Method of characteristics: theoretical and numerical applications

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CEMRACS 2015

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Outline

DiPLoMa origins

Once upon a time in 2011...

the "basmac" project was proposed
to the 2011 CEMRACS session.
It was the beginning of
an amazing research activity.
It was aimed at studying
the low Mach number regime.

So was born the CDMATH group.

Models and numerical aspects

LMNC model (version 2011)

$$\begin{cases} \nabla\cdot\mathbf{u} = \dfrac{\beta(h,p_0)}{p_0}\Phi, & (1a) \\ \rho(h,p_0)\times\left[\partial_t h + \mathbf{u}\cdot\nabla h\right] = \Phi, & (1b) \\ \rho(h,p_0)\times\left[\partial_t\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] - \nabla\cdot\sigma(\mathbf{u}) + \nabla\bar{p} = \rho(h,p_0)\mathbf{g}. & (1c) \end{cases}$$

Equation of state: stiffened gas law for a monophasic fluid

$$\rho(h,p_0) = \frac{\gamma}{\gamma-1}\frac{p_0+\pi}{h-q}$$

Dimension: 1

Numerical scheme: MOC (Matlab)

Models and numerical aspects

LMNC model (version 2012)

$$
\begin{cases}
\nabla\cdot \mathbf{u} = \dfrac{\beta(h,p_0)}{p_0}\Phi, & (1a)\\
\rho(h,p_0)\times\left[\partial_t h + \mathbf{u}\cdot\nabla h\right] = \Phi, & (1b)\\
\rho(h,p_0)\times\left[\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] - \nabla\cdot\sigma(\mathbf{u}) + \nabla\bar{p} = \rho(h,p_0)\mathbf{g}. & (1c)
\end{cases}
$$

Equation of state: stiffened gas law with phase change

$$
\rho(h,p_0) = \frac{\gamma(h)}{\gamma(h)-1}\,\frac{p_0+\pi(h)}{h-q(h)}
$$

Dimension: 1

Numerical scheme: INTMOC (Fortran)

Models and numerical aspects

LMNC model (version 2013)

$$\begin{cases} \nabla\cdot \mathbf{u} = \dfrac{\beta(h,p_0)}{p_0}\Phi, & \text{(1a)} \\ \rho(h,p_0)\times\left[\partial_t h + \mathbf{u}\cdot\nabla h\right] = \Phi, & \text{(1b)} \\ \rho(h,p_0)\times\left[\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] - \nabla\cdot\sigma(\mathbf{u}) + \nabla\bar{p} = \rho(h,p_0)\mathbf{g}. & \text{(1c)} \end{cases}$$

Equation of state: tabulated law

$$\rho \in \mathbb{R}_7[h]$$

Dimension: 1

Numerical scheme: MOC (Fortran)

Models and numerical aspects

LMNC model (version 2014)

$$\begin{cases} \nabla\cdot\mathbf{u} = \dfrac{\beta(h,p_0)}{p_0}\Phi, & \text{(1a)}\\ \rho(h,p_0)\times\left[\partial_t h + \mathbf{u}\cdot\nabla h\right] = \Phi, & \text{(1b)}\\ \rho(h,p_0)\times\left[\partial_t\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] - \nabla\cdot\sigma(\mathbf{u}) + \nabla\bar{p} = \rho(h,p_0)\mathbf{g}. & \text{(1c)} \end{cases}$$

Equation of state: stiffened gas/tabulated law

$$\rho(h,p_0) = \frac{\gamma(h)}{\gamma(h)-1}\,\frac{p_0+\pi(h)}{h-q(h)} \quad / \quad \rho\in\mathbb{R}_7[h]$$

Dimension: 2

Numerical scheme: FreeFem++ (convect)

Models and numerical aspects

LMNC model (version 2015)

$$\begin{cases} \nabla\cdot\mathbf{u} = \dfrac{\beta(h,p_0)}{p_0}\left[\Phi + \nabla\cdot\left(\lambda(h,p_0)\nabla T(h,p_0)\right)\right], & \text{(1a)} \\ \rho(h,p_0)\times\left[\partial_t h + \mathbf{u}\cdot\nabla h\right] = \Phi + \nabla\cdot\left(\lambda(h,p_0)\nabla T(h,p_0)\right), & \text{(1b)} \\ \rho(h,p_0)\times\left[\partial_t\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] - \nabla\cdot\sigma(\mathbf{u}) + \nabla\bar{p} = \rho(h,p_0)\mathbf{g}. & \text{(1c)} \end{cases}$$

Equation of state: stiffened gas/tabulated law

$$\rho(h,p_0) = \frac{\gamma(h)}{\gamma(h)-1}\,\frac{p_0+\pi(h)}{h-q(h)} \quad / \quad \rho\in\mathbb{R}_7[h]$$

Dimension: 1/2/3

Numerical scheme: MOC (Fortran)/FreeFem++ (convect)

Models and numerical aspects

LMNC model (version 201?)

$$\begin{cases} \nabla\cdot\mathbf{u} = -\dfrac{P_0'(t)}{\rho\big(h,P_0(t)\big)c^2\big(h,P_0(t)\big)} + \dfrac{\beta\big(h,P_0(t)\big)}{P_0(t)}\Phi, & \text{(1a)} \\ \rho\big(h,P_0(t)\big)\times\big[\partial_t h + \mathbf{u}\cdot\nabla h\big] = \Phi + P_0'(t), & \text{(1b)} \\ \rho\big(h,P_0(t)\big)\times\big[\partial_t\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\big] - \nabla\cdot\sigma(\mathbf{u}) + \nabla\bar{p} = \rho\big(h,P_0(t)\big)\mathbf{g}. & \text{(1c)} \end{cases}$$

Equation of state: stiffened gas/tabulated law

$$\rho\big(h,P_0(t)\big) = \frac{\gamma\big(h,P_0(t)\big)}{\gamma\big(h,P_0(t)\big)-1}\,\frac{P_0(t)+\pi\big(h,P_0(t)\big)}{h-q\big(h,P_0(t)\big)} \quad / \quad \rho\in\mathbb{R}_7[h,P_0(t)]$$

Dimension: 1/2/3

Numerical scheme: MOC (Fortran)/FreeFem++ (convect)

From Paris with love

When? 5.–6. November 2015

Where? Univ. Paris Descartes

About? Low Mach and low Froude flows

Addressed to whom? Anybody interested in theoretical and numerical aspects

And? Poster session (applications before 25. September)

Method of characteristics

Purpose: designing an accurate numerical scheme for smooth functions of advection equations while satisfying physical constraints at the discrete level.

Advection equation

$$\partial_t \mathrm{Y} + \mathbf{U} \cdot \nabla \mathrm{Y} = f.$$

Method of characteristics

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathrm{Y}\big(t, \mathcal{X}(t; s, \mathbf{x})\big)\right] = f\big(t, \mathcal{X}(t; s, \mathbf{x})\big),$$

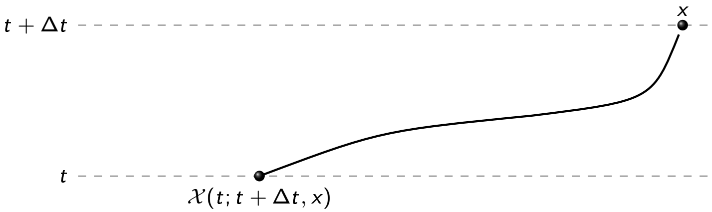
for $\mathcal{X}$ solution to:

$$\begin{cases} \dfrac{\mathrm{d}\mathcal{X}}{\mathrm{d}t} = \mathbf{U}\big(t, \mathcal{X}(t; s, \mathbf{x})\big), \\ \mathcal{X}(s; s, \mathbf{x}) = \mathbf{x}. \end{cases}$$

Physical constraints

This also reads

$$\mathrm{Y}(t+\Delta t, \mathbf{x}) = \mathrm{Y}\big(t, \mathcal{X}(t; t+\Delta t, \mathbf{x})\big) + \int_t^{t+\Delta t} f\big(\sigma, \mathcal{X}(\sigma; t+\Delta t, \mathbf{x})\big)\,\mathrm{d}\sigma,$$



- If $f = 0$, Y is constant along the characteristic curves: **maximum principle**.
- If $f > 0$, Y is monotone-increasing along the characteristic curves: **positivity principle**.

Applications

Abstract Bubble Vibration model (P., DIE, 26(1-2), 59-80, 2013)

$$\begin{cases} \partial_t \mathrm{Y} + \nabla\phi \cdot \nabla \mathrm{Y} = 0, \\ \Delta\phi = \psi(t)\left[\mathrm{Y} - \dfrac{1}{|\Omega|}\displaystyle\int_\Omega \mathrm{Y}(t,\mathbf{y})\,\mathrm{d}\mathbf{y}\right] \end{cases}$$

Explicit solution in 1D for $\Omega = (0,1)$

$$\mathrm{Y}(t,x) = \mathrm{Y}^0\left(\Theta_t^{-1}(x)\right)$$

where

$$\Theta_t(x) = \frac{\displaystyle\int_0^x e^{\Psi(t)\mathrm{Y}^0(y)}\mathrm{d}y}{\displaystyle\int_0^1 e^{\Psi(t)\mathrm{Y}^0(y)}\mathrm{d}y}$$

Applications

Low Mach Nuclear Core model (Bernard et al, M2AN, 48(06), 1639-1679, 2014)

$$\begin{cases} \partial_t h + v\partial_y h = \frac{\beta_\ell \Phi(y)}{p_0}(h - q_\ell), \\ \partial_y v = \frac{\beta_\ell \Phi(y)}{p_0}. \end{cases}$$

Explicit solution in 1D for $\Omega = (0,1)$

$$h(t,y) = q_\ell + v(y) \times \begin{cases} \dfrac{h_0\left(\Theta^{-1}(\Theta(y) - t)\right) - q_\ell}{v\left(\Theta^{-1}(\Theta(y) - t)\right)}, & \text{if } \Theta(y) \geq t, \\ \dfrac{h_e\left(t - \Theta(y)\right) - q_\ell}{v_e}, & \text{otherwise,} \end{cases}$$

with $v(y) = v_e + \dfrac{\beta_\ell}{p_0}\displaystyle\int_0^y \Phi(z)\,\mathrm{d}z$ and $\Theta(y) = \displaystyle\int_0^y \frac{\mathrm{d}z}{v(z)}$.

Settings

Given a mesh size Δx, a time step Δt and the corresponding time-space grid (t^n, x_i), we design a numerical scheme based on the resolution of the two steps of the method of characteristics (MOC schemes). We consider here a backward method.

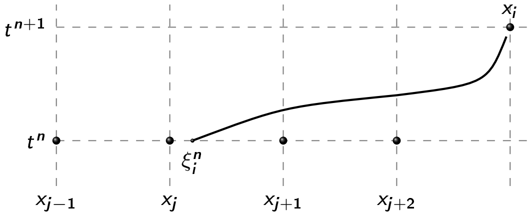
① **Time step**: yields an approximation of $\xi_i^n := \mathcal{X}(t^n; t^{n+1}, x_i)$ with

$$\begin{cases} \dfrac{\mathrm{d}\mathcal{X}}{\mathrm{d}t} = \mathbf{U}\big(t, \mathcal{X}(t; t^{n+1}, x_i)\big), \\ \mathcal{X}(t^{n+1}; t^{n+1}, x_i) = x_i. \end{cases}$$

② **Space step**: yields an interpolated value of $\mathrm{Y}\big(t^n, \xi_i^n)\big)$ to compute

$$\mathrm{Y}(t^{n+1}, x_i) = \mathrm{Y}\big(t^n, \mathcal{X}(t^n; t^{n+1}, x_i)\big) + \int_{t^n}^{t^{n+1}} f\big(\sigma, \mathcal{X}(\sigma; t^{n+1}, x_i)\big)\,\mathrm{d}\sigma,$$

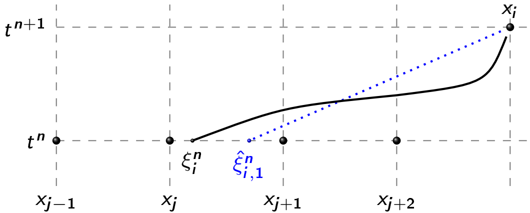
MOC_1 scheme



Taylor expansion:

$$\mathcal{X}(t^n; t^{n+1}, x_i) = \mathcal{X}(t^n; t^n, x_i) + \Delta t \cdot \partial_s \mathcal{X}(t^n; t^n, x_i) + \mathcal{O}(\Delta t^2).$$

MOC_1 scheme



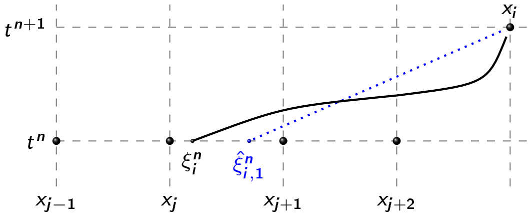
Taylor expansion:

$$\mathcal{X}(t^n; t^{n+1}, x_i) = \mathcal{X}(t^n; t^n, x_i) + \Delta t \cdot \partial_s \mathcal{X}(t^n; t^n, x_i) + \mathcal{O}(\Delta t^2).$$

Using $\partial_s \mathcal{X}(s; s, \mathbf{x}) = -\nabla_x \mathcal{X}(s; s, \mathbf{x}) \mathbf{U}(s, \mathbf{x}) = -\mathbf{U}(s, \mathbf{x})$, we set:

$$\xi_{i,1}^n = x_i - u(t^n, x_i)\Delta t.$$

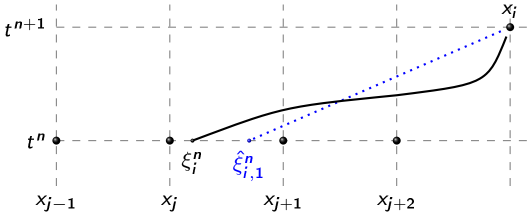
MOC$_1$ scheme



Setting $\theta = \dfrac{x_{j+1} - \xi_{i,1}^n}{\Delta x}$, we finally compute

$$Y_i^{n+1} = \theta Y_j^n + (1-\theta) Y_{j+1}^n + \Delta t \cdot f(t^{n+1}, x_i).$$

MOC_1 scheme

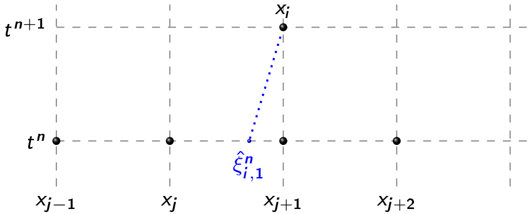


Setting $\theta = \dfrac{x_{j+1} - \xi_{i,1}^n}{\Delta x}$, we finally compute

$$Y_i^{n+1} = \theta Y_j^n + (1-\theta) Y_{j+1}^n + \Delta t \cdot f(t^{n+1}, x_i).$$

The scheme is unconditionally stable, consistent at order 1 and satisfies the maximum principle (for $f = 0$).

MOC_1 scheme

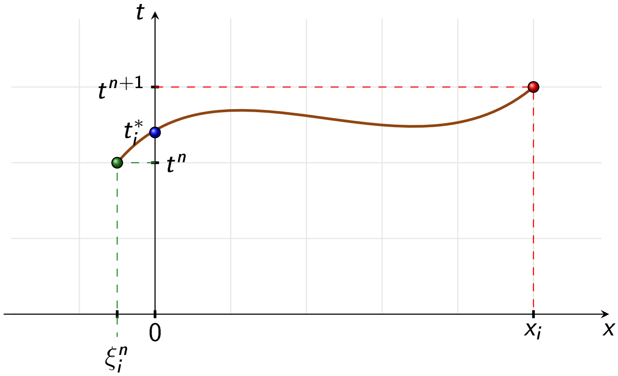


For $f = 0$ and a constant velocity $u_0 > 0$, if a CFL condition $\Delta t \leq \Delta x / u_0$ is imposed, we recover the standard upwind scheme.

$$j = i - 1,\ \xi^n_{i,1} = x_i - u_0 \Delta t,\ \theta = u_0 \frac{\Delta t}{\Delta x},\ Y_i^{n+1} = u_0 \frac{\Delta t}{\Delta x} Y^n_{i-1} + \left(1 - u_0 \frac{\Delta t}{\Delta x}\right) Y_i^n.$$

Boundary conditions

Dirichlet: $Y(t, 0) = Y_e(t)$



Resolution of $\mathcal{X}(t_i^*; t^{n+1}, x_i) = 0$ by means of a fixed-point method.

Towards higher orders: the MOC_2 scheme

Goal: reaching order 2 while preserving the maximum principle

① 2nd-order Approximation $\xi_{i,2}^n$ of the foot of the characteristic curve ξ_i^n

② 2nd-order interpolation procedure to compute $\Upsilon(t^n, \xi_{i,2}^n)$

Issue: no linear scheme of order $p \geq 2$ is monotonicity-preserving (see for instance Leveque, 1992)

Trick: variable stencil through a nonlinear criterion to choose between two potential interpolation processes

Computation of the foot ξ_i^n

Step ①

$$\mathcal{X}(t^n; t^{n+1}, x_i) = \mathcal{X}(t^n; t^n, x_i) + \Delta t \cdot \partial_s \mathcal{X}(t^n; t^n, x_i) + \frac{\Delta t^2}{2} \partial_{ss} \mathcal{X}(t^n; t^n, x_i) + \mathcal{O}(\Delta t^3).$$

Properties of the characteristic flow

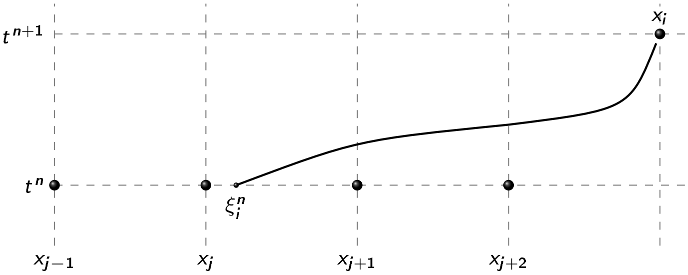
$$\partial_s \mathcal{X}(s; s, \mathbf{x}) = -\nabla_x \mathcal{X}(s; s, \mathbf{x}) \mathbf{U}(s, \mathbf{x}) = -\mathbf{U}(s, \mathbf{x}),$$
$$\partial_{ss}^2 \mathcal{X}(s; s, \mathbf{x}) = -\partial_t \mathbf{U}(s, \mathbf{x}) - \partial_s \mathcal{X}^T(s; s, x) \nabla_x \mathbf{U}(s, \mathbf{x}).$$

Hence

$$\xi_i^n = x_i - u_i^n \Delta t + \frac{\Delta t^2}{2} [u_i^n \partial_x u_i^n - \partial_t u_i^n] + \mathcal{O}(\Delta t^3),$$
$$\xi_{i,2}^n = x_i - \Delta t \frac{3u_i^n - u_{i-1}^n}{2} + \frac{\Delta t^2}{2} u_i^n \partial_x u_i^n.$$

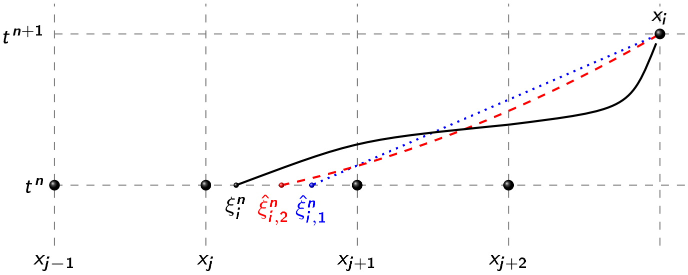
Interpolation procedure

Step ②



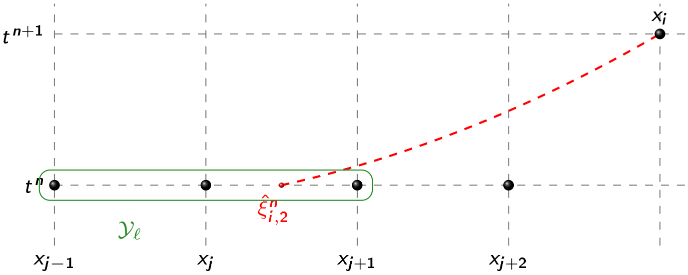
Interpolation procedure

Step ②



Interpolation procedure

Step ②



Interpolation procedure

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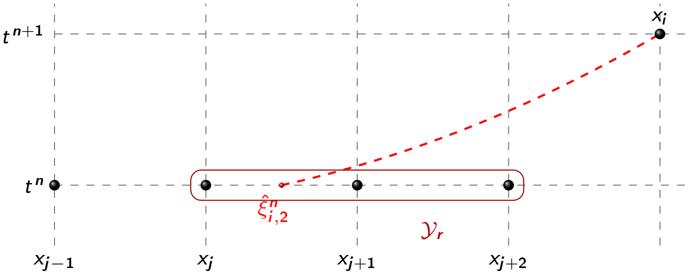
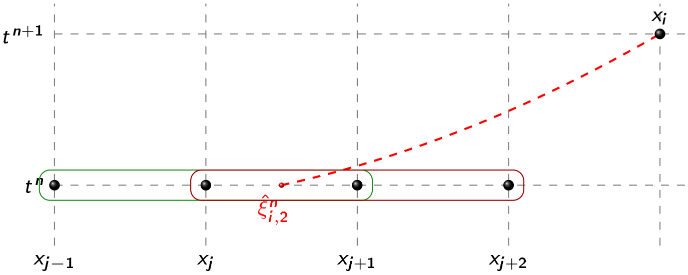


Interpolation procedure

Step ②



Trick: adaptive stencil

How to select the relevant scheme?

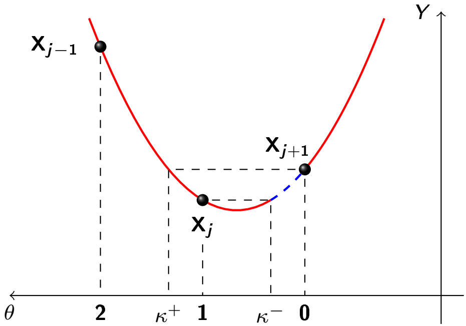
We set $\theta_{ij}^n = \dfrac{x_{j+1} - \xi_{i,2}^n}{\Delta x}$. The scheme reads

$$
\begin{aligned}
Y_i^{n+1} = \alpha_{ij}^n & \Bigg[\overbrace{-\frac{\theta_{ij}^n(1-\theta_{ij}^n)}{2} Y_{j-1}^n + \theta_{ij}^n(2-\theta_{ij}^n) Y_j^n + \frac{(1-\theta_{ij}^n)(2-\theta_{ij}^n)}{2} Y_{j+1}^n}^{\mathcal{Y}_\ell(\theta_{ij}^n)} \Bigg] \\
& + (1-\alpha_{ij}^n) \Bigg[\underbrace{\frac{\theta_{ij}^n(1+\theta_{ij}^n)}{2} Y_j^n + \left[1 - \left(\theta_{ij}^n\right)^2\right] Y_{j+1}^n - \frac{\theta_{ij}^n(1-\theta_{ij}^n)}{2} Y_{j+2}^n}_{\mathcal{Y}_r(\theta_{ij}^n)} \Bigg]
\end{aligned}
$$

We must satisfy

$$Y_i^{n+1} \in \left[\min_{k \in \mathcal{V}(j)} Y_k^n, \max_{k \in \mathcal{V}(j)} Y_k^n \right], \quad \mathcal{V}(j) = \{j, j+1\}.$$

How to select the relevant scheme?



For a constant velocity u_0 and under a CFL condition $\Delta t \leq \Delta x/u_0$, the left scheme is the Beam-Warming scheme (if $u_0 > 0$) or the Lax-Wendroff scheme (if $u_0 < 0$).

How to select the relevant scheme?

The left scheme (resp. the "right" scheme) satisfies the maximum principle iff

$$\theta_{ij}^n \notin (\kappa_\ell^-, \kappa_\ell^+) \qquad \text{(resp. } (\kappa_r^-, \kappa_r^+)\text{)},$$

with

$$\kappa_\ell^- = \frac{2(Y_{j+1}^n - Y_j^n)}{Y_{j-1}^n - 2Y_j^n + Y_{j+1}^n}, \qquad \kappa_r^- = \frac{2(Y_{j+1}^n - Y_j^n)}{Y_j^n - 2Y_{j+1}^n + Y_{j+2}^n},$$

$$\kappa_\ell^+ = \frac{Y_{j-1}^n - 4Y_j^n + 3Y_{j+1}^n}{Y_{j-1}^n - 2Y_j^n + Y_{j+1}^n}, \qquad \kappa_r^+ = \frac{Y_{j+2}^n - Y_j^n}{Y_j^n - 2Y_{j+1}^n + Y_{j+2}^n}.$$

(P., DCDS-S, 5(3), 641-656, 2012)

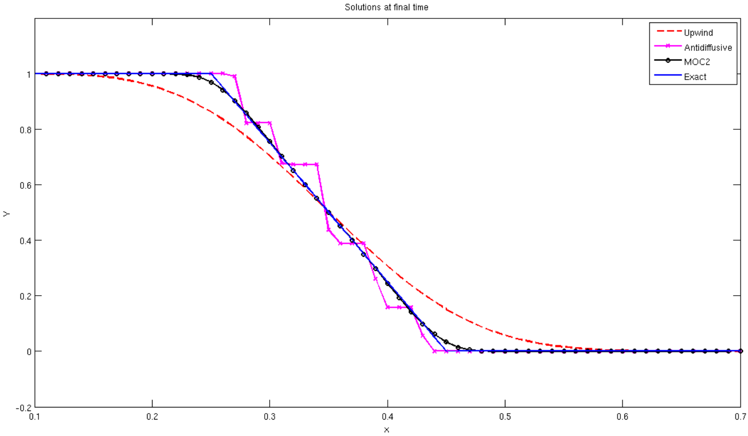
How to select the relevant scheme?

In $Y_i^{n+1} = \alpha_{ij}^n \mathcal{Y}_\ell(\theta_{ij}^n) + (1-\alpha_{ij}^n)\mathcal{Y}_r(\theta_{ij}^n)$, α_{ij}^n is determined like this

- If $\theta_{ij}^n \notin (\kappa_\ell^-, \kappa_\ell^+) \cup (\kappa_r^-, \kappa_r^+)$, we set
$$\alpha_{ij}^n = \frac{1+\theta_{ij}^n}{3}$$
- If $\theta_{ij}^n \notin (\kappa_\ell^-, \kappa_\ell^+)$ but $\theta_{ij}^n \in [\kappa_r^-, \kappa_r^+]$, we set
$$\alpha_{ij}^n = 1$$
- If $\theta_{ij}^n \notin (\kappa_r^-, \kappa_r^+)$ but $\theta_{ij}^n \in [\kappa_\ell^-, \kappa_\ell^+]$, we set
$$\alpha_{ij}^n = 0$$
- If $\theta_{ij}^n \in [\kappa_\ell^-, \kappa_\ell^+] \cap [\kappa_r^-, \kappa_r^+]$, we set
$$\alpha_{ij}^n = \theta_{ij}^n,\ \mathcal{Y}_\ell(\theta_{ij}^n) = Y_j^n,\ \mathcal{Y}_r(\theta_{ij}^n) = Y_{j+1}^n$$

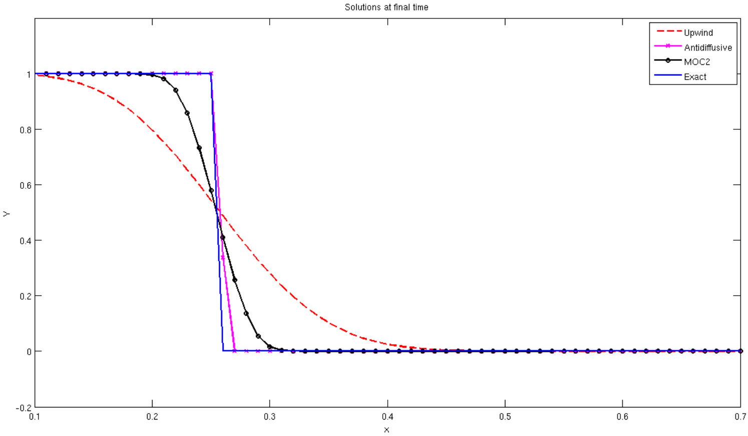
Numerical results

Example: Transport of a volume fraction



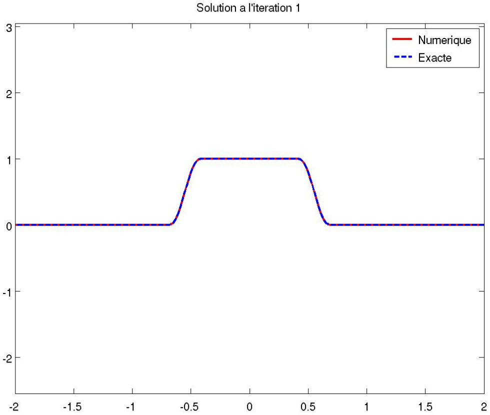
Numerical results

Example: Transport of a volume fraction



Numerical results

Example: Transport with source term



Numerical results

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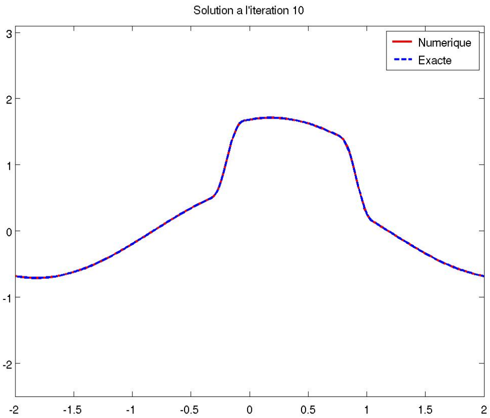

Numerical results

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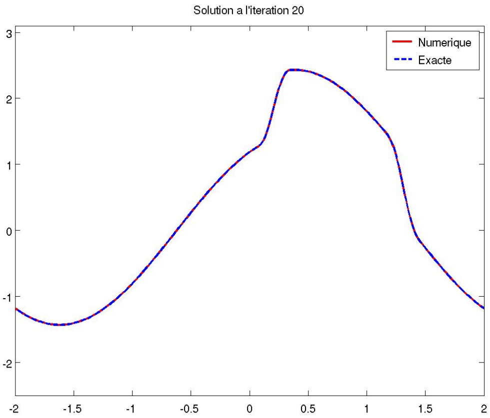

Numerical results

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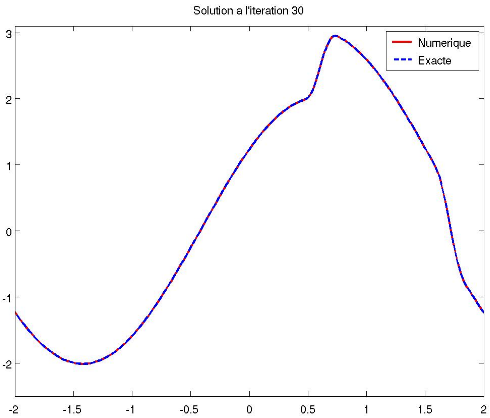

Numerical results

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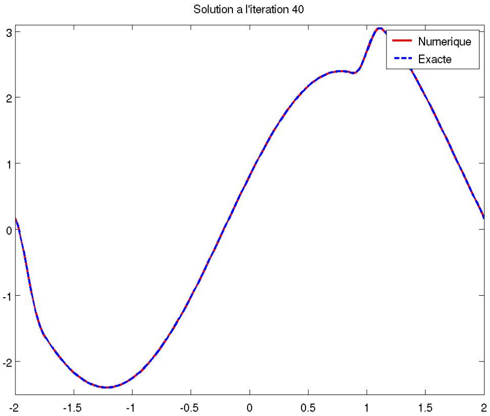

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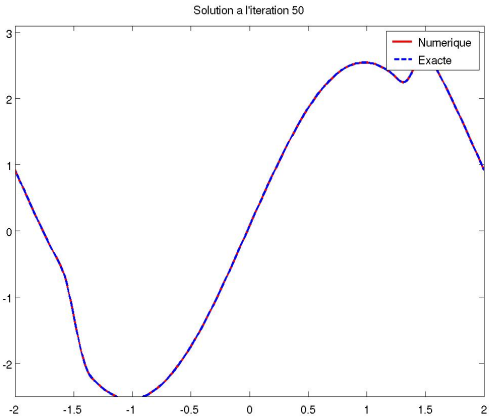

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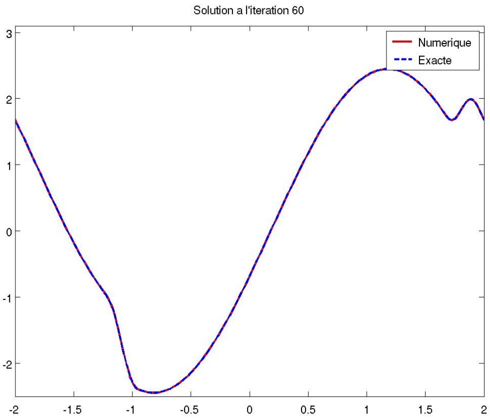
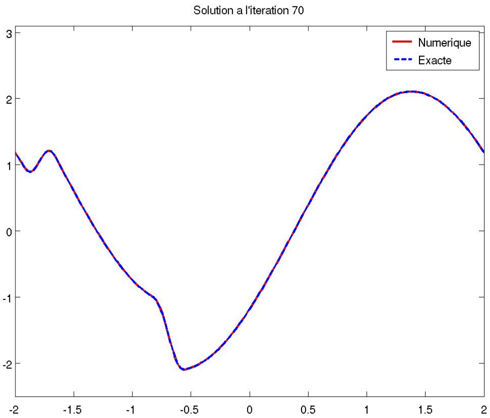


Numerical results

Example: Transport with source term



Numerical results

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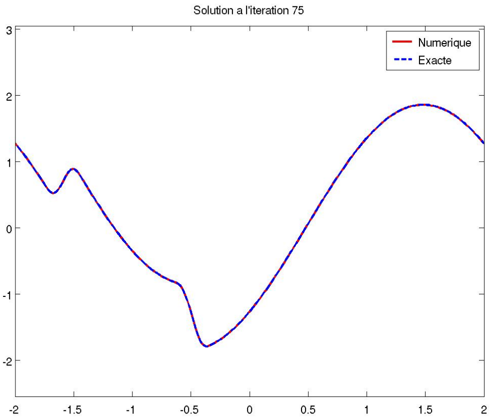

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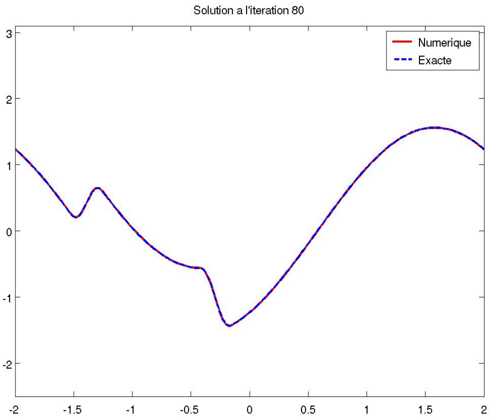

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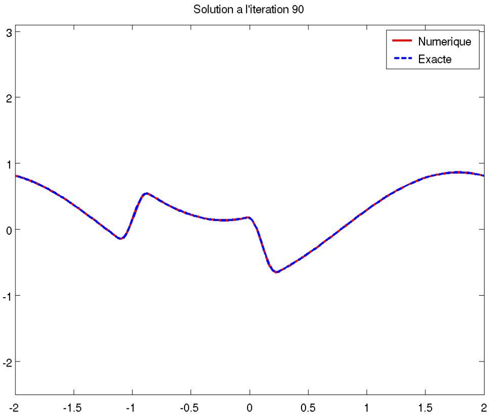

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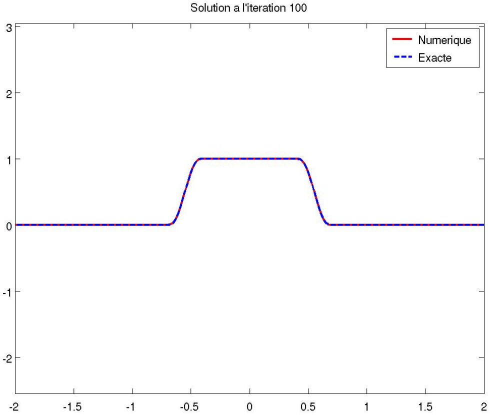
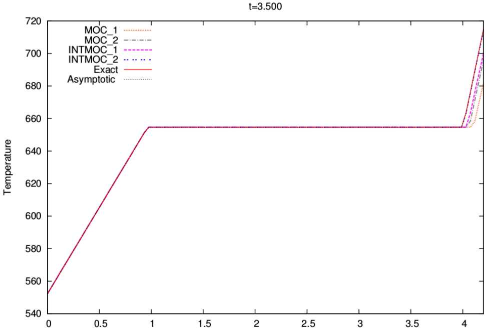


The INTMOC version

In the LMNC-SG model, we have to deal with

$$\rho(h,p_0)\left[\partial_t h + v\partial_y h\right] = \Phi, \quad \rho(h,p_0) = \frac{p_0}{\beta(h)\cdot\big(h-q(h)\big)}$$

As β and q are piecewise constant, it is easy to determine the primitive function R of $h \mapsto \rho(h,p_0)$ as well as its inverse R^{-1}.



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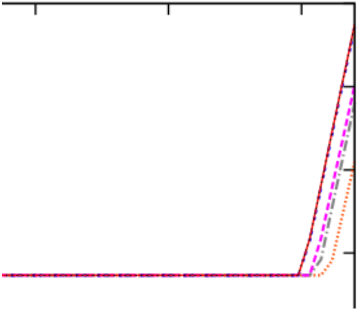

Diffusion

In the λ-LMNC model, we have to deal with

$$\partial_t h + v\partial_y h = \frac{\Phi + \lambda\partial^2_{yy} h}{\rho(h, p_0)}$$

First attempt

$$h_i^{n+1} = h(t^n, \xi_i^n) + \Delta t \frac{\Phi(t^n, \xi_i^n)}{\rho\big(h(t^n, \xi_i^n), p_0\big)} + \frac{\lambda \Delta t}{\rho\big(h(t^n, \xi_i^n), p_0\big)} \underbrace{\partial^2_{yy} h(t^n, \xi_i^n)}_{\approx \theta \partial^2_{yy} h_j^n + (1-\theta)\partial^2_{yy} h_{j+1}^n}$$

Stability condition: $\Delta t \preccurlyeq \Delta y^2$

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$$h_i^{n+1} = h(t^n, \xi_i^n) + \Delta t \frac{\Phi(t^n, \xi_i^n)}{\rho\big(h(t^n, \xi_i^n), p_0\big)} + \frac{\lambda \Delta t}{\rho\big(h(t^n, \xi_i^n), p_0\big)} \partial^2_{yy} h_i^{n+1}$$

The resulting linear system involves a tridiagonal M-matrix. The Thomas algorithm enables to invert in a $\mathcal{O}(N_y)$ procedure.

Thank you for your attention