Residual equilibrium schemes for some nonlinear PDEs

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Numerical Methods for Hyperbolic Systems with source terms and applications
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Motivations

Several applications involve PDEs which admit nontrivial stationary solutions, like *convection-diffusion equations*

$$\partial_t U = \nabla_x \cdot (A(U) + \nabla_x N(U)),$$

hyperbolic balance laws

$$\partial_t U + \nabla_x \cdot F(U) = R(U),$$

or *kinetic equations*

$$\partial_t f + v \cdot \nabla_x f = Q(f).$$

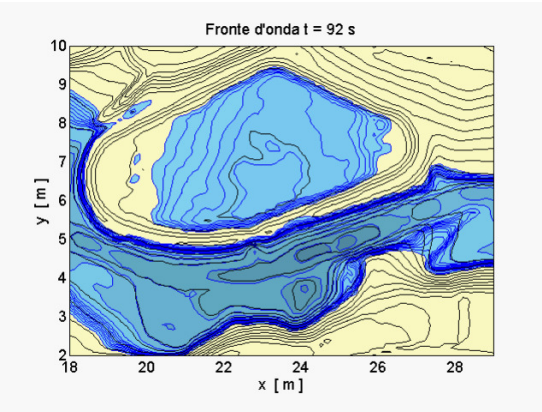
- In many situations, such systems of equations stabilize onto a large-time behavior which is characterized by an accurate balancing between the different terms appearing in the PDE.

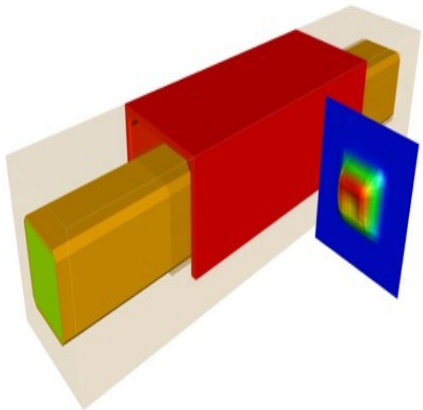
Some examples

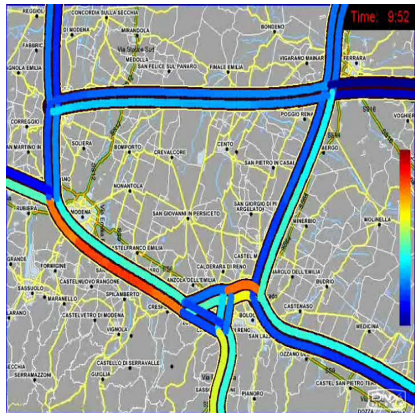
- Shallow water equations
- Porous media
- Hydrodynamic models for semiconductors
- Traffic flow models

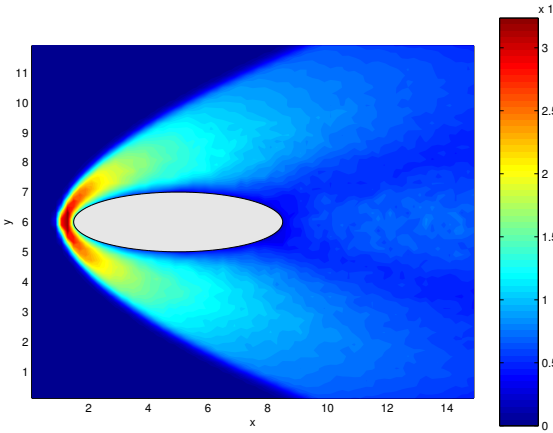
  ⋮

- Kinetic equations (Fokker-Planck, Boltzmann-like)
- Convection-diffusion equations (biology, economy, sociology, . . .)









Steady state preserving methods

- The construction of numerical schemes which preserves such stationary solutions is challenging and depends strongly on the particular problem studied.
- For kinetic equations, one often is interested in schemes which preserve the steady state solution of the collision operator (Gaussian profiles, power laws, etc...). This is related to the velocity discretization and typically is tackled with the aim of *conservative and entropic approximation* [1].
- For balance laws, there is a large literature on the so called *well-balanced schemes* [2], namely schemes which capture the balance between the transport terms and the other ones. This, in general, is related to the construction of suitable numerical fluxes in space.

[1] P.Degond, L.Pareschi, G.Russo, Mod. Sim. Sci. Eng. Tech., Birkhüser '04
G.Dimarco, L.Pareschi, Acta Numerica, '14
[2] F.Bouchut, Frontiers in Mathematics, Birhüser '04
L.Gosse, SEMA SIMAI Springer Series '13

Outline

1. Preliminaries
   - Motivations
2. Residual equilibrium schemes
   - Fokker-Planck equations
   - General formulation
   - Nonlinear parabolic problems
   - Nonlinear Boltzmann equations
   - Shallow water equations
3. Local residual equilibrium schemes
   - Residual equilibrium schemes with limiters
   - Shallow water equations
4. Final considerations

Fokker-Planck equations

As a prototype example we consider the one-dimensional Fokker-Planck equation

Fokker-Planck equation

$$\frac{\partial f}{\partial t} = L(f), \qquad L(f) = \frac{\partial}{\partial v}\left[vf + T\frac{\partial f}{\partial v}\right], \quad v \in \mathbb{R}.$$

- Equilibrium solution are characterized by Gaussian distributions

$$M = \frac{\rho}{\sqrt{2\pi T}} \exp\left(\frac{-v^2}{2T}\right),$$

  where $\rho = \int_{\mathbb{R}} f\, dv$.
- The construction of schemes which preserves the equilibrium states is non trivial, the most famous example is given by the *Chang-Cooper method* [3]
- Extensions of the Chang-Cooper idea to high order and to more general nonlinear Fokker-Planck equations are very difficult [4]

[3] J.S. Chang, G. Cooper, JCP '70

[4] C.Buet, S.Cordier, P.Degond, S.Dellacherie, M.Lemou, L.Mieussens, K-C.Le Thanh ('98-'07)

Micro-macro decomposition

Let us consider a change of variables thanks to the *micro-macro decomposition*

$$g = f - M,$$

with M the Maxwellian equilibrium and g such that $\int_{\mathbb{R}^3} g\,\phi\,dv = 0$, $\phi = 1, v, |v|^2$. Since $L(M) = 0$ we have

$$L(f) = L(g) + L(M) = L(g),$$

and therefore, being M time independent, we obtain the equivalent formulation

$$\frac{\partial g}{\partial t} = L(g).$$

Now the only admissible equilibrium state is $g \equiv 0$.

- The construction of numerical approximations of L, say L_h for a discretization parameter h, such that $L_h(0) = 0$ is straightforward even with high order of accuracy.
- Discretizing $L(f)$ and $L(g)$ at the numerical level is not equivalent.

A semi-discrete scheme

Let us now consider a semi-discrete scheme applied to the original Fokker-Planck problem

$$\frac{\partial f_h}{\partial t} = L_h(f_h).$$

In general, this scheme does not preserve the steady state since $L_h(M_h) \neq 0$, where M_h is our target discrete equilibrium state.
We can rewrite

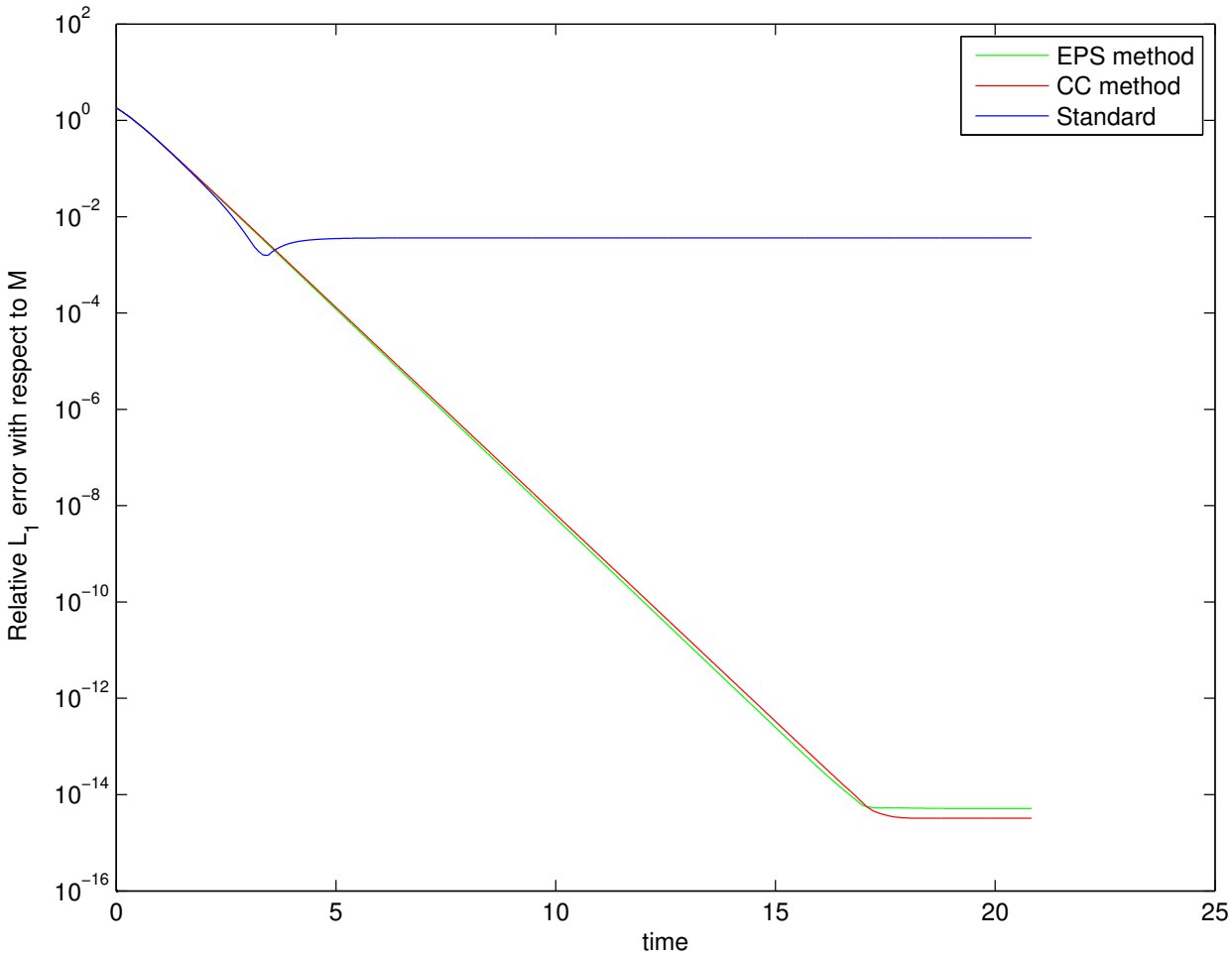
$$L_h(f_h) = \underbrace{L_h(g_h)}_{\text{equilibrium preserving}} + \underbrace{L_h(M_h)}_{\text{residual equilibrium}} .$$

Therefore, in the original variables, the equilibrium preserving semi-discrete scheme can be re-written as

$$\frac{\partial f_h}{\partial t} = L_h(f_h) - L_h(M_h) =: \tilde{L}_h(f_h),$$

which clearly preserves $f_h = M_h$ as equilibrium state.

Example of second order schemes



Plot of $\|f - M\|_1 / \|M\|_1$ for standard central difference (blue), Chang-Cooper (red) and residual equilibrium (green) with $N = 50$ grid points in $[-5, 5]$

General formulation

Suppose we have a differential problem of the form

$$u' = G(u),$$

where $G(u) = 0$ implies $u(t) = u^{eq}(t)$, with $u^{eq}(t)$ is a given equilibrium state. Let G_h be an order q approximation of $G(u)$, hereafter called the *underlying method*, which originates the approximated problem

$$u_h' = G_h(u_h).$$

Given the discrete equilibrium state $u_h^{eq}(t)$ we define the *residual equilibrium* as

$$r_h(t) = G_h(u_h^{eq}(t)),$$

note that $r_h(t) = O(h^q)$ and define the new order q approximation

$$\widetilde{G}_h(u) := G_h(u) - r_h(t).$$

The *residual equilibrium approximation* is then given by[5]

$$u_h' = \widetilde{G}_h(u_h).$$

[5] L.Pareschi, T.Rey, preprint '15

Nonlinear parabolic problems

Let us now consider a general problem of the form

Nonlinear parabolic equation

$$\frac{\partial u}{\partial t} = \nabla_x \cdot (A(x,u) + \nabla_x N(u)), \qquad x \in \Omega \subseteq \mathbb{R}^d.$$

- Coefficients: $A(x,u) = xu(1 \pm u), \quad N(u) = u.$
  Equilibrium solution: (*Fermi-Dirac*):

$$u^{eq}(x) = \frac{1}{\beta e^{x^2/2\sigma} \pm 1}.$$

- Coefficients: $A(x,u) = xu \quad N(u) = |u|^m.$
  Equilibrium solution: (*Barrenblatt-Pattle*)

$$u^{eq}(x) = \left(C - \frac{m-1}{2m}|x|^2\right)_+^{1/(m-1)}.$$

2D porous media

- We apply the residual equilibrium method using as underlying scheme the finite volume upwind approach by Chainais and Peng [6].
- We choose $d = 2$, $m = 5$, $\Omega = [-10, 10] \times [-10, 10]$.
- Initial condition. Sum of Gaussians:

$$u(x) = \begin{cases} e^{\frac{-1}{6-|x-c_0|}} & |x - c_0| < 6, \\ e^{\frac{-1}{6-|x-c_1|}} & |x - c_1| < 6 \end{cases}$$

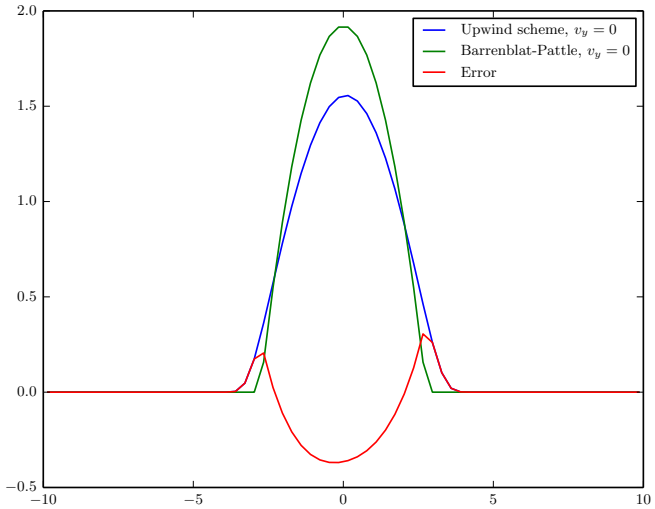
  with $c_0 = (2, -2)$ and $c_1 = (-2, 2)$.
- Related approaches: Bessemoulin-Chatard, M., and Filbet, F. SISC '12, Carrillo, J. a., Chertock, A., and Huang, Y. preprint '14, Cancés, C., and Guichard, C. Math. Comp. '15.

[6] C.Chainais, Y. Peng, M3AS '04

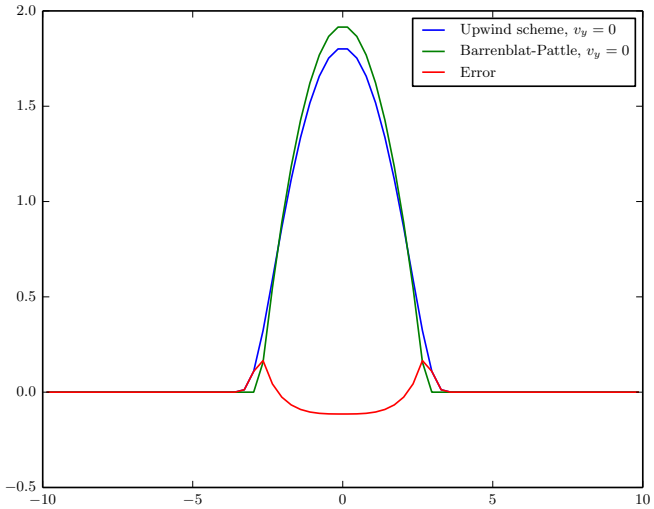
Test case

Standard vs Residual Equilibrium

Standard

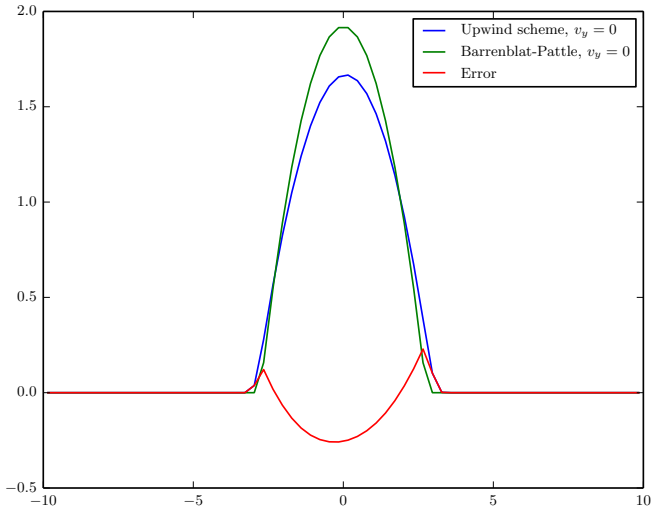


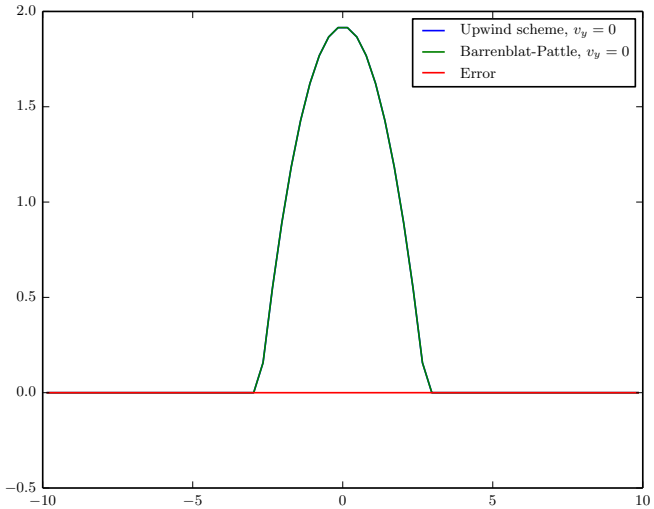
$t = 0.1$



$t = 0.5$

Res. Eq.





The Boltzmann case

The residual equilibrium method applies also to Boltzmann equations

Homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = Q(f, f).$$

The operator $Q(f, f)$ characterizes the particles interactions and reads

$$Q(f, f) = \int_{\mathbb{R}^3 \times S^2} B(|v - v_*|, n)[f(v')f(v'_*) - f(v)f(v_*)]\, dv_*\, dn$$

where

$$v' = v + \frac{1}{2}(v - v_*) + \frac{1}{2}|v - v_*|n, \quad v'_* = v + \frac{1}{2}(v - v_*) - \frac{1}{2}|v - v_*|n,$$

and $B(|v - v_*|, n)$ is a nonnegative collision kernel.

- The equilibrium states are again described by Gaussian distributions M.

Residual equilibrium and micro-macro

Given a discretized operator Q_h we get the *residual equilibrium approximation*

$$\frac{\partial f_h}{\partial t} = \tilde{Q}_h(f_h, f_h),$$

with

$$\tilde{Q}_h(f_h, f_h) = Q_h(f_h, f_h) - r_h$$

and $r_h = Q_h(M_h, M_h)$.
Even in this case the approach can be related to the *micro-macro decomposition* $g = f - M$, which at the semi-discrete level gives

$$\frac{\partial g_h}{\partial t} = \mathcal{L}_h(M_h, g_h) + Q_h(g_h, g_h),$$

where $\mathcal{L}_h(M_h, g_h) = Q_h(g_h, M_h) + Q_h(M_h, g_h)$ and which has $g_h \equiv 0$ as equilibrium state.

Residual equilibrium spectral methods

Using Fourier-Galerkin spectral method [7] as underlying method we derive

Residual equilibrium spectral method

$$\frac{\partial g_N}{\partial t} = \mathcal{L}_N(M_N, g_N) + Q_N(g_N, g_N),$$
$$f_N = M_N + g_N,$$

where

$$M_N := \mathcal{P}_N M, \quad g_N := \mathcal{P}_N g, \quad \mathcal{L}_N(M_N, g_N) := \mathcal{P}_N \mathcal{L}(M_N, g_N),$$

and $\mathcal{P}_N$ is the orthogonal projection in the inner L^2-product on the space of trigonometric polynomials of degree N.

- It is immediate to see that $g_N \equiv 0$ is an admissible local equilibrium of the spectral scheme and therefore $f_N = M_N$ is a local equilibrium state.

[7] L. Pareschi, G. Russo, SINUM '00 - C. Mouhot, L. Pareschi, Math. Comp. '05

Spectral accuracy

It can be proved that $Q_N(M_N, M_N)$ is spectrally close to 0 since we have [8]

Lemma

$$||Q_N(M_N, M_N)||_2 \leq \frac{C}{N^{r-2}} \left(||M||_{H^r_p} + ||Q(M_N, M_N)||_{H^r_p} \right), \quad \forall\, r \geq 2.$$

From this we obtain consistency and spectral accuracy

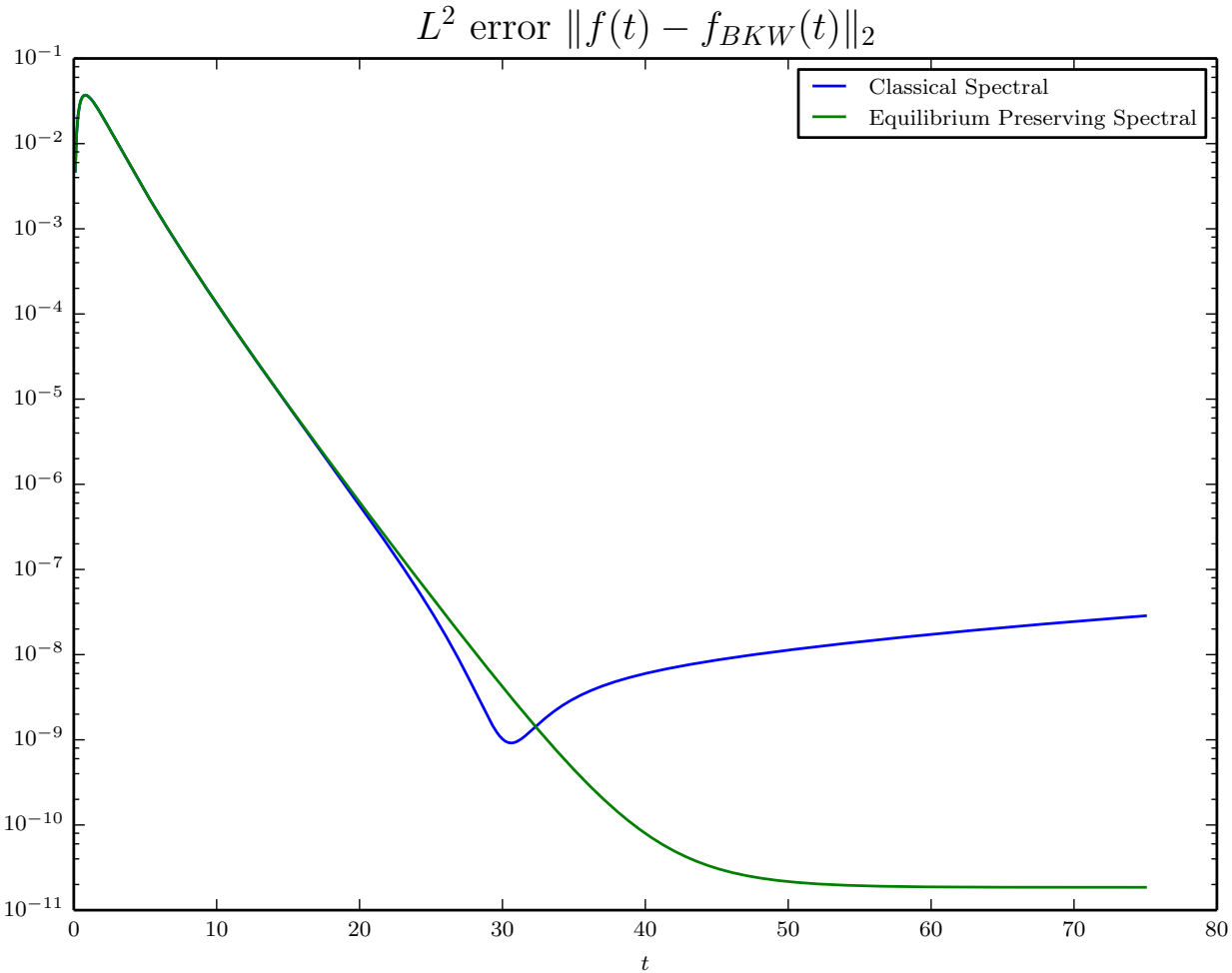
Theorem

Let $f \in H^r_p([-\pi, \pi]^3)$, $r \geq 0$ *then*

$$||Q(f,f) - \mathcal{L}_N(M_N, g_N) - Q_N(g_N, g_N)||_2 \leq \frac{C}{N^r} \left(||f||_{H^r_p} + ||Q(f_N, f_N)||_{H^r_p} + ||M||_{H^r_p} + ||Q(M_N, M_N)||_{H^r_p} \right).$$

[8] F.Filbet, T.Rey, L.P. CRAS '14

A numerical example: BKW solution



Long time behavior of the L_1-error for the BKW solution [9] (Maxwell molecules in dimension $d = 2$) with $N_v = 64$ and $v \in [-8, 8]$.

[9] A.V.Bobylev, Dokl. Akad. Nauk. SSSR '75

Shallow water

The residual equilibrium approach can be applied also to some systems of balance laws like the one-dimensional shallow water equations

Shallow water

$$\begin{cases} \partial_t h + \partial_x (hu) = 0, \\ \partial_t (hu) + \partial_x \left(hu^2 + \frac{1}{2} g h^2 \right) = -gh\, \partial_x B, \end{cases}$$

where $g > 0$ is the gravitational constant and $B \geq 0$ is the bottom profile.
The steady state solutions are characterized by the equations

$$hu = C_1, \qquad \frac{1}{2} u^2 + g(h + B) = C_2,$$

where C_1 and C_2 are constants determined by the boundary conditions.

A numerical example

We used Lax-Friedrichs with Van Leer's flux limiters as underlying method and consider a *perturbation of the steady state* as test case[10].

$\Omega = [0, 1]$, no flux at the boundaries

Bottom topography:

$$B(x) = \begin{cases} 0.25\left(\cos(\pi(x - 0.5)/0.1 + 1\right), & |x - 0.5| < 0.1 \\ 0 & \text{otherwise} \end{cases}$$

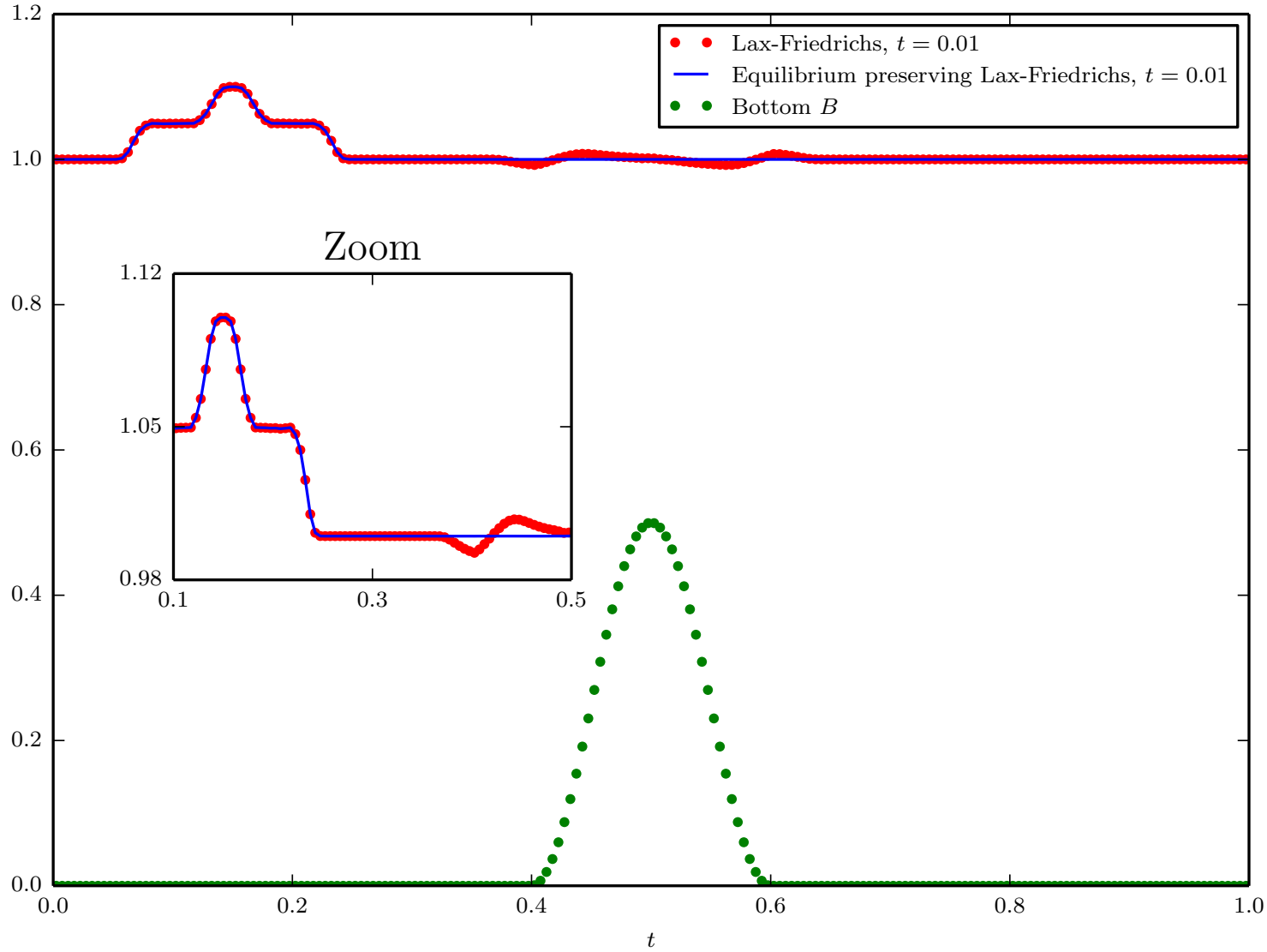
Initial condition:

$$(h(x), u(x)) = (1 + \varepsilon(x) - B(x), 0)\,,$$

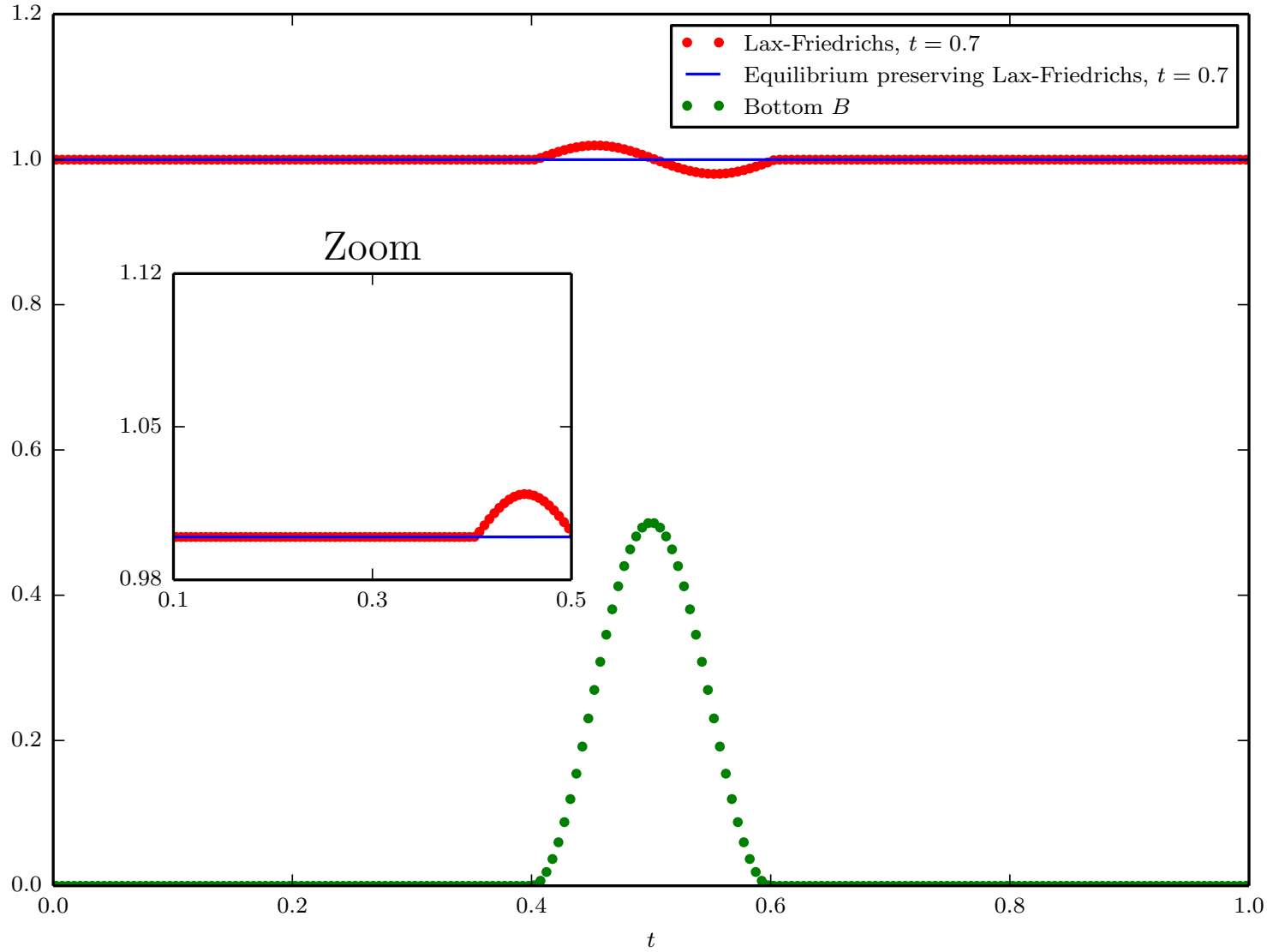
with $\varepsilon(x) = 0.1$ if $0.1 < x < 0.2$ and 0 elsewhere.

Equilibrium : $(h^{eq}(x), u^{eq}(x)) = (1, 0)$.

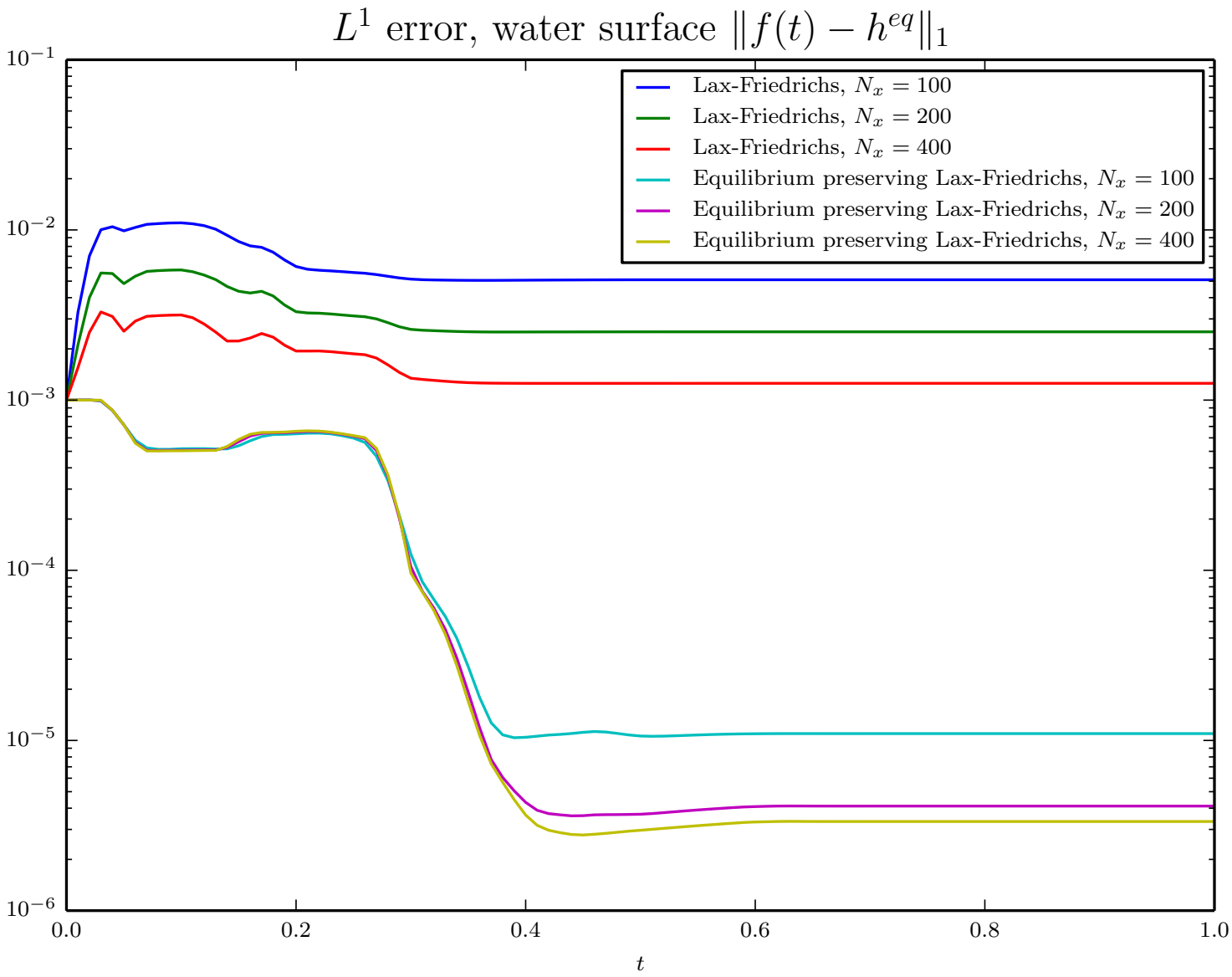
[10] R.J. LeVeque, JCP '98



Evolution of the water height at time $t = 0.01$ for the standard (red circles) and the residual equilibrium (blue line) Lax-Friedrichs method.



Evolution of the water height at time $t = 0.7$ for the standard (red circles) and the residual equilibrium (blue line) Lax-Friedrichs method.



Time evolution of the L^1 error with respect to the equilibrium.

Local residual equilibrium schemes

Let us consider a semi-discrete scheme of the general form

$$\frac{\partial u_i}{\partial t} + \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x} = 0$$

where $F_{i\pm1/2}$ are the edge fluxes for the i-th cell and

$$u_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t)\, dx,$$

is the cell average of the solution.
Let us denote with $F^{std}_{i\pm1/2}$ the *standard fluxes*. If we denote by u^{eq}_i the cell average of the equilibrium state we can define the *equilibrium preserving fluxes* as $F^{wb}_{i\pm1/2}$ as

$$F^{wb}_{i\pm1/2} = F^{std}_{i\pm1/2} - F^{eq}_{i\pm1/2},$$

where $F^{eq}_{i\pm1/2}$ is defined as $F^{std}_{i\pm1/2}$ by replacing u_i with u^{eq}_i.

- This flux is equilibrium preserving, however it may loose some good properties of the original flux. These properties, of course, are recovered asymptotically since the flux preserves the exact steady state solution.

A flux-limiter approach

The idea is to switch between the two fluxes using a flux-limiter based on an equilibrium indicator. We use the standard flux where the solution is far from equilibrium and the well-balanced flux where the solution is close to equilibrium. The resulting flux can be written as

$$F_{i\pm1/2} = F^{std}_{i\pm1/2} - \phi_{i\pm1/2}(F^{std}_{i\pm1/2} - F^{wb}_{i\pm1/2}) = F^{std}_{i\pm1/2} - \phi_{i\pm1/2}F^{eq}_{i\pm1/2},$$

where $\phi_{i\pm1/2} = \phi(r_{i\pm1/2}) \geq 0$ is the *flux limiter* and

$$r_{i\pm1/2} = \frac{u_{i\pm1/2} - u^{eq}_{i\pm1/2}}{u^{eq}_{i\pm1/2}} \quad \text{with} \quad u_{i\pm1/2} = \frac{u_{i\pm1} + u_i}{2}, \; u^{eq}_{i\pm1/2} = \frac{u^{eq}_{i\pm1} + u^{eq}_i}{2}$$

is the *equilibrium indicator*.

- Therefore, when the limiter is close to zero (far from equilibrium), the flux is represented by the standard scheme. Similarly, when the limiter is close to 1 (equilibrium solution), it is represented by the well balanced scheme.

Transcritical flow with shock

We consider again the high-resolution Lax-Friedrichs methods as underlying method and test the residual equilibrium method with limiter for a *transcritical flow*.

$\Omega = [0, 25]$, inflow $hu = 0.18$ on $x = 0$, outflow $h = 0.33$ on $x = 25$

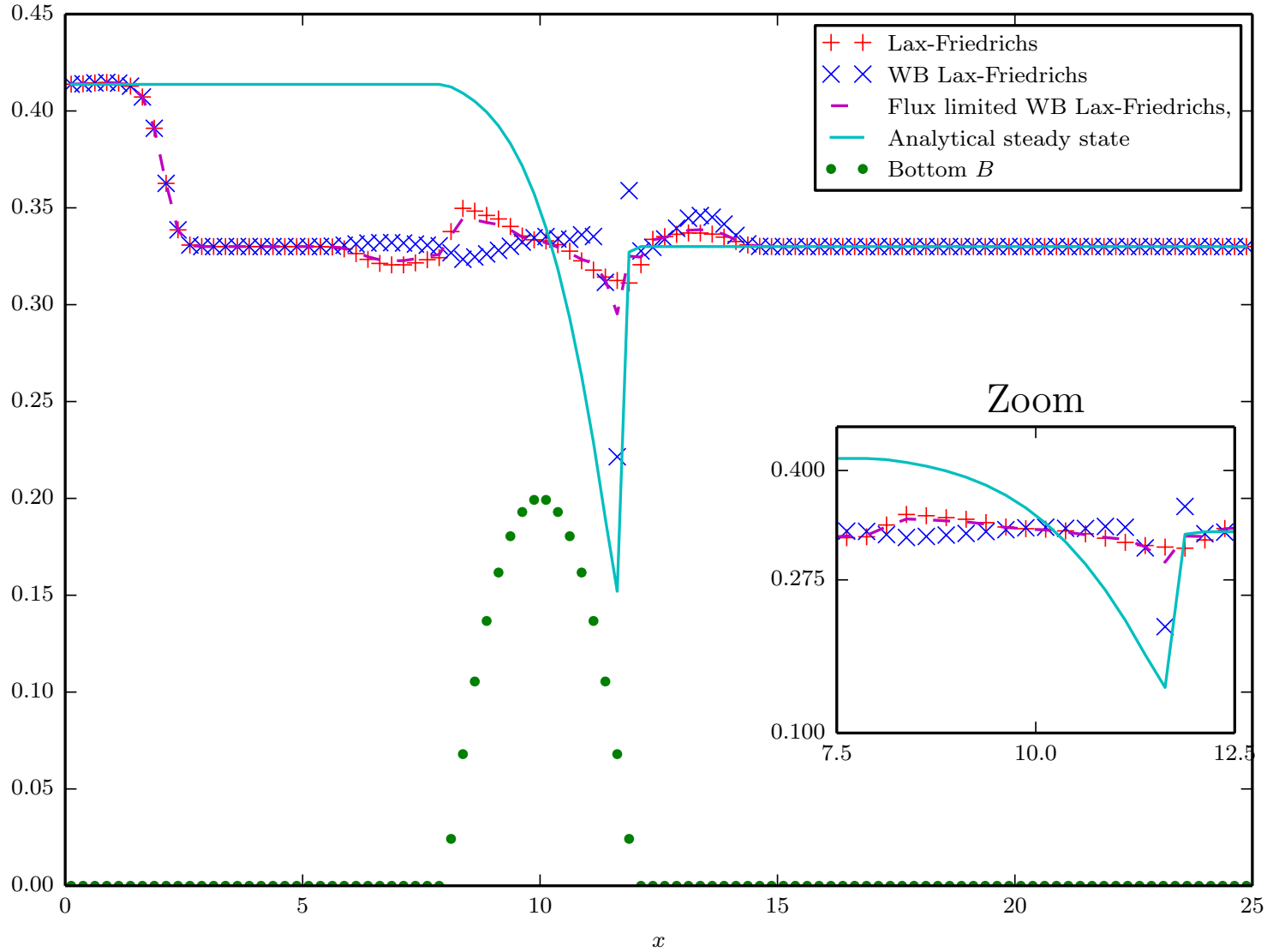
Bottom topography:

$$B(x) = \begin{cases} \left(0.20.05(x10)^2\right), & |x - 10| < 2 \\ 0 & \text{otherwise} \end{cases}$$

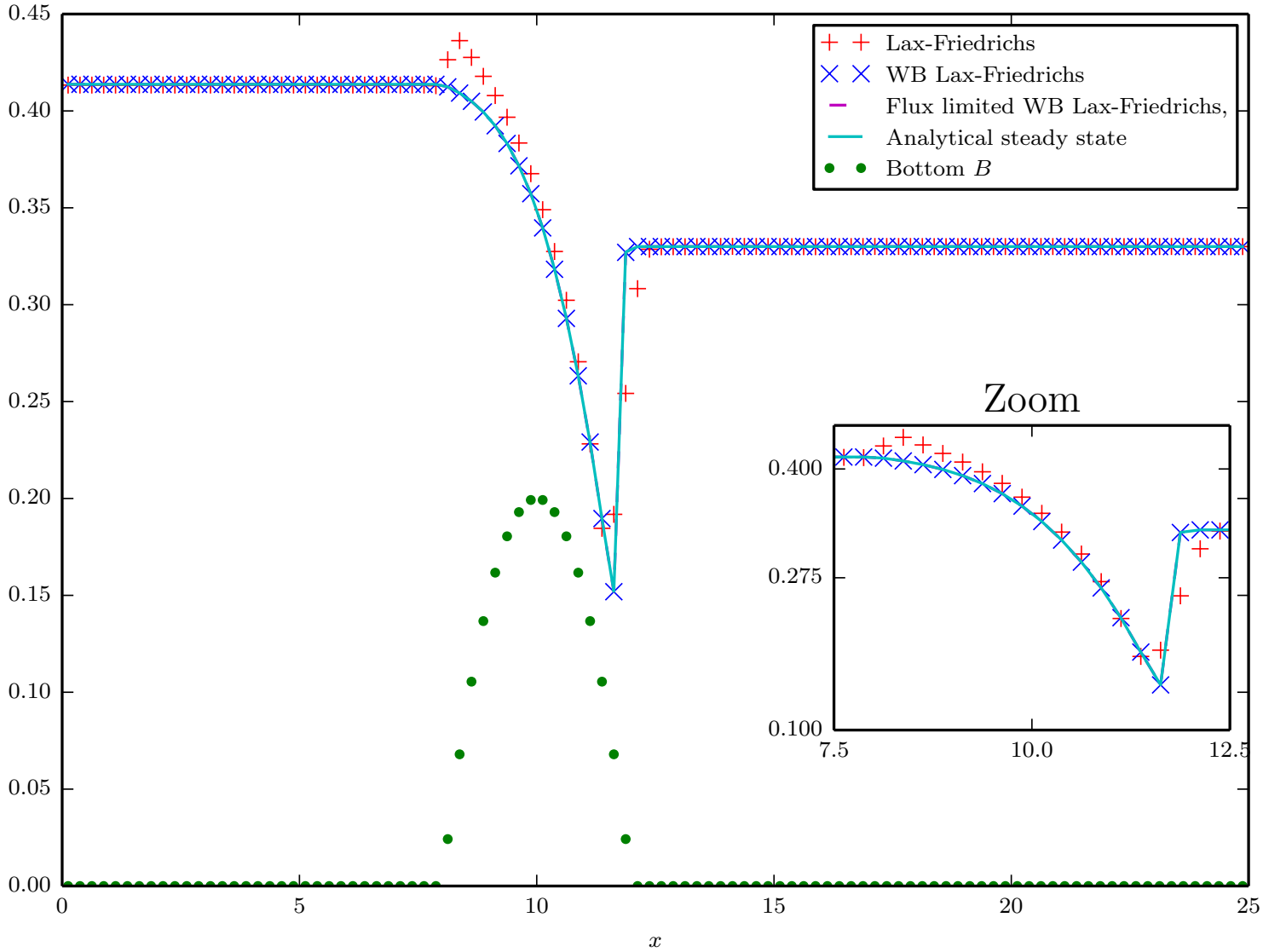
Initial condition:

$$(h(x), u(x)) = (0.33 - B(x), 0)\,.$$

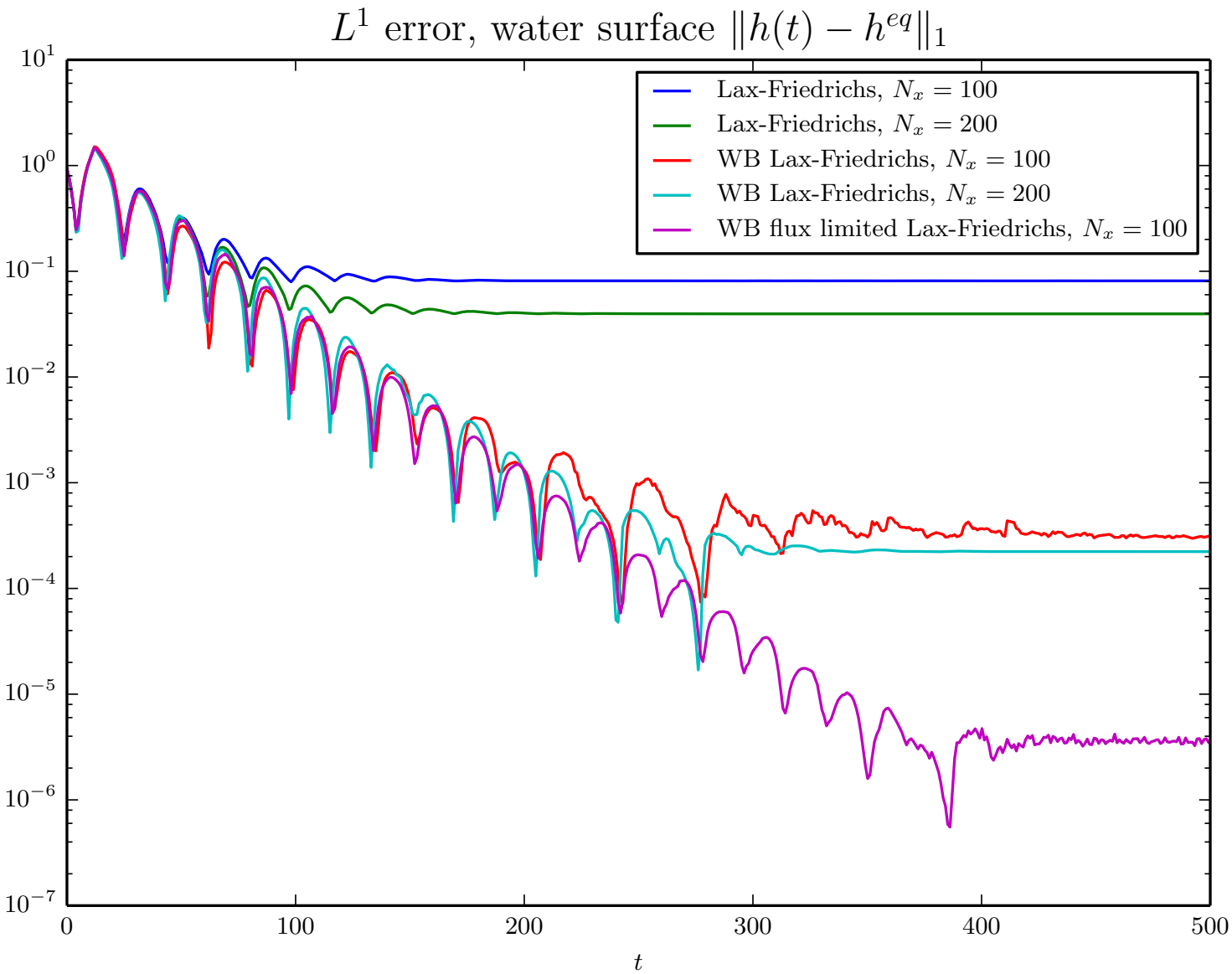
Equilibrium : $(h^{eq}(x), u^{eq}(x))$ solution of a nonlinear equation.



Evolution of the water height at time $t = 1$ for the standard (red plus), the residual equilibrium (blue cross) and flux-limited residual equilibrium (magenta dashed line)



Evolution of the water height at time $t = 500$ for the standard (red plus), the residual equilibrium (blue cross) and flux-limited residual equilibrium (magenta dashed line)



Time evolution of the L^1 error with respect to the equilibrium.

Final considerations

The *residual equilibrium method* represent a powerful tool for the construction of steady state preserving schemes.

- It applies to most PDEs where an explicit steady state can be computed either analytically or numerically.
- The order of accuracy depends on the underlying method.
- It is easy to embed the method in an existing scheme.
- The use of suitable flux-limiters permits to recover the properties of the underlying scheme (if needed).

Research directions :

- Stability for nonlinear problems, better characterization of the flux-limiter, ...
- Applications of the residual equilibrium schemes to other degenerate diffusion equations (capturing power laws seems challenging) and to other fields where well-balancing is relevant, like semiconductors, chemotaxis, etc.