Source Terms

Matilde Tozzi

Seminar Course - Fundamentals of Wave Simulation - Solving Hyperbolic Systems of PDEs

January 2024

Table of contents

1. From Conservation Laws to Balance Laws

2. Godunov-Strang splitting
   - The Advection-Reaction Equation
   - The Unsplit Method
   - Godunov Splitting
   - General Formulation
   - Strang Splitting
   - Accuracy

3. Implicit Methods and Choice of ODE Solver

4. Stiff and Singular Source Terms and the Associated Numerical Difficulties

From Conservation Laws to Balance Laws

Our reference equation is

$$q_t + f(q)_x = \psi(q) \tag{1}$$

where

- the homogeneous equation $q_t + f(q)_x = 0$ is **hyperbolic**
- $\psi(q)$ (the **source terms**) don't depend on derivatives of q
  - $\Rightarrow q_t = \psi(q)$ is an independent system of ODEs

The Advection-Reaction Equation

A standard example that will be used to illustrate the following numerical methods is the **advection-reaction equation**

$$q_t + \bar{u} q_x = -\beta q. \tag{2}$$

It can be seen as the model for the transport along a flow of a radioactive substance, where

- β is the **decay rate**
- $\bar{u}$ is the (constant) **transport speed**
- $q(x, 0) = \mathring{q}(x)$ is the **initial condition**.

The Advection-Reaction Equation

A standard example that will be used to illustrate the following numerical methods is the **advection-reaction equation**

$$q_t + \bar{u} q_x = -\beta q. \tag{2}$$

It can be seen as the model for the transport along a flow of a radioactive substance, where

- β is the **decay rate**
- $\bar{u}$ is the (constant) **transport speed**
- $q(x, 0) = \mathring{q}(x)$ is the **initial condition**.

Exact solution

Along the characteristic $\frac{dx}{dt} = \bar{u}$ we have $\frac{dq}{dt} = -\beta q$ and it follows that

$$q(x, t) = e^{-\beta t} \mathring{q}(x - \bar{u} t). \tag{3}$$

The Advection-Reaction Equation: Plot

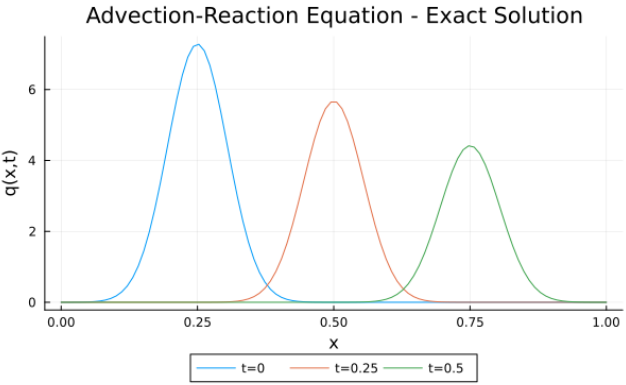

Figure: Evolution of the exact solution of the advection-reaction equation with $\bar{u} = 1$, $\beta = 1$, and $\mathring{q} = \text{Gaussian}(0.25, 0.003)$.

The Unsplit Method

Dor this specific example we can easily compute an **unsplit method**

$$
\begin{aligned}
q_t &= -\bar{u} q_x - \beta q \\
\frac{Q_i^{n+1} - Q_i^n}{\Delta t} &= -\bar{u} \frac{Q_i^n - Q_{i-1}^n}{\Delta x} - \beta Q_i^n \\
Q_i^{n+1} &= Q_i^n - \bar{u} \frac{\Delta t}{\Delta x} (Q_i^n - Q_{i-1}^n) - \Delta t \beta Q_i^n
\end{aligned}
$$

which is first-order accurate and stable for $0 < \bar{u} \frac{\Delta t}{\Delta x} \leq 1$.

Taylor Expansion of the Exact Solution

Note

The full Taylor expansion of (2) can be written formally as

$$e^{-\Delta t(\bar{u}\partial_x+\beta)}q(x,t) := q(x,t+\Delta t) = \\ = \sum_{j=0}^{\infty} \frac{(\Delta t)^j}{j!} \partial_t^j q(x,t) = \sum_{j=0}^{\infty} \frac{(\Delta t)^j}{j!} (-\bar{u}\partial_x - \beta)^j q(x,t). \tag{4}$$

The operator $e^{-\Delta t(\bar{u}\partial_x+\beta)}$ is called **solution operator** for the equation (2) over a time step of length Δt.

Godunov Splitting

In the case of the advection equation, we can split it into two subproblems:

$$\text{Problem A: } q_t + \bar{u} q_x = 0, \tag{5}$$

$$\text{Problem B: } q_t = -\beta q. \tag{6}$$

The idea is to solve the two problems in an alternating manner, using standard solving stategies, e.g.:

$$\text{A-step: } Q_i^* = Q_i^n - \frac{\bar{u}\Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n), \tag{7}$$

$$\text{B-step: } Q_i^{n+1} = Q_i^* - \beta \Delta t Q_i^*. \tag{8}$$

Unsplit Method vs Godunov Splitting

One may think that given that both Q_i^* and Q_i^{n+1} are calculated using Δt, the solution is valid for time $2\Delta t$, but it is not really the case: in fact if we combine the two stages and eliminate Q_i^*, we obtain

$$Q_i^{n+1} = Q_i^n - \frac{\bar{u}\Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) - \beta\Delta t Q_i^n + \frac{\bar{u}\beta\Delta t^2}{\Delta x}(Q_i^n - Q_{i-1}^n),$$

which differs from the unsplit method for the last term:

$$Q_i^{n+1} = Q_i^n - \bar{u}\frac{\Delta t}{\Delta x}(Q_i^n - Q_{i-1}^n) - \Delta t\beta Q_i^n$$

Commuting vs Non-commuting operators

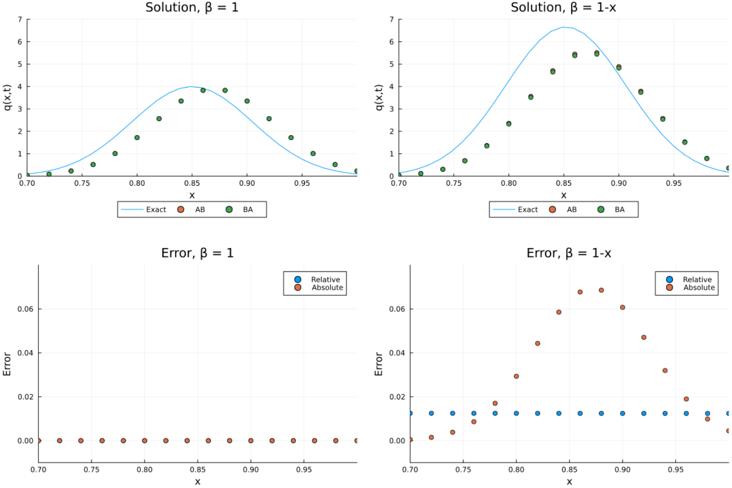

Figure: Comparison between the exact solution of the advection-reaction equation and the split method with the two different orders of steps. The problem has $\bar{u} = 1$, $\mathring{q} = \text{Gaussian}(0.25, 0.003)$, $\Delta x = \Delta t = 0.02$, $t = 0.6$.

General Formulation

Consider the more general formulation

$$q_t = (\mathcal{A} + \mathcal{B})q \tag{9}$$

where $\mathcal{A}$ and $\mathcal{B}$ can be differential operators. We assume that they don't explicitly depend on t, so that we can write

$$q_{tt} = (\mathcal{A} + \mathcal{B})q_t = (\mathcal{A} + \mathcal{B})^2 q \tag{10}$$

If we Taylor expand the solution at time t and use the notation defined in (4), we easily get to

$$q(x, \Delta t) = \sum_{j=0}^{\infty} \frac{\Delta t^j}{j!} (\mathcal{A} + \mathcal{B})^j q(x, 0) = e^{\Delta t(\mathcal{A}+\mathcal{B})} q(x, 0). \tag{11}$$

General Formulation II

With **Godunov splitting**, we obtain

$$q^*(x, \Delta t) = e^{\Delta t \mathcal{A}} q(x, 0) \tag{12}$$

and

$$q^{**}(x, \Delta t) = e^{\Delta t \mathcal{B}} q^*(x, \Delta t) = e^{\Delta t \mathcal{B}} e^{\Delta t \mathcal{A}} q(x, 0). \tag{13}$$

The splitting error is then

$$q(x, \Delta t) - q^{**}(x, \Delta t) = (e^{\Delta t(\mathcal{A}+\mathcal{B})} - e^{\Delta t \mathcal{B}} e^{\Delta t \mathcal{A}}) q(x, 0). \tag{14}$$

If we Taylor expand q^{**}, we obtain

$$q^{**}(x, \Delta t) = (I + \Delta t(\mathcal{A}+\mathcal{B}) + \frac{1}{2}\Delta t^2(\mathcal{A}^2 + 2\mathcal{B}\mathcal{A} + \mathcal{B}^2) + \dots) q(x, 0). \tag{15}$$

Strang Splitting

With the **Strang splitting** we are approximating $e^{\Delta t(\mathcal{A}+\mathcal{B})}$ by $e^{\frac{1}{2}\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}e^{\frac{1}{2}\Delta t\mathcal{A}}$. The Taylor expansion shows in fact that

$$e^{\frac{1}{2}\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}e^{\frac{1}{2}\Delta t\mathcal{A}} = I+\Delta t(\mathcal{A}+\mathcal{B})+\frac{1}{2}\Delta t^2(\mathcal{A}^2+\mathcal{A}\mathcal{B}+\mathcal{B}\mathcal{A}+\mathcal{B}^2)+\mathcal{O}(\Delta t^3). \tag{16}$$

After n time steps we obtain

$$Q^n = \underbrace{(e^{\frac{1}{2}\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}e^{\frac{1}{2}\Delta t\mathcal{A}})(e^{\frac{1}{2}\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}e^{\frac{1}{2}\Delta t\mathcal{A}})\dots(e^{\frac{1}{2}\Delta t\mathcal{A}}e^{\Delta t\mathcal{B}}e^{\frac{1}{2}\Delta t\mathcal{A}})}_{n \text{ times}}Q^0. \tag{17}$$

Strang Splitting II

Another way of obtaining the same result is

$$\begin{aligned} Q^1 &= e^{\Delta t \mathcal{A}} e^{\Delta t \mathcal{B}} Q^0 \\ Q^2 &= e^{\Delta t \mathcal{B}} e^{\Delta t \mathcal{A}} Q^1 \\ &\vdots \end{aligned} \tag{18}$$

It is essentially the same, but with Δt instead of $\frac{1}{2}\Delta t$.

- **Pros**: computationally cheaper (fewer function evaluations)
- **Cons**: difficult to implement with variable time steps, needs an even number of iterations

Implicit Methods and Choice of ODE Solver

If the ODE $q_t = \psi(q)$ is **stiff** (i.e. such that an extremely small time step is required to solve it with an explicit numerical method), then an **implicit** method is needed. The usual choice is the **trapezoidal rule**:

$$Q_i^{n+1} = Q_i^* + \frac{\Delta t}{2}[\psi(Q_i^*) + \psi(Q_i^{n+1})]. \tag{19}$$

Another nice property of the split methods is that they only require the ODE part to be solved implicitly: the hyperbolic part can still be solved with explicit methods.

Stiff and Singular Source Terms

If the source term is concentrated in space, it is called **stiff** in analogy with the the ODEs.
We say that the solution is evolving on a **slow manifold** in state space and perturbing the solution causes it to produce a rapid response. A very simple example is

$$u'(t) = -\frac{u(t)}{\tau} \tag{20}$$

where $u \equiv 0$ is the slow manifold.

Numerical Difficulties

The trapezoidal rule seems to work fine for ODEs, but fails for hyperbolic equations with stiff source terms. If we consider (20), the trapezoidal methods yields

$$U^{n+1} = \left(\frac{1 - \frac{1}{2}\frac{\Delta t}{\tau}}{1 + \frac{1}{2}\frac{\Delta t}{\tau}} \right) U^*. \tag{21}$$

On the slow manifold ($U^* = 0$), then $U^{n+1} = 0$ and we remain in the slow manifold. In any other case, if $-\frac{\Delta t}{\tau} \to -\infty$, then $U^{n+1} = -U^*$ and this means that the coefficient in (21) makes the solution oscillate.

Numerical Difficulties II

This is due to the fact that the trapezoidal rule is an **A-stable** method: the stability region is the left half plane, but the problem requires an **L-stable** method, where the stability function approaches zero as the step size goes to infinity.

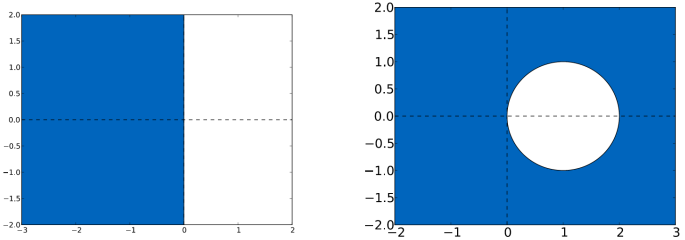

Figure: Stability region of the trapezoidal rule (left) and implicit Euler (right)

Backward Differentiation Formulas

The **BDF** (Backward Differentiation Formulas) methods have this characteristic and the simplest one is the backward Euler method. In fact for (20)

$$U^{n+1} = U^* - \frac{\Delta t}{\tau} U^{n+1} \Rightarrow U^{n+1} = \left(\frac{1}{1 + \frac{\Delta t}{\tau}} \right) U^*. \tag{22}$$

This time the coefficient approaches zero for $\frac{\Delta t}{\tau} \to \infty$. However, the implicit Euler method is only first-order accurate.

Bibliography

[1] R. J. LeVeque, *Finite Volume Methods for Hyperbolic Problems*. Cambridge: Cambridge University Press, 2002.

[2] https://github.com/matilde-t/SeminarCourse-FundamentalsOfWaveSimulation

[3] https://github.com/clawpack/apps/tree/master/fvmbook/chap17

[4] https://github.com/clawpack/riemann_book

[5] B. L. Byron, *On Padé approximations to the exponential function and A-stable methods for the numerical solution of initial value problems.* Waterloo, Ontario: University of Waterloo, 1969.

[6] https://commons.wikimedia.org/wiki/File:Stability_region_for_trapezoidal_method.svg

[7] https://commons.wikimedia.org/wiki/File:Stability_region_for_BDF1.svg