} = e^z,$$

Identity obtained observing that $\int_0^1 e^{cz} dc = (e^z - 1)/z$:

$$e^z = 1 + z \int_0^1 e^{cz} dc.$$

Using exact Fourier interpolation, the error is due to the use of quadrature rule to compute the integral:

$$R(z) = 1 + z \sum_{\ell=1}^s b_{\ell} e^{c_{\ell} z}.$$

Therefore:

$$\rho = R(-i\xi a).$$

Optimal quadrature formulas: given s stages, choose the scheme of order s with the largest stability region.

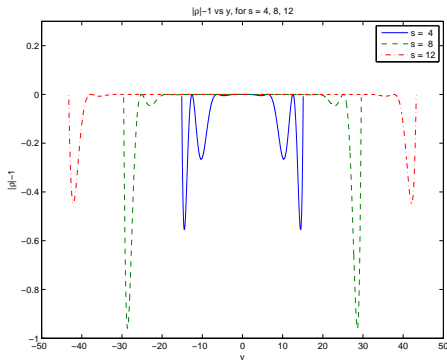
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The function $|\rho| - 1$ is given by



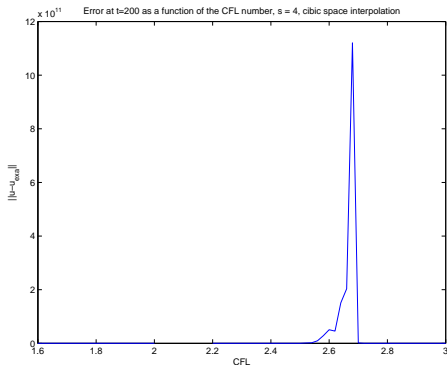
The bad news

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For example: using a third degree polynomial (4th order space interpolation) rather than Fourier interpolation, $s = 8$, one obtains instability in a neighborhood of $a = 2.6$.



The instability disappears for larger values of a , up to about the theoretical value $a^* = 4.81$.

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Possible solutions (work in progress):

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- reformulate the whole stability theory replacing Fourier interpolation by polynomial interpolations

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- check stability of different stencils and let nonlinear reconstruction choose the stable stencil
- reformulate the whole stability theory replacing Fourier interpolation by polynomial interpolations
- Basic question: is this of any use, or there is no way to make such conservative correction stable in practice?

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Thank you !

Maurizio, Roberto and Giovanni in 2002

