Preserving exactly equilibrium solutions to obtain accurate off-equilibrium simulations

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with

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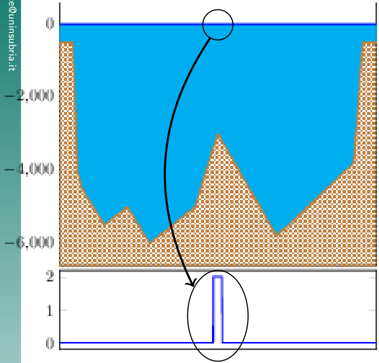
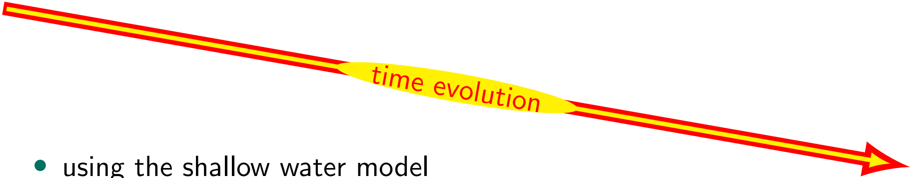
A tsunami wave across the Atlantic?





- using the shallow water model

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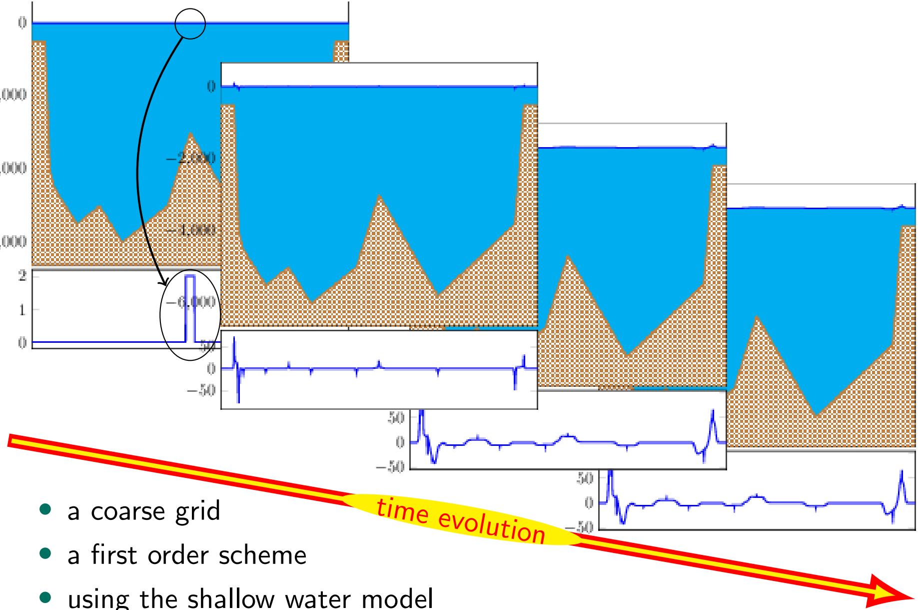

- a coarse grid
- a first order scheme
- using the shallow water model

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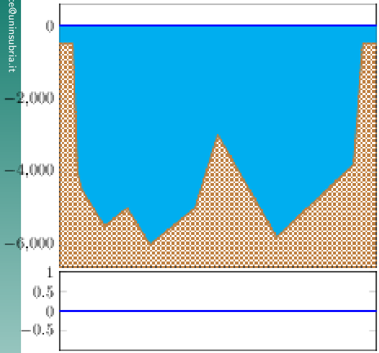
A quiet Atlantic ocean?



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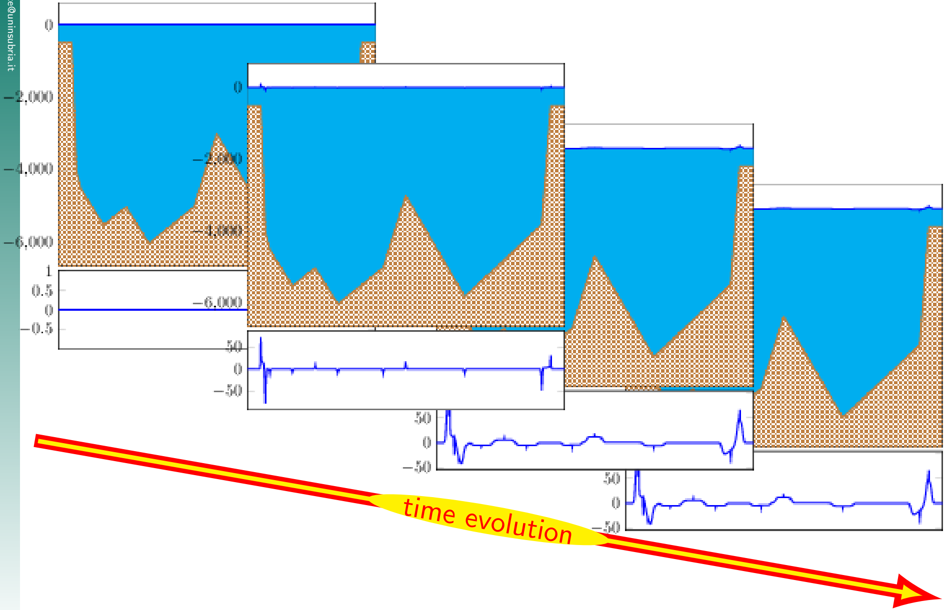

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Finite Volume Schemes for hyperbolic balance laws

$$\boxed{\frac{\partial u}{\partial t} + \nabla_x \cdot f(u) = s(u)} \qquad \text{(balance law)}$$

$$\overline{u}_j(t) := \frac{1}{|\Omega_j|}\int_{\Omega_j} u(t,x)\mathrm{d}x \qquad \text{(cell average)}$$

Average (balance law) on Ω_j, obtaining the semi-discrete formulation:

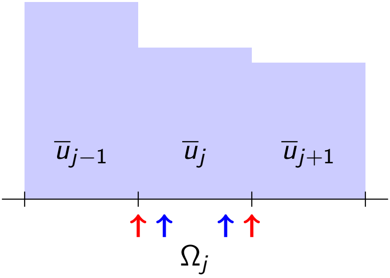
$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\overline{u}_j = -\frac{1}{|\Omega_j|}\int_{\partial\Omega_j} f(u(t,\gamma)) \cdot \vec{n}(\gamma)\mathrm{d}\gamma + \frac{1}{|\Omega_j|}\int_{\Omega_j} s(u(t,x))\mathrm{d}x} \qquad \text{(SD)}$$

Quadrature and reconstruction

Approximate the integrals with numerical quadratures

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{u}_j = \dots \sum_{\mathrm{e}_{jk}} \sum_{q=1}^{Q} w_q f(u(t,\gamma_q)) \cdot \vec{n}(\gamma_q) \dots \sum_{q=1}^{Q^2} \widetilde{w}_q s(u(t,x_q))$$

- Know the cell averages
- Need the point values



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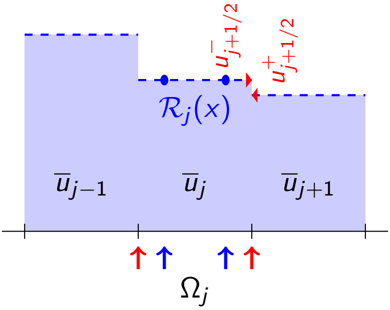
- Know the cell averages
- Need the point values
- Choose a reconstruction:

$$\mathcal{R}_j(x) \text{ s.t. } \int_{\Omega_j} \mathcal{R}_j(x)\mathrm{d}x = \overline{u}_j$$



- ... and use it to feed
  - ➔ the numerical quadrature for the source term
  - ➔ the numerical fluxes at interfaces $F_{j+1/2} = \mathcal{F}\left(u^-_{j+1/2}, u^+_{j+1/2}\right)$

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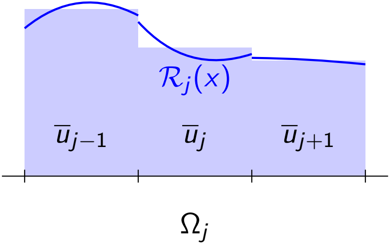
Higher order schemes

- Choose a reconstruction:

$$\mathcal{R}_j(x) \text{ s.t. } \int_{\Omega_j} \mathcal{R}_j(x)\mathrm{d}x = \overline{u}_j$$

- and such that, for $i = \pm 1, \pm 2, \ldots,$

$$\mathcal{R}_j(x) \text{ s.t. } \int_{\Omega_{j+i}} \mathcal{R}_j(x)\mathrm{d}x = \overline{u}_{j+i}$$



- in practice use "Essentially Non Oscillatory" reconstructions, which locally trade accuracy for non-oscillatory propeties (ENO, WENO, CWENO[1], ...).
  CWENO is particularly efficient when many reconstruction points per cell are required.

[1] Levy, Puppo, Russo (1998–2002); M.S., Puppo, Visconti, ... (2016–2021)

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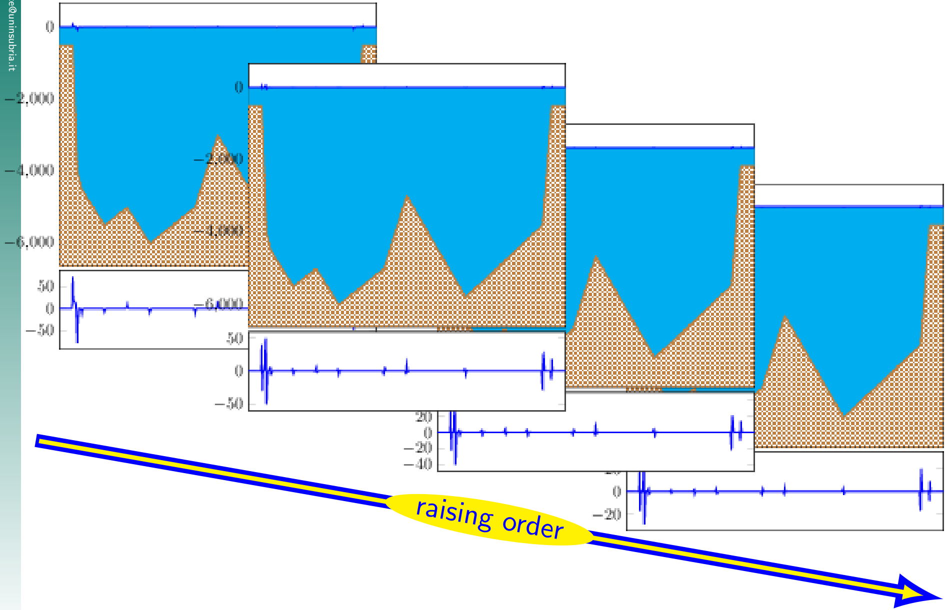
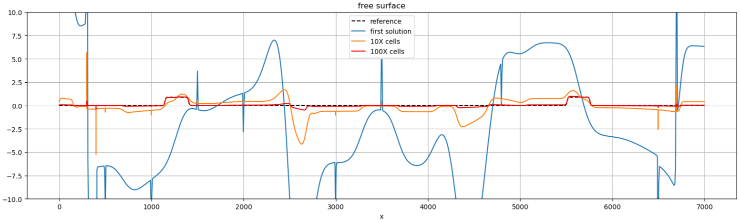
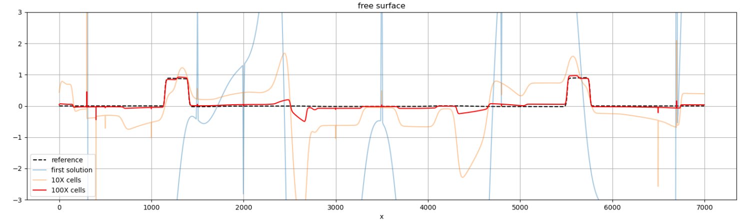
A tsunami across the Ocean (take 2)



Only grid refinement seems to help



but we cannot discretize the Atlantic with 1 meter cells!



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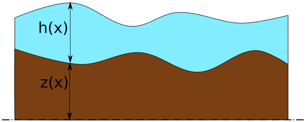
Steady states of the Shallow Water model

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



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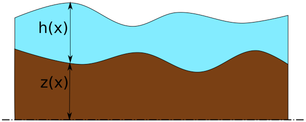

$\partial_t = 0$ $\Rightarrow$

$$\begin{cases} \partial_x q = 0 \\ \partial_x \left(q^2/h + \frac{1}{2} g h^2 \right) = -gh \partial_x Z \end{cases}$$

They are called "lake at rest" when $q = 0$:

$$q(t,x) = 0 \qquad \text{and} \qquad \partial_x \left(\tfrac{1}{2} g h^2 \right) = -gh \partial_x Z$$

i.e.

$$\Rightarrow h(x) + Z(x) = C$$

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Origin of numerical storms

Exact steady state:

$$\partial_x f(u) = s(u)$$

In the numerical scheme

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{u}_j = -\underbrace{\left[\mathcal{F}_{j+1/2}(\overline{u}_\bullet) - \mathcal{F}_{j-1/2}(\overline{u}_\bullet)\right]}_{\partial_x f(u)+\mathcal{O}(\Delta \mathrm{x}^p)} \quad + \quad \underbrace{\mathcal{S}_j(\overline{u}_\bullet)}_{s(u)+\mathcal{O}(\Delta \mathrm{x}^p)}$$

and in general

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\overline{u}_j\right|_{\substack{\text{lake}\\ \text{at}\\ \text{rest}}} = \mathcal{O}(\Delta \mathrm{x}^p) - \mathcal{O}(\Delta \mathrm{x}^p) \neq 0$$

Well balanced schemes

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{u}_j = \mathcal{H}_j(\overline{u}_\bullet)$$

- A scheme is called well balanced if

$$\mathcal{H}_j(\overline{u}_\bullet)\Big|_{\substack{\text{steady}\\\text{state}}} = 0$$

so that $\overline{u}^n_\bullet$ steady $\Rightarrow \overline{u}^{n+1}_\bullet = \overline{u}^n_\bullet +$ machine precision

The well-balanced property can be satisfied w.r.to all equilibria, to a class of equilibria, to a single equilibrium, etc

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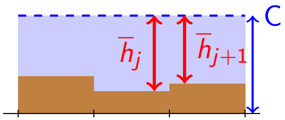
One of the culprits: the reconstruction

On lake at rest, free surface $\eta = h + Z$ is flat,
but reconstruction is applied to h and q



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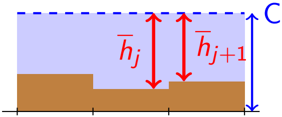
$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{h}_j = \mathcal{F}^h_{j+1/2}(\overline{u}_\bullet) - \mathcal{F}^h_{j-1/2}(\overline{u}_\bullet)$$

where (e.g. first order)

$$\mathcal{F}^h_{j+1/2}(\overline{u}_\bullet) = \tfrac{1}{2}(q^-_{j+1/2} + q^+_{j+1/2}) - D_{j+1/2}(h^+_{j+1/2} - h^-_{j+1/2})$$

where D^h is the numerical dissipation term.
For a lake at rest (first order p-wise constant):



$$\begin{aligned}\mathcal{F}^h_{j+1/2}(\overline{u}_\bullet) &= \tfrac{1}{2}(\cancelto{0}{q^-_{j+1/2}} + \cancelto{0}{q^+_{j+1/2}}) - D_{j+1/2}(h^+_{j+1/2} - h^-_{j+1/2}) \\ &= -D_{j+1/2}\left[(\cancel{C} - \overline{Z}_{j+1}) - (\cancel{C} - \overline{Z}_j)\right] \\ &\neq 0 \qquad \text{unless the bottom is flat}\end{aligned}$$

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Towards well-balanced schemes

- Design a well balanced reconstruction $\mathcal{R}_j(x; \overline{u}_\bullet)$ that
  - are accurate of order p on general data
  - on steady states, we have no jumps at interfaces

Key idea: reconstruct perturbations w.r.to equilibria of interest

[2] Audusse et al. (2004)
Noelle, Pankratz, Puppo, Natvig (2006)
Cravero, Puppo, M.S., Visconti (2018)
[3] Levy, Puppo, Russo (1998–2002); M.S., Puppo, Visconti, . . . (2016–2021)

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  Key idea: reconstruct perturbations w.r.to equilibria of interest
- Design a well balanced quadrature[2] such that
  - → are consistent and accurate of order p on general data
  - → $$\frac{\mathrm{d}}{\mathrm{d}t}\overline{u}_j\Big|_{\text{steady state}} = \underbrace{-[\mathcal{F}_{j+1/2}(\overline{u}_\bullet) - \mathcal{F}_{j-1/2}(\overline{u}_\bullet)]}_{\cancel{-\partial_x f(u)}+\mathcal{O}(\Delta x^p)} + \underbrace{\mathcal{S}_j(\overline{u}_\bullet)}_{\cancel{s(u)}+\mathcal{O}(\Delta x^p)} \quad = 0$$

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- There are alternatives like source upwinding or path-conservative schemes, but high order versions invariably require many reconstruction points inside the cell, so we have found that CWENO[3] class reconstructions are most useful

[2] Audusse et al. (2004)
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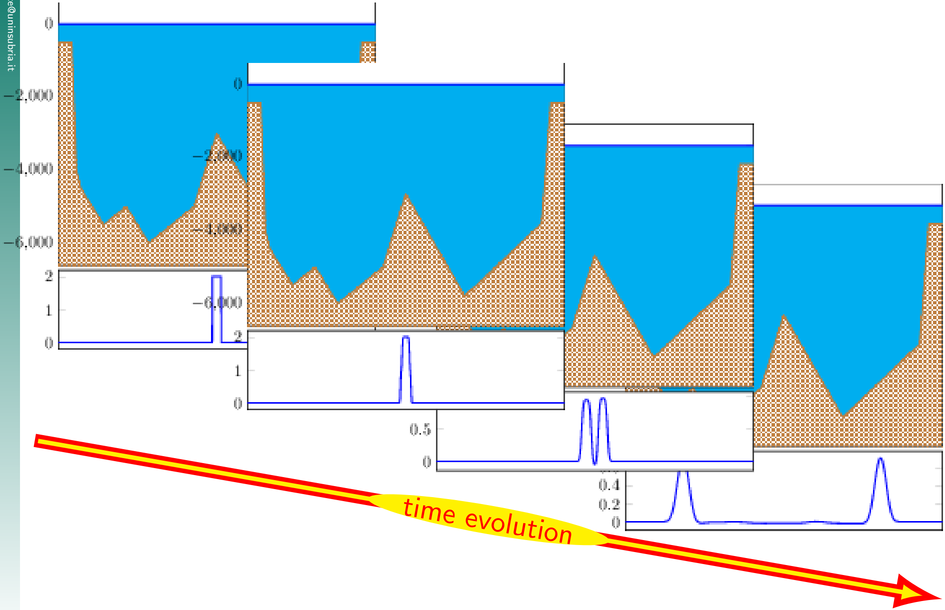
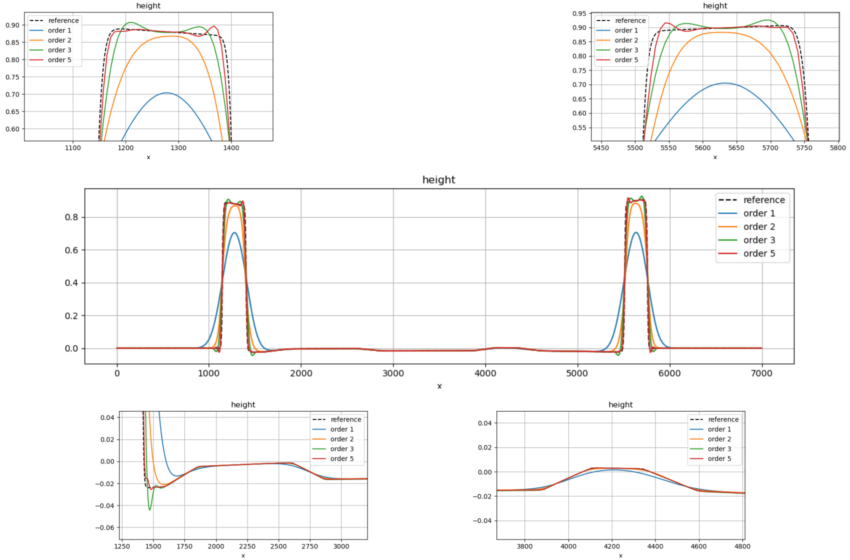
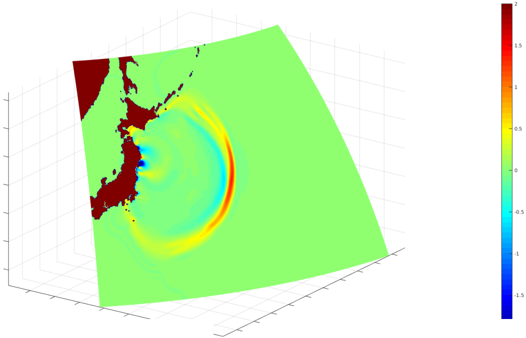
A tsunami across the Ocean (take 3)

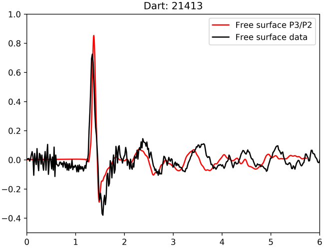


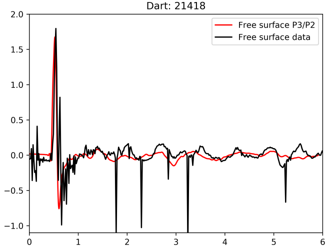
Comparing different orders



2d with Coriolis force for the Tohoku tsunami







Castro, M.S. (2018)

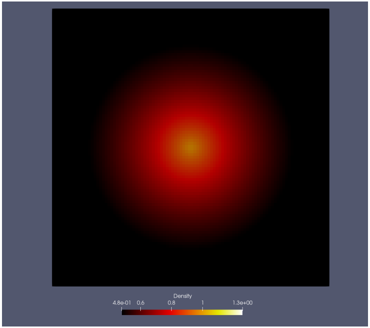
Euler gas dynamics with external gravity

Some more examples

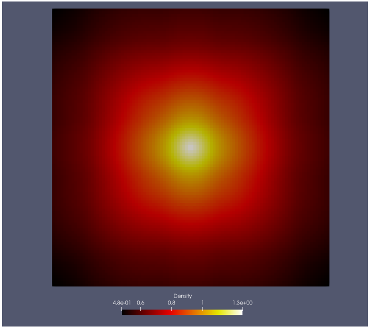
An isothermal atmosphere?

Spherically symmetric gas cloud initially in isothermal equilibrium.

Initial state:
isothermal equilibrium

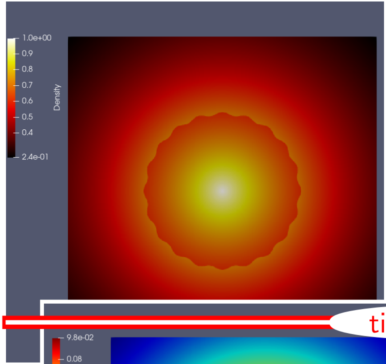


Evolution:
numerically equilibrium is lost

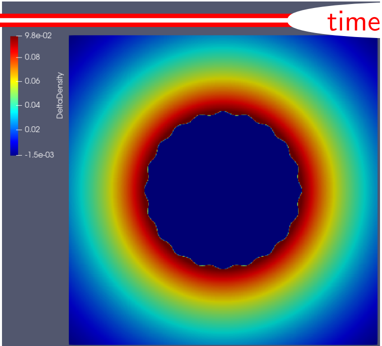


The scheme is not well-balanced!

A perturbed isothermal atmosphere??



time evolution



Note the change in range of colorbars

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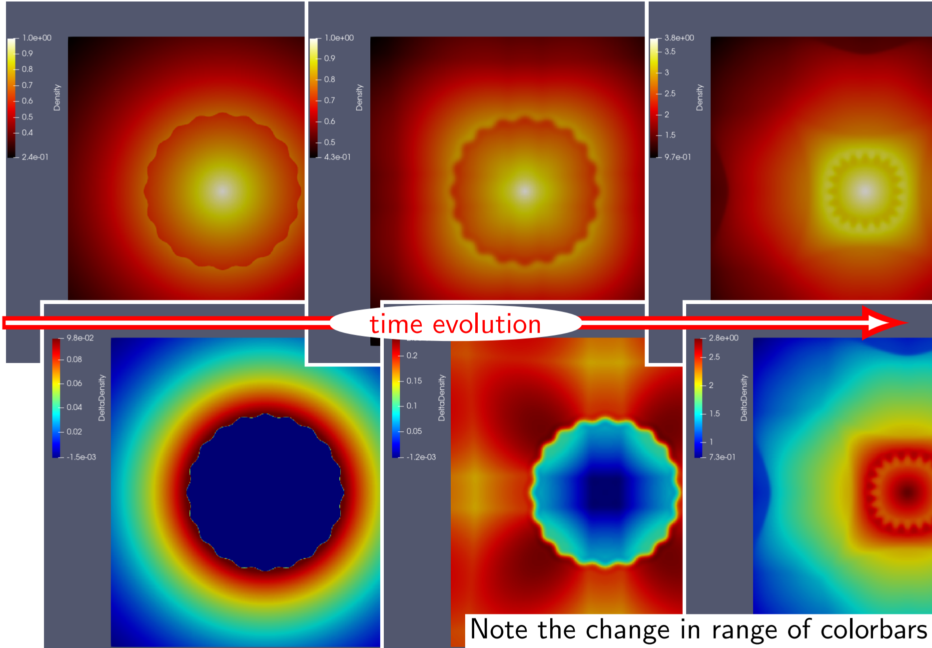
A perturbed isothermal atmosphere??



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Steady states of Euler+gravity

The system

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho v) & = 0 \\ \partial_t (\rho v) + \nabla \cdot (\rho v \otimes v + pI) & = -\rho \nabla \Phi \\ \partial_t E + \nabla \cdot (v(E+p)) & = -\rho v \nabla \Phi \end{cases}$$

has very large families of hydrostatic equilibria satisfying

$$\boxed{v(x,t) \equiv 0} \qquad \boxed{\nabla p^{\text{eq}} = -\rho^{\text{eq}} \nabla \Phi}$$

For example:

- isothermal athmospheres:

$$\rho^{\text{iso}}(x) = \frac{e^{-\Phi(x)/T_{eq}}}{T_{eq}} \qquad p^{\text{iso}}(x) = e^{-\Phi(x)/T_{eq}}.$$

- polytropic equilibria:

$$\rho^{\text{poly}}(x) = \left(1 - \tfrac{\nu-1}{\nu}\Phi(x)\right)^{\frac{1}{\nu-1}} \qquad p^{\text{poly}}(x) = (\rho(x))^{\nu}.$$

- and many more ...

Euler+gravity: well-balanced reconstruction

- introduce fluctuations

$$r(x,t) = \rho(x,t) - \rho^{\text{eq}}(x) \qquad \pi(x,t) = p(x,t) - p^{\text{eq}}(x)$$

- compute $\overline{r}_j$ and $\overline{\pi}_j$ from the data $\overline{\rho}_\bullet, \overline{m}_\bullet, \overline{E}_\bullet$
- Reconstruct $\overline{r}$, $\overline{\pi}$ and $\overline{\rho v}$ to get $r^\pm_{j+1/2}$, $\pi^\pm_{j+1/2}$, $(\rho v)^\pm_{j+1/2}$
- Then set

$$\begin{aligned}
\rho^\pm_{j+1/2} &= r^\pm_{j+1/2} + \rho^{\text{eq}}(x_{j+1/2}) \\
p^\pm_{j+1/2} &= \pi^\pm_{j+1/2} + p^{\text{eq}}(x_{j+1/2}) \\
E^\pm_{j+1/2} &= \tfrac{1}{2}{(\rho v)^\pm_{j+1/2}}^2 / \rho^\pm_{j+1/2} + p^\pm_{j+1/2}/(\gamma - 1)
\end{aligned}$$

Klingenberg, Puppo, M.S. (2019)

Higher order extension

Pointwise

$$E(x) = \frac{1}{2}\frac{m(x)^2}{\rho(x)} + \frac{p(x)}{\gamma - 1} \quad \rightsquigarrow \quad p(x) = (\gamma - 1)\left(E(x) - \tfrac{1}{2}\tfrac{m(x)^2}{\rho(x)}\right)$$

where $m = \rho v$, but on cell averages

$$\overline{p}_j = (\gamma - 1)\left(\overline{E}_j - \tfrac{1}{2}\tfrac{\overline{m}_j^2}{\overline{\rho}_j}\right) + \mathcal{O}(\Delta \mathrm{x}^2)$$

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$$\overline{p}_j = (\gamma - 1)\left(\overline{E}_j - \tfrac{1}{2}\frac{\overline{m}_j^2}{\overline{\rho}_j}\right) + \mathcal{O}(\Delta x^2)$$

Solution:

- reconstruct $E_j(x)$, $m_j(x)$, $\rho_j(x)$ from their cell averages
- choose an appropriate (Gaussian) quadrature rule and compute

$$\overline{p}_j \approx \sum_{q=0}^{N_q} w_q p(x_q) = \sum_{q=0}^{N_q} w_q (\gamma - 1)(E_j(x) - \tfrac{1}{2}\frac{m_j(x)^2}{\rho_j(x)})$$

with the desired accuracy (CWENO useful here!)

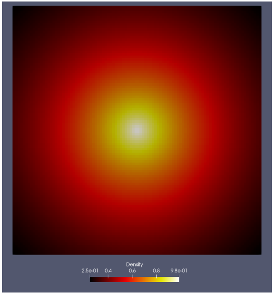
Klingenberg, Puppo, M.S. (2019)

An isothermal atmosphere!

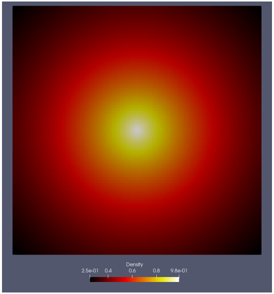
Using

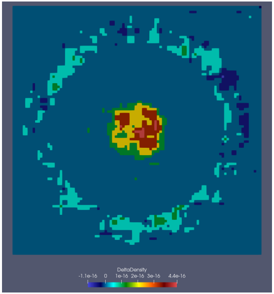
- well-balanced reconstruction
- well-balanced quadrature for the source,

Initial state:
isothermal equilibrium

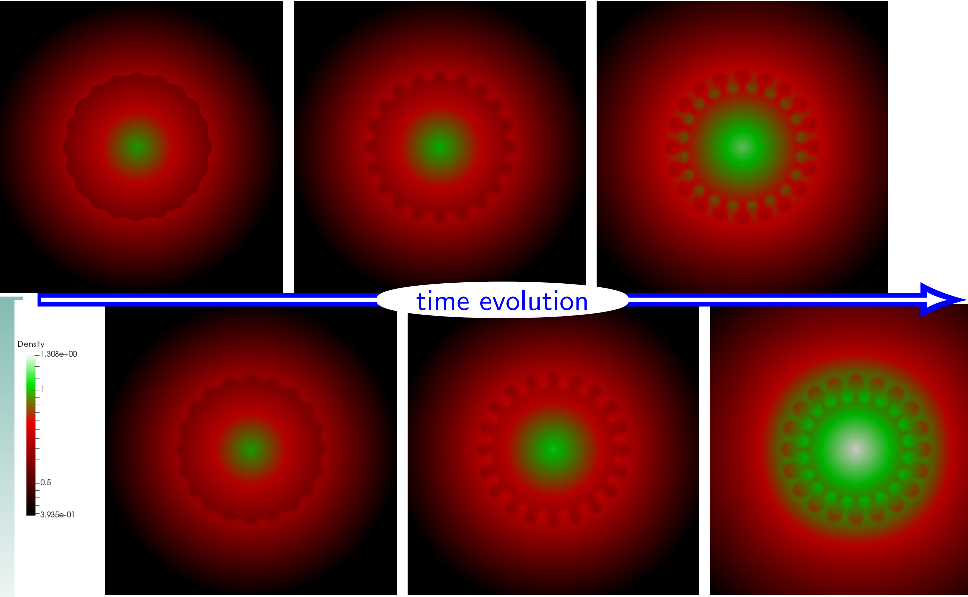


Evolution:
steady state is preserved up to 10^{-16}





A quasi-isothermal atmosphere!



Euler gas dynamics with external gravity

Some more examples

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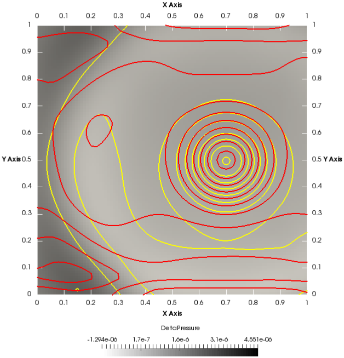
Windy athmospheres for Euler+gravity

The technique can be extended to "windy steady states", i.e.

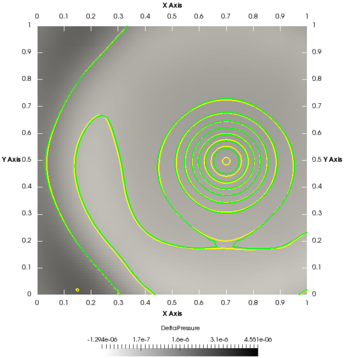
- $\nabla p = -\rho \nabla \Phi$
- constant $\vec{v}(x,t)$ s.t. $\vec{v} \cdot \nabla \Phi = 0$

Density (grayscale) and density perturbation (contours, yellow=reference)

WB on isothermal



WB on windy isothermal



Klingenberg, Puppo, M.S. (2019)

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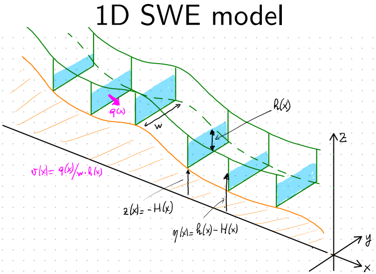
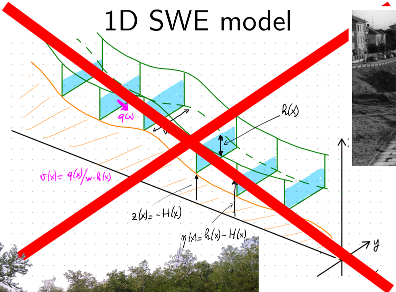
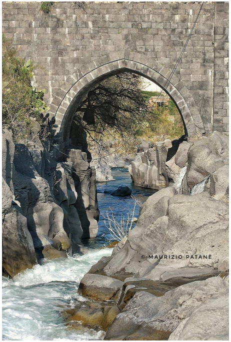
Shallow water for non-rectangular sections

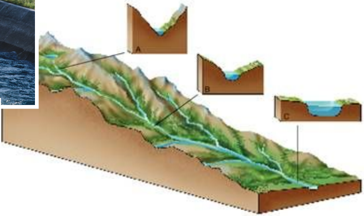


Shallow water for non-rectangular sections

1D SWE model







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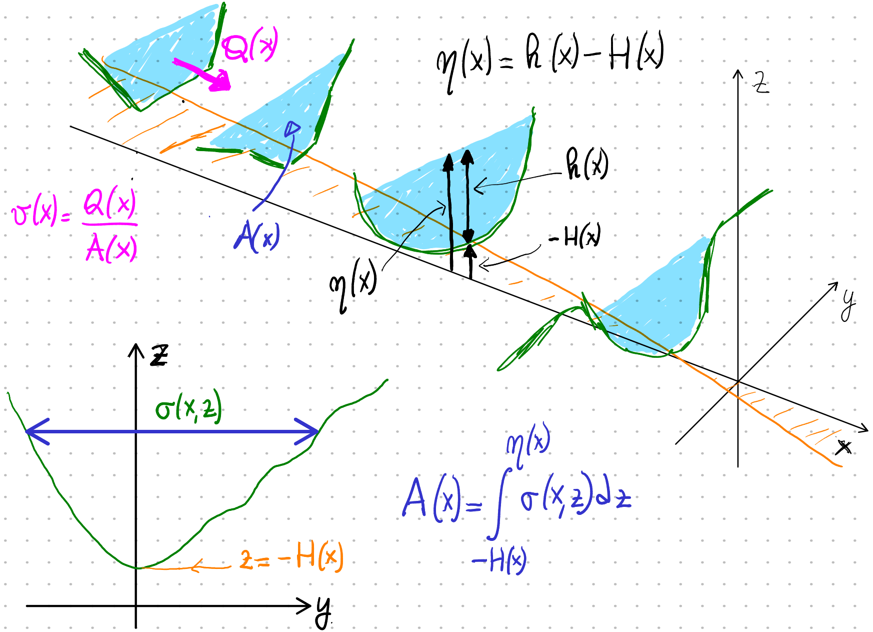
Channel topography and cross-section



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Shallow water for non-rectangular sections (2)

$A(t,x)$ wet area at location x, time t

$Q(t,x)$ discharge at location x, time t

$\eta(t,x)$ free surface height at location x, time t

The model can be written as[4] is

$$\begin{cases} \dfrac{\partial A}{\partial t} + \dfrac{\partial Q}{\partial x} = 0 \\ \dfrac{\partial Q}{\partial t} + \dfrac{\partial}{\partial x}\left(\dfrac{Q^2}{A}\right) = -gA\dfrac{\partial \eta}{\partial x} \end{cases}$$

$$A(x) = \int_{Z(x)}^{\eta(x)} \sigma(x,z)\mathrm{d}z$$

Well-balanced scheme:[5]

- convert $A \leftrightarrow h \leftrightarrow \eta$ at machine-precision
- reconstruct fluctuations from a lake-at-rest
- deduce reconstruction of free surface η
- path-conservative approach instead of w.b. quadrature

[4] Gouta-Maurel – Int. J. Numer. Meth. Fluid (2002)

[5] Escalante, Castro, M.S. (2021)

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Rainy shallow-water model

Model presented by O. Lakkis at 2018 CSMM in Como

$$\begin{cases} \partial_t h + \partial_x q = R(t,x) \\ \partial_t q + \partial_x \left({q^2}/{h} + \frac{1}{2} g h^2 \right) = -gh\partial_x z - \kappa(t,h,q)\frac{q}{h} \end{cases}$$

where

- $R(t,x)$ is the contribution of rain (and possibly runoff for fluvial case)
- κ models the change in momentum due to the added water, assuming that the incoming water has zero velocity

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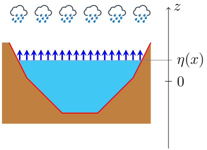
"filling the lake" solution:
$R(t,x) = R(t)$ and



$$\begin{cases} h(t,x) + Z(x) = C(t) \\ q(t,x) = 0 \end{cases} \quad \text{where } C(t) = C(0) + \int_0^t S(\tau)\mathrm{d}\tau$$

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Well-balanced scheme on "filling the lake"

- The Runge-Kutta scheme of a semidiscrete scheme for SWE, applied to the $R(t)$ term is
$$\sum_{k=1}^{\sigma} b_k \begin{pmatrix} R(t_n+c_k\Delta t) \\ 0 \end{pmatrix}$$
is a quadrature rule in time for $\int_0^{\Delta t} S(\tau)\mathrm{d}\tau$.
- Any w.b. scheme on lake-at-rests for SWE is automatically well-balanced on the "filling the lake" provided that $S(t)$ is polynomial of degree up to the accuracy of the rule with nodes c_k and weights b_k.

order	1	2	3	5	7	9
N=25	4.3e-16		2.3e-15			
N=50	3.6e-15		2.0e-14			
N=100	3.4e-15	5.0e-15	5.3e-15	5.1e-15	1.5e-14	2.4e-14

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Conclusions and perspectives

There are many well-balancing techniques (w.b. quadrature, source upwinding, path-conservative schemes) but the common motivation is that

only preserving exactly the equilibria
we can see small perturbations of equilibria

using a coarse grid, thus being able to perform computations in a fast, cheap (and eco-friendly) way

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Well-balancing is just an instance of a more general approach to numerics, which includes asymptotic preserving schemes, divergence-free discretizations, structure-preserving schemes, etc

Thankyou for your kind attention!






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