Some issues in the semi-Lagrangian treatment of second-order balance laws

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joint works with L. Bonaventura



Outline



Introduction

- Some basic concepts in SL and FFSL schemes
- The general idea in treating diffusion operators



The case of variable-coefficient operators in divergence form

- General construction of the schemes
- Discretization in advective form
- Discretization in conservative form

Nonlinear conservation laws with a viscosity term

- Solvability of the implicit scheme
- Entropic behaviour of the scheme
- Numerical tests

Basic concepts on SL schemes - hyperbolic case

Model equation: linear, constant-coefficient advection

$$egin{cases} u_t(x,t)+\mathsf{a} u_x(x,t)=0\ u(x,0)=u_0(x) \end{cases}$$

Representation formula

$$u(x,t)=u_0(x-at)$$

Semi-Lagrangian (SL) schemes stem from the so-called **Courant–Isaacson–Rees (CIR) method** ('52) which discretizes the representation formula (instead of the equation)

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General principle of SL schemes



Advection of the solution along characteristics:

$$u(x_j, t_{n+1}) = u(x_j - a\Delta t, t_n)$$

A numerical strategy I[V] is used to reconstruct the value at $x_j - a\Delta t$.

Construction of SL schemes

Semi-Lagrangian (SL) discretization $v_i^{n+1} = I[V^n](x_i - a\Delta t)$

The most classical choice for the interpolation I[V] is a symmetric Lagrange interpolation on a structured uniform mesh:



Various other options are possible, among which Galerkin projection

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General principle of FFSL schemes



Mass balance in the **control volume** $\Omega_j = [x_{j-1/2}, x_{j+1/2}]$:

$$\int_{\Omega_{j}} u(t_{n+1}) dx = \int_{\Omega_{j}} u(t_{n}) dx + \int_{x_{j-1/2}-a\Delta t}^{x_{j-1/2}} u(t_{n}) dx - \int_{x_{j+1/2}-a\Delta t}^{x_{j+1/2}} u(t_{n}) dx$$

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Construction of FFSL schemes

Flux-Form Semi-Lagrangian (FFSL) discretization

$$v_j^{n+1} = v_j^n + \frac{1}{\Delta x} \left(\int_{x_{j-1/2}-a\Delta t}^{x_{j-1/2}} R[V^n](x) dx - \int_{x_{j+1/2}-a\Delta t}^{x_{j+1/2}} R[V^n](x) dx \right)$$

As in a conventional **FV** scheme, the reconstruction R[V] preserves the average on each cell $[x_{j-1/2}, x_{j+1/2}]$ and reconstructs with high order smooth solutions

$$\xrightarrow{\qquad } \begin{array}{c} \overbrace{\qquad } \begin{array}{c} \overbrace{\qquad } \begin{array}{c} \overbrace{\qquad } \\ \overbrace{\qquad } \\ x_{l-3/2} \end{array} \xrightarrow{\qquad } \begin{array}{c} \overbrace{\qquad } \\ x_{l-1/2} \end{array} \xrightarrow{\qquad } \begin{array}{c} \overbrace{\qquad } \\ x_{l} \end{array} \xrightarrow{\qquad } \begin{array}{c} \overbrace{\qquad } \\ x_{l+1/2} \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ x_{l+3/2} \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \overbrace{\qquad } \\ \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \\ \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \end{array} \xrightarrow{} \end{array} \xrightarrow{\qquad } \begin{array}{c} \end{array} \xrightarrow{} \end{array} \xrightarrow{\qquad } \end{array} \xrightarrow{\qquad } \begin{array}{c} \end{array} \xrightarrow{} \end{array} \xrightarrow{} \end{array} \xrightarrow{} \end{array} \xrightarrow{} \end{array} \xrightarrow{\qquad } \begin{array}{c} \end{array} \xrightarrow{} \begin{array}{c} \end{array} \xrightarrow{} \end{array}$$

Theoretical results

• SL: multidimensional and high-order implementations can be easily constructed; theoretical results available for Galerkin projection and symmetric Lagrange interpolation in the variable coefficient case

Theoretical results

- SL: multidimensional and high-order implementations can be easily constructed; theoretical results available for Galerkin projection and symmetric Lagrange interpolation in the variable coefficient case
- FFSL: more complex in higher dimension; theoretical results available in one space dimension by exploiting the relationship with the SL case

Stochastic representation formula

The generalization of the concept of characteristics to **diffusion operators in trace form** may be performed in a stochastic framework

- Feynman–Kac formula: generalizes the representation formula by characteristics to the second-order case. Its use in numerical schemes was first proposed by Kushner in the 70s.
- It is a **stochastic representation formula**, but since it represents the solution as an expectation, its result is purely deterministic.
- It can be extended to more general situations, including second-order Dynamic Programming Equations ([KD01, CF95])
- Numerical implementation is performed via the **stochastic weak Euler scheme**, some high-order extension [F10]

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Deterministic interpretation (1)

A deterministic construction of this technique may be given via the Taylor expansion:

$$u(x_j + a\Delta t + \sigma\sqrt{2\Delta t}) = u(x_j) + \Delta t \ au_x(x_j) + \sqrt{2\Delta t} \ \sigma u_x(x_j) + \Delta t \ \sigma^2 u_{xx}(x_j)\sigma + O(\Delta t^{3/2}) + O(\Delta t^2)$$

$$u(x_j + a\Delta t - \sigma\sqrt{2\Delta t}) = u(x_j) + \Delta t \ au_x(x_j) - \sqrt{2\Delta t} \ \sigma u_x(x_j) + \Delta t \ \sigma^2 u_{xx}(x_j)\sigma - O(\Delta t^{3/2}) + O(\Delta t^2)$$

Taking the mean value we get:

$$\frac{1}{2} \left[u(x_j + a\Delta t + \sigma\sqrt{\Delta t}) + u(x_j + a\Delta t - \sigma\sqrt{\Delta t}) \right] = u(x_j) + \Delta t \left[au_x(x_j) + \sigma^2 u_{xx}(x_j)\sigma \right] + O(\Delta t^2)$$

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Deterministic interpretation (2)



• A first **upwinding** of magnitude *a* Δ*t* follows the **advection** (if advection occurs)

Deterministic interpretation (2)



- A first upwinding of magnitude a Δt follows the advection (if advection occurs)
- A second symmetric upwinding of magnitude $\sigma\sqrt{2\Delta t}$ is related to the diffusion

Operators in divergence form

The stochastic framework of the Feynman–Kac formula is **unsuitable to treat operators in divergence form**. To study the extension of this technique, we use the

Model equation: linear, second-order balance law

$$u_t + au_x = (\nu(x)u_x)_x \tag{1}$$

(formally, this equation can be put in the advective form

$$u_t + (a - \nu_x(x))u_x = \nu(x)u_{xx}$$

although a SL discretization of this latter equation would lose the conservative character and require the knowledge of ν_x)

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Operators in divergence form

In the model problem proposed:

- Variable-coefficient **advection terms** may be included without technical problems if **first-order consistency** is enough
- The diffusivity has **no dependence on** *t* (again, it can be extended to **time dependent diffusivity** if first-order schemes are OK)
- For the moment, we work in a **single space dimension** (extension to higher dimensions is possible, but not trivial for the conservative scheme)

General construction of the schemes

At the level of **consistency**, the analysis [BF14] can be based on the

General structure

$$u(x_j, t_{n+1}) \approx A_j^+ u(x_j - a\Delta t + \delta_j^+, t_n) + A_j^- u(x_j - a\Delta t - \delta_j^-, t_n).$$
(2)

- We have **four free parameters** to be consistent with the evolution operator
- (2) should be regarded as a **time discretization** (no space reconstruction is introduced yet)
- In general, we don't expect that the consistency rate could go beyond the unity

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Consistency

First order consistency conditions for the approximation (2)

$$\begin{cases} A_i^+ + A_i^- = 1 + O(\Delta t^2) \\ A_i^+ \delta_i^+ - A_i^- \delta_i^- = \Delta t \, \nu_x(x_i) + O(\Delta t^2) \\ A_i^+ \delta_i^{+2} + A_i^- \delta_i^{-2} = 2\Delta t \, \nu(x_i) + O(\Delta t^2) \\ A_i^+ \delta_i^{+3} - A_i^- \delta_i^{-3} = O(\Delta t^2). \end{cases}$$

• In the case of constant viscosity, we obtain again

$$\delta_{j}^{+} = \delta_{j}^{-} = \sqrt{2\Delta t \nu}, \quad A_{j}^{+} = A_{j}^{-} = 1/2$$

- Extension to a generic dimension: relatively straightforward [BF14]
- Extension to **higher order consistency**: some existing works for trace operators [F10], very difficult in general

Stability not proved in general, except for

- Monotone space discretizations (in this case the scheme is monotone and L^{∞} stable)
- **Constant diffusivity** (in this case the scheme is the convex combination of stable schemes)

Advective scheme – abstract formulation

Equation (1) can be treated in this form way by keeping $A_j^{\pm} = 1/2$ and defining two (different) displacements δ_i^{\pm} :

$$u(x_j, t_{n+1}) \approx \frac{1}{2}u(x_j - a\Delta t + \delta_j^+, t_n) + \frac{1}{2}u(x_j - a\Delta t - \delta_j^-, t_n)$$

with the δ^{\pm} defined as **solutions of**

$$\delta_{j}^{\pm}=\sqrt{2\Delta t \
u \left(x_{j}\pm\delta_{j}^{\pm}
ight)}$$

(the resulting time discretization is **first-order**, **nonconservative**). Note that the **difference between** δ_j^+ and δ_j^- generates the **additional advection term**:

$$\frac{1}{2}(\delta_j^+ - \delta_j^-) = \Delta t \,\nu_x(x_j) + O\left(\Delta t^2\right).$$

Fully discrete advective scheme

Fully discrete scheme

$$v_j^{n+1} = \frac{1}{2}I[V^n](x_j + \delta_j^+) + \frac{1}{2}I[V^n](x_j - \delta_j^-)$$

where (under reasonable assumptions) the displacements δ_j^\pm can be computed via the iteration

$$\delta_j^{\pm (k+1)} = \sqrt{2\Delta t \ \nu \left(x_j \pm \delta_j^{\pm (k)}\right)}$$

• For a space interpolation of degree r, the consistency error is

$$L(\Delta x, \Delta t) = O\left(\Delta t + \frac{\Delta x^{r+1}}{\Delta t}\right)$$

• Few iterations required to compute δ_j^\pm without degrading the consistency rate

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Flux-form scheme

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SL for second-order balance laws

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Nonlinear conservation laws - construction of the scheme

Model equation: nonlinear conservation law

 $u_t + f(u)_x = \nu u_{xx}$

The advective form of the equation is

$$u_t + f'(u)u_x = \nu u_{xx},$$

which is naturally discretized by the

Non-conservative scheme

$$v_{j}^{n+1} = \frac{1}{2} I[V^{n}](x_{j} - \Delta t f'(v_{j}^{n+1}) - \sqrt{2\Delta t \nu}) + \frac{1}{2} I[V^{n}](x_{j} - \Delta t f'(v_{j}^{n+1}) + \sqrt{2\Delta t \nu})$$

 v_i^{n+1} and the speed of propagation are unknown (the scheme is implicit).

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Convergence of the iterative solver

The scheme computes the solution V^{n+1} as a solution of **a system of** scalar fixed point equations:

$$V=T(V),$$

in which T depends on V^n and has **decoupled** components. Partial derivatives of the transformation T are given by

$$\frac{\partial T_j}{\partial v_j^{n+1}} = -\frac{\Delta t f''(v_j^{n+1})}{2} \left[l'[V^n] \left(x_j - \Delta t f'(v_j^{n+1}) - \sqrt{2\Delta t \nu} \right) + l'[V^n] \left(x_j - \Delta t f'(v_j^{n+1}) + \sqrt{2\Delta t \nu} \right) \right]$$

and are therefore "small" (i.e., T is a contraction) for Δt small enough.

A unilateral bound on the incremental ratio

Despite being non-conservative, an indication on the **correct entropic behaviour of the scheme** may be obtained by a **unilateral bound on the incremental ratio** of the numerical solution. If \overline{D}_j is a suitably defined incremental ratio at the foot of the characteristic ending at (x_j, t_n) , then

$$\frac{v_{j+1}^{n+1}-v_j^{n+1}}{\Delta x} = \frac{\bar{D}_j^n}{1+\Delta t \bar{D}_j^n f''(\eta)}$$

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which entails that, **uniformly wrt** ν :

for a convex flux (f" > 0), the maximum value of the derivative (if positive) decreases strictly from t_n to t_{n+1}

A unilateral bound on the incremental ratio

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$$\frac{v_{j+1}^{n+1} - v_j^{n+1}}{\Delta x} = \frac{\bar{D}_j^n}{1 + \Delta t \bar{D}_j^n f''(\eta)}$$

which entails that, **uniformly wrt** ν :

- for a convex flux (f" > 0), the maximum value of the derivative (if positive) decreases strictly from t_n to t_{n+1}
- for a concave flux (f'' < 0), the minimum value of the derivative (if negative) increases strictly from t_n to t_{n+1}

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1-D numerical tests – Burgers' equation

$$u_t + \left(\frac{u^2}{2}\right)_x = \nu u_{xx}, \quad t \in [0, 0.8], \quad \nu = 10^{-3}$$



100 nodes, $\Delta t = 0.05$, Courant number $\lesssim 5$

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1-D numerical tests – LWR equation

$$u_t + \left(\frac{u-u^2}{2}\right)_x = \nu u_{xx}, \quad t \in [0, 1.2], \quad \nu = 10^{-3}$$



100 nodes, $\Delta t = 0.05$, Courant number $\lesssim 2.5$

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 $u = 10^{-3}$, 100 imes 100 nodes, $\Delta t =$ 0.1, Courant number \lesssim 10

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 $u = 10^{-3}$, 100 imes 100 nodes, $\Delta t =$ 0.1, Courant number \lesssim 10

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 $u = 10^{-3}$, 100 imes 100 nodes, $\Delta t =$ 0.1, Courant number \lesssim 10

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 $u = 10^{-3}$, 100 imes 100 nodes, $\Delta t =$ 0.1, Courant number \lesssim 10

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- Construction of a general approach to treat diffusion terms in SL schemes, **both** in trace and divergence form
- Nonconservative structure, but conservative version is in progress (1D ok, multi-D ?)
- Various extensions to nonlinear problems: porous media eqn, turbulent viscosity for atmospherical models, viscous nonlinear conservation laws
- Flux-form version of the scheme for nonlinear conservation laws in progress
- Good overall numerical accuracy, but only first-order convergence wrt time

References

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Thank you for your attention!

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Thank you for your attention! (but...)

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Part 2

Highlights from my (scientific) life with Maurizio

"You are Ferretti of the Falcone–Ferretti paper? Wow." (Santiago de Compostela, 2005)

Literature

- 1 book
- 6 papers on journals
- 5 proceedings
- 2 editorials

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- Uncountable set, but
- 2 conferences with social ballroom dancing

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- Uncountable set, but
- 2 conferences with social ballroom dancing
- 1 conference reached by sailing boat

- Uncountable set, but
- 2 conferences with social ballroom dancing
- 1 conference reached by sailing boat
- 1 conference staying in a double bed room

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Image: A math a math

"...il signor Severino Pinzelleri..."

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"...il signor Severino Pinzelleri..."

• Verbatim translation: "...Mr. Severino Pinzelleri..."

"...il signor Severino Pinzelleri..."

- Verbatim translation: "...Mr. Severino Pinzelleri..."
- Actual translation: "...Mr. John Smith..." (antonomasia)

"...con tutti i cazzimbiccheri..."

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"...con tutti i cazzimbiccheri..."

• Verbatim translation: untranslatable

"...con tutti i cazzimbiccheri..."

- Verbatim translation: untranslatable
- Actual translation: "...with all the bells'n'whistles..."

"Salutace Biancaneve!"

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"Salutace Biancaneve!"

• Verbatim translation: "Best regards to Snow White!"

"Salutace Biancaneve!"

- Verbatim translation: "Best regards to Snow White!"
- Actual translation: "Don't even think of it, no hope! "

"Questo è un problema intricato"

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"Questo è un problema intricato"

• Verbatim translation: "This is an intricate problem"

"Questo è un problema intricato"

- Verbatim translation: "This is an intricate problem"
- Actual translation: "This is an intricate problem.

"Questo è un problema intricato"

- Verbatim translation: "This is an intricate problem"
- Actual translation: "This is an intricate problem. You do the computations"

(as a chairman) "What about error estimates?"

(as a chairman) "What about error estimates?"

• Verbatim translation: not required

(as a chairman) "What about error estimates?"

- Verbatim translation: not required
- Actual translation: "Come on, guys. Doesn't *really* anyone have a question?"

"Vediamoci alle... (ora t_0)"

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"Vediamoci alle... (ora t_0)"

• Verbatim translation: "Let's meet at... (time t_0)"

"Vediamoci alle... (ora t_0)"

- Verbatim translation: "Let's meet at... (time t₀)"
- Actual translation: "I will be there at some time $t \in [t_0 + 30m, +\infty)$ "

Cheers, Maurizio!



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