Explicit / implicit methods for some advection dominated problems of transport and flow in porous media

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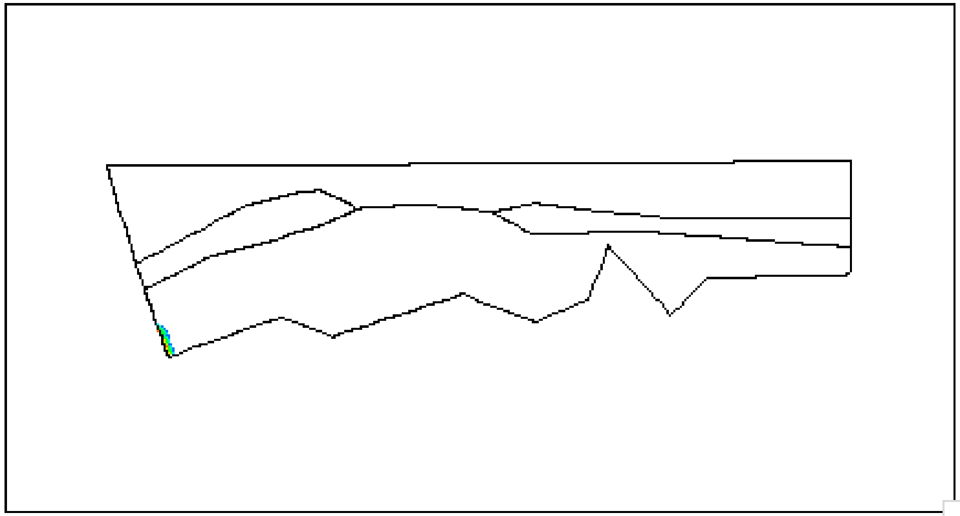
P. Frolkovič: *Application of level set method for groundwater flow with moving boundary*. Adv. Wat. Res., 2012
P. Frolkovič, K. Mikula, J. Urbán: *Semi-implicit finite volume level set method for advective motion of interfaces in normal direction*. Appl. Num. Meth., 2014
T. Kmeťo: *Semi-implicit numerical methods for the solution of advection equation.* Dipl. Thesis, 2014

Motivation

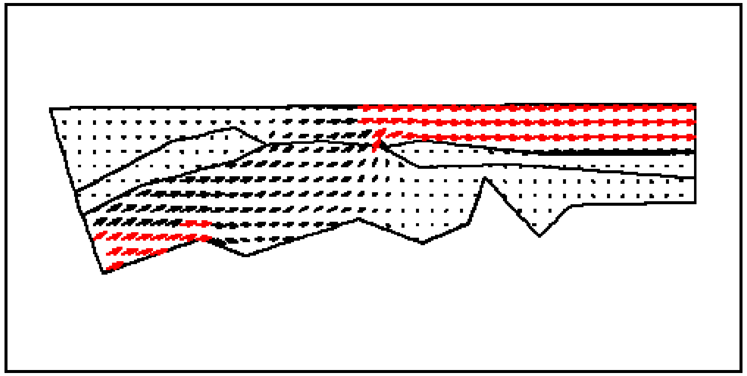
Advection dominated equations

$$\Theta \partial_t (Rc) + \vec{V} \cdot \nabla c - \nabla \cdot D \nabla c = F \,, \quad \nabla \cdot \vec{V} = 0$$

- contaminant transport



Time dependant inflow concentration



Stationary groundwater flow

P. Frolkovič, M. Lampe, G. Wittum: *Numerical simulation of contaminant transport in groundwater using software tools of r3t.* Comp. Vis. Sc., 2012, to appear

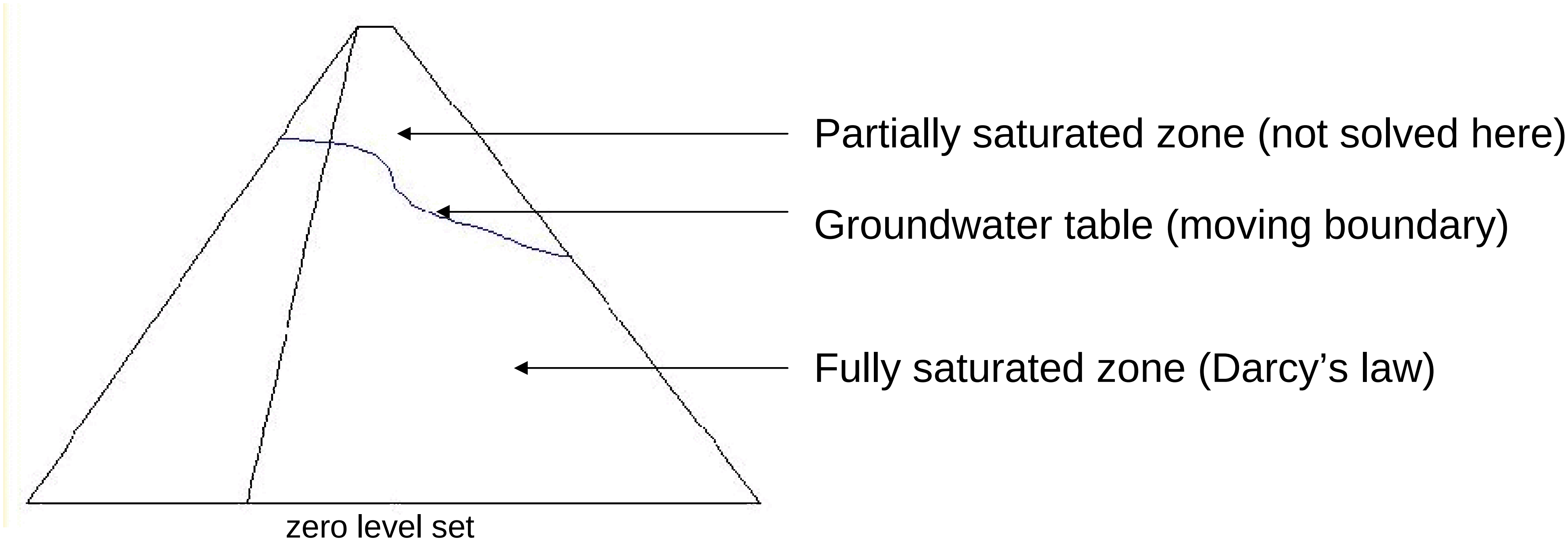
P. Frolkovič, J. Kačur: *Semi-analytical solutions of contaminant transport equation with nonlinear sorption in 1D*, Computational Geosciences, 2006

Motivation

Level set method

$$\partial_t \phi + \vec{V} \cdot \nabla \phi = 0\,, \quad \nabla \cdot \vec{V} = 0$$

- moving boundaries and/or interfaces



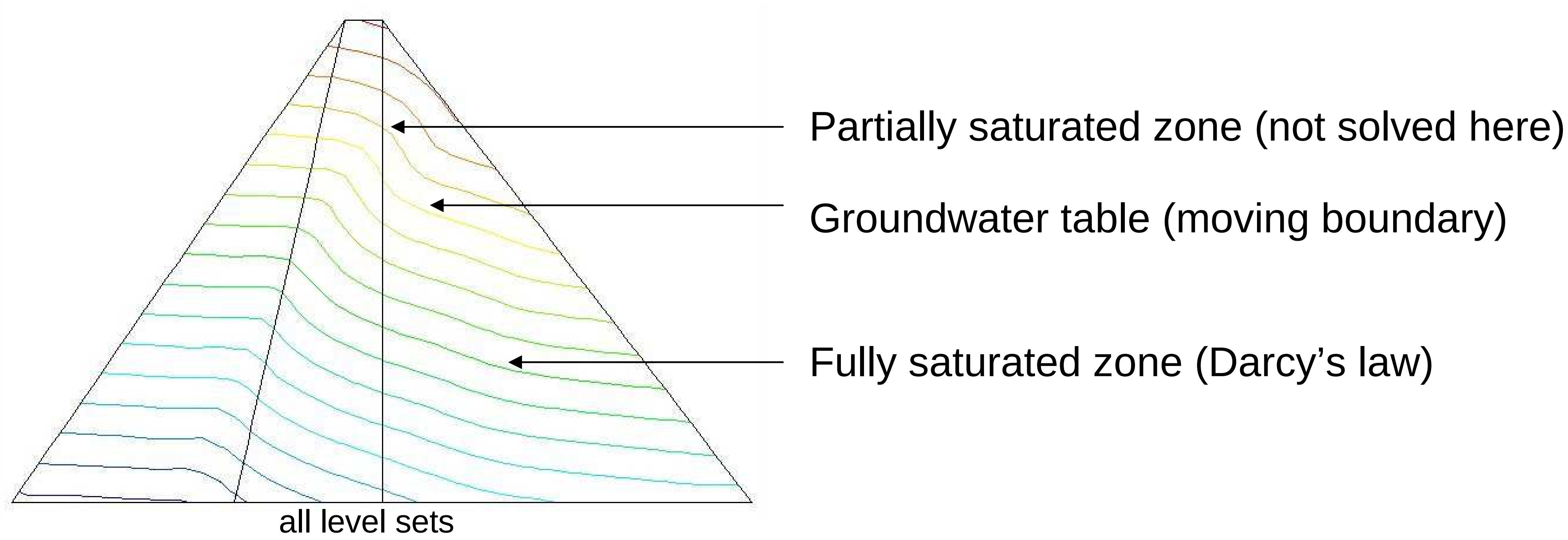
P. Frolkovič: *Application of level set method for groundwater flow with moving boundary*. Advances in Water Resources, 2012

Motivation

Level set method

$$\partial_t \phi + \color{red}{\vec{V} \cdot \nabla \phi} = 0\,, \quad \nabla \cdot \vec{V} = 0$$

- moving boundaries and/or interfaces

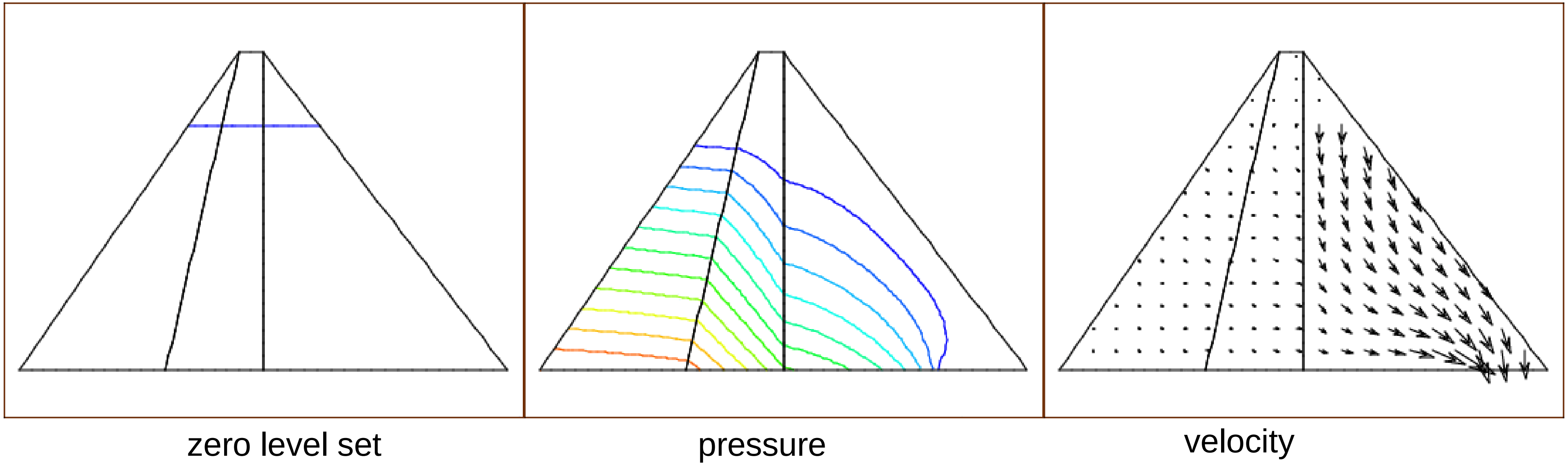


P. Frolkovič: *Application of level set method for groundwater flow with moving boundary*. Advances in Water Resources, 2012

Motivation

Moving groundwater table

$$\partial_t \phi + \vec{V} \cdot \nabla \phi = 0, \quad \vec{V} = -K\left(\nabla p - \rho \vec{g}\right), \quad \nabla \cdot \vec{V} = 0$$



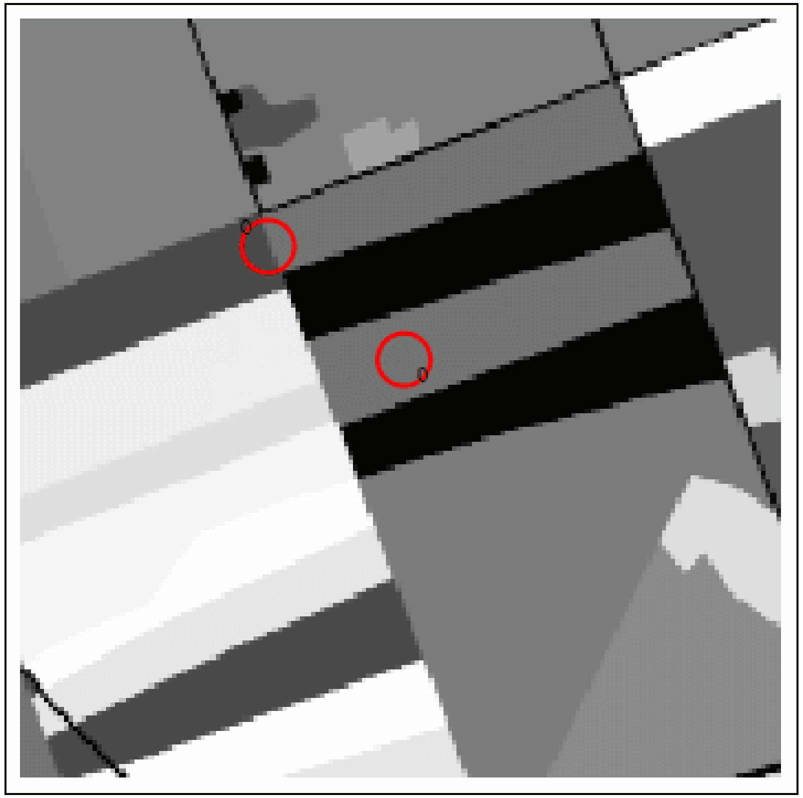
- extension of flow velocity to whole domain
- boundary conditions on implicitly given interface
  - immersed interface methods

P. Frolkovič: *Application of level set method for groundwater flow with moving boundary*. Advances in Water Resources, 2012

Motivation

Interfaces moving in normal direction

$$\partial_t \phi + s\frac{\nabla \phi}{|\nabla \phi|} \cdot \nabla \phi = 0,$$



P. Frolkovič, K. Mikula, J. Urbán: Semi-implicit finite volume level set method for advective motion of interfaces in normal direction. Appl. Num. Meth. 2014

General scheme

1D advection

$$\partial_t c + V\partial_x c = 0, \quad c(x,0) = c^0(x)$$

- equivalent ``balance law'' formulation

$$\partial_t c + \partial_x (Vc) - c\,\partial_x V = 0, \quad c(x,0) = c^0(x)$$

- space discretization

$$c(x_i)\partial_x V(x_i) \approx c_i \frac{V_{i+\frac{1}{2}} - V_{i-\frac{1}{2}}}{\Delta x}$$

$$\partial_x(c(x_i)V(x_i)) \approx \frac{c_{i+\frac{1}{2}}V_{i+\frac{1}{2}} - c_{i-\frac{1}{2}}V_{i-\frac{1}{2}}}{\Delta x}$$

General scheme

Properties

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- obtained also by finite volume discretization in 2D/3D
  - in this form it is conservative
- particular scheme obtained by choice of

$$c_{i+\frac{1}{2}}^{n-1/2} \approx c(\frac{1}{2}(x_i + x_{i+1}), \frac{1}{2}(t^{n-1} + t^n)) \quad \text{and} \quad c_i^{n-1/2}$$

- explicit or implicit or explicit/implicit:
  - c_i^{n-1} are known, c_i^n are unknowns
- high-resolution form in the space discretization
  - involves 2nd and 1st order form, “limiters”

Implicit schemes

1st order implicit upwind

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- central difference?

$$c_{i+\frac{1}{2}}^{n-1/2} = \frac{1}{2}\left(c_i^n + c_{i+1}^n\right), \qquad c_i^{n-1/2} = c_i^n$$

Implicit schemes

1st order implicit upwind

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- central difference?

$$c_{i+\frac{1}{2}}^{n-1/2} = \frac{1}{2}\left(c_i^n + c_{i+1}^n\right), \qquad c_i^{n-1/2} = c_i^n$$

- upwind difference $V > 0$

$$c_{i+\frac{1}{2}}^{n-1/2} = c_i^n \qquad \boxed{c_i^n\left(1 + \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\right) = c_{i-1}^n \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x} + c_i^{n-1}}$$

- a system of linear algebraic eq's, here it is simple
- positive coefficients scheme for arbitrary time step

Implicit schemes

<u>Comparison of 3 implicit schemes</u>

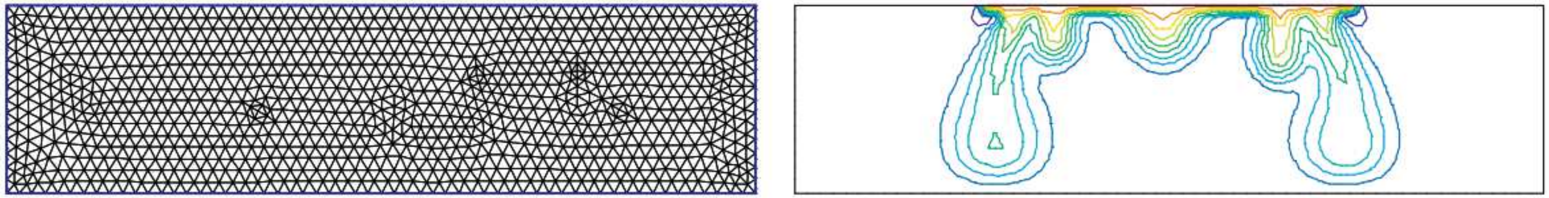
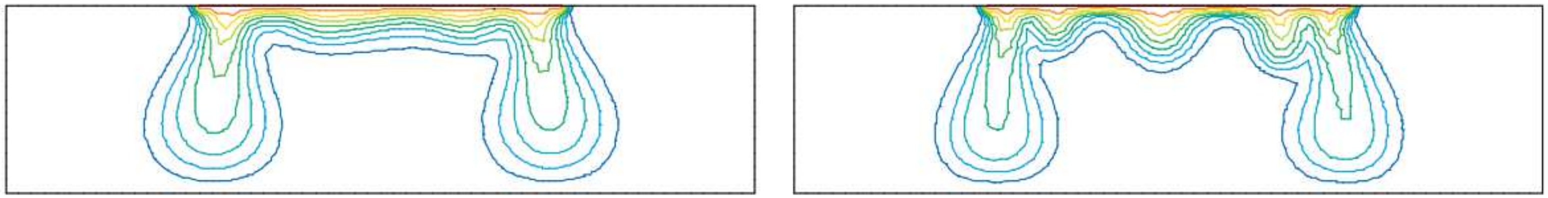


Figure 4. Grid and numerical solution for no upwind.

Stabilizing the Elder example by full upwind resulted in qualitatively very different numerical results. As full upwind added an unnecessary large amount of "artificial" diffusion, the numerical solution was during time simulation too diffusive that resulted into a different number of the fingers for this grid. On the other hand, the simple algorithm of partial upwind scheme gave analogous numerical results with respect to no upwind method, but with no oscillations presented (see the Figure 5).



P. Frolkovič, H. De Schepper: *Numerical modelling of convection dominated transport coupled with density driven flow in porous media*, Adv. Wat. Res.,2001

Implicit schemes

Advantage

- fully coupled with other implicit terms

Disadvantage

- poor resolution for pure advection

Explicit schemes

1st order upwind

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- upwind difference for $V > 0$

$$c_{i+\frac{1}{2}}^{n-1/2} = c_i^{n-1} \text{ and } c_i^{n-1/2} = c_i^{n-1}$$

Explicit schemes

1st order upwind

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- upwind difference for $V > 0$

$$c_{i+\frac{1}{2}}^{n-1/2} = c_i^{n-1} \text{ and } c_i^{n-1/2} = c_i^{n-1}$$

- explicit definition of unknowns

$$\color{red}{c_i^n} = c_{i-1}^{n-1}\frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x} + c_i^{n-1}\left(1 - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\right)$$

- positive coefficients scheme for restricted time step

Explicit schemes

1st order upwind

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

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- positive coefficients scheme for restricted time step
  - a remedy - flux-based method of characteristics

Explicit schemes

1st order explicit upwind

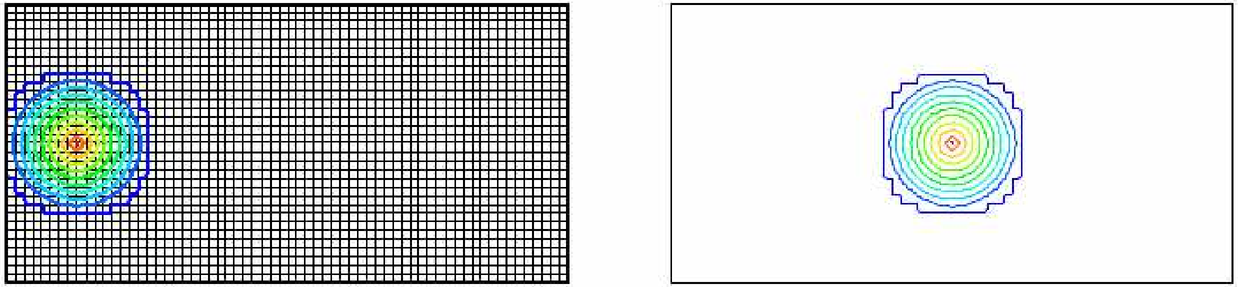


Fig. 1. Grid with interpolated initial condition C_0 (the left picture) and the numerical solution of the explicit method (16) at $t = 3/4$, if the Courant number $\mathcal{C}$ is equal to 1 (the right picture). The minimum of the solution is 0 and the maximum is 1.

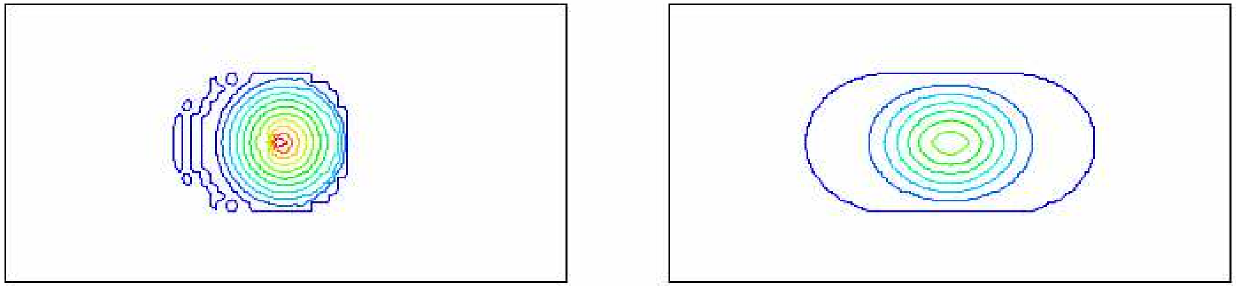


Fig. 2. Numerical solution of the explicit method (16) if $\mathcal{C} = 24/23 > 1$ (the left picture, the minimum is -0.125 and the maximum is 1.12) and for $\mathcal{C} = 0.5$ (the right picture, the minimum is 0 and the maximum is 0.659).

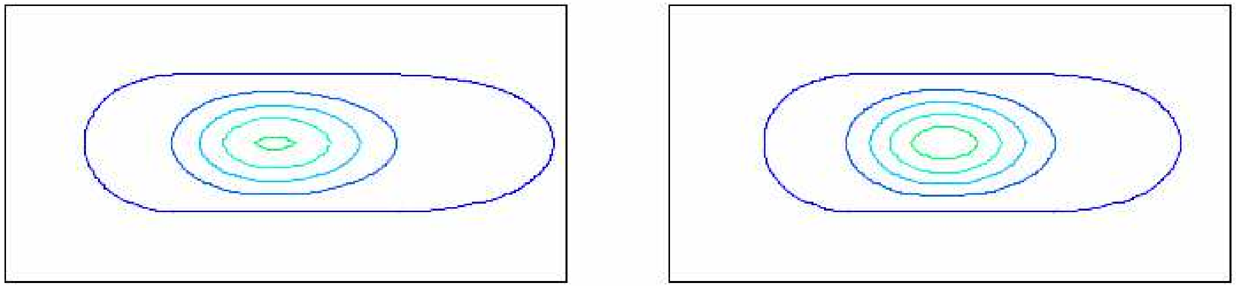


Fig. 3. Numerical solution of the implicit method (15) if $\mathcal{C} = 24/23 > 1$ (the left picture, the maximum is 0.419) and with $\mathcal{C} = 0.5$ (the right picture, the maximum is 0.469).

P. Frolkovič: *Flux-based method of characteristics for contaminant transport in flowing groundwater*, Comp. Vis. Sc., 2002

Explicit schemes

2nd order accurate upwind

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- general idea like “finite Taylor series” for $V > 0$

$$c_{i+\frac{1}{2}}^{n-1/2} = c_i^{n-1} + \frac{\Delta x}{2}\partial_x c_i^{n-1} + \frac{\Delta t}{2}\partial_t c_i^{n-1},$$

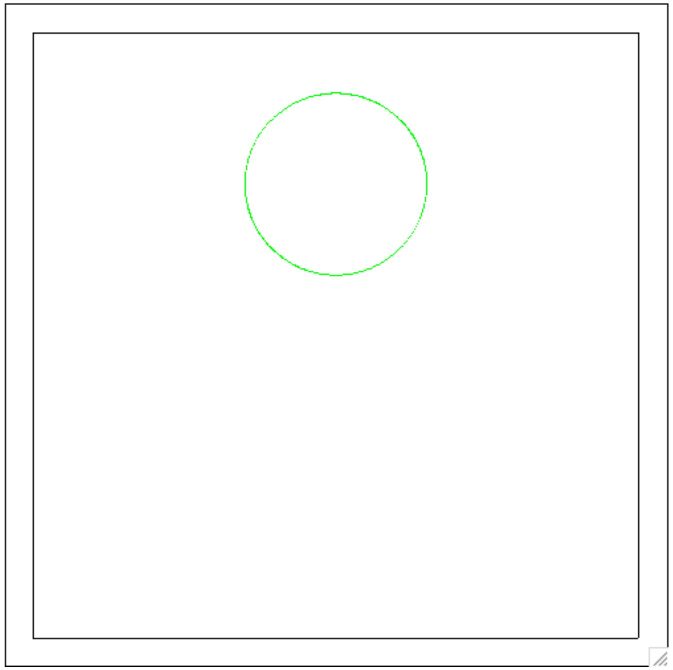
$$c_{i+\frac{1}{2}}^{n-1/2} = c_i^{n-1} + \frac{\Delta x}{2}\partial_x c_i^{n-1} - \frac{\Delta t}{2} V_i \partial_x c_i^{n-1},$$

$$c_{i+\frac{1}{2}}^{n-1/2} = c_i^{n-1} + \left(\frac{\Delta x - \Delta t V_i}{2}\right)\frac{c_{i+1}^{n-1} - c_{i-1}^{n-1}}{2\Delta x}$$

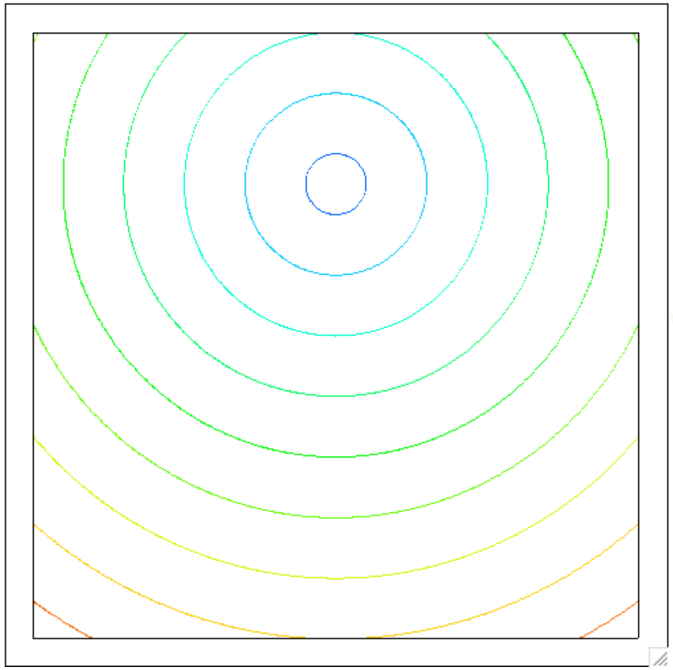
Explicit schemes

Level set method

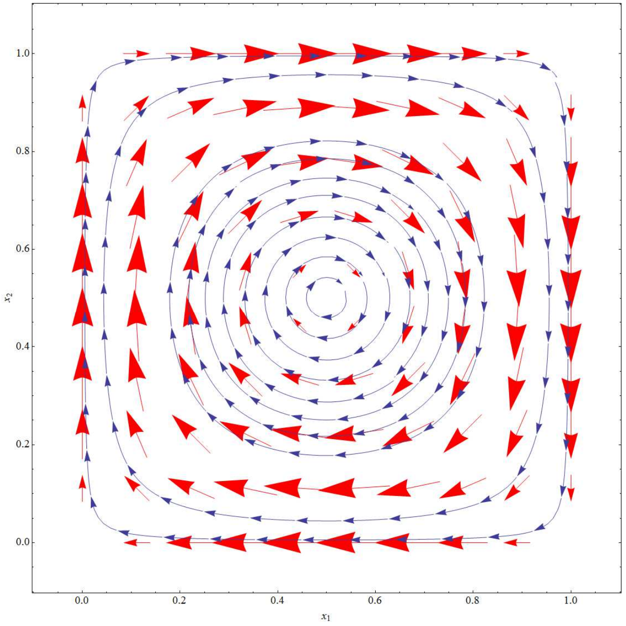
$$\partial_t \phi + \vec{V} \cdot \nabla \phi = 0$$



zero level set



many level sets

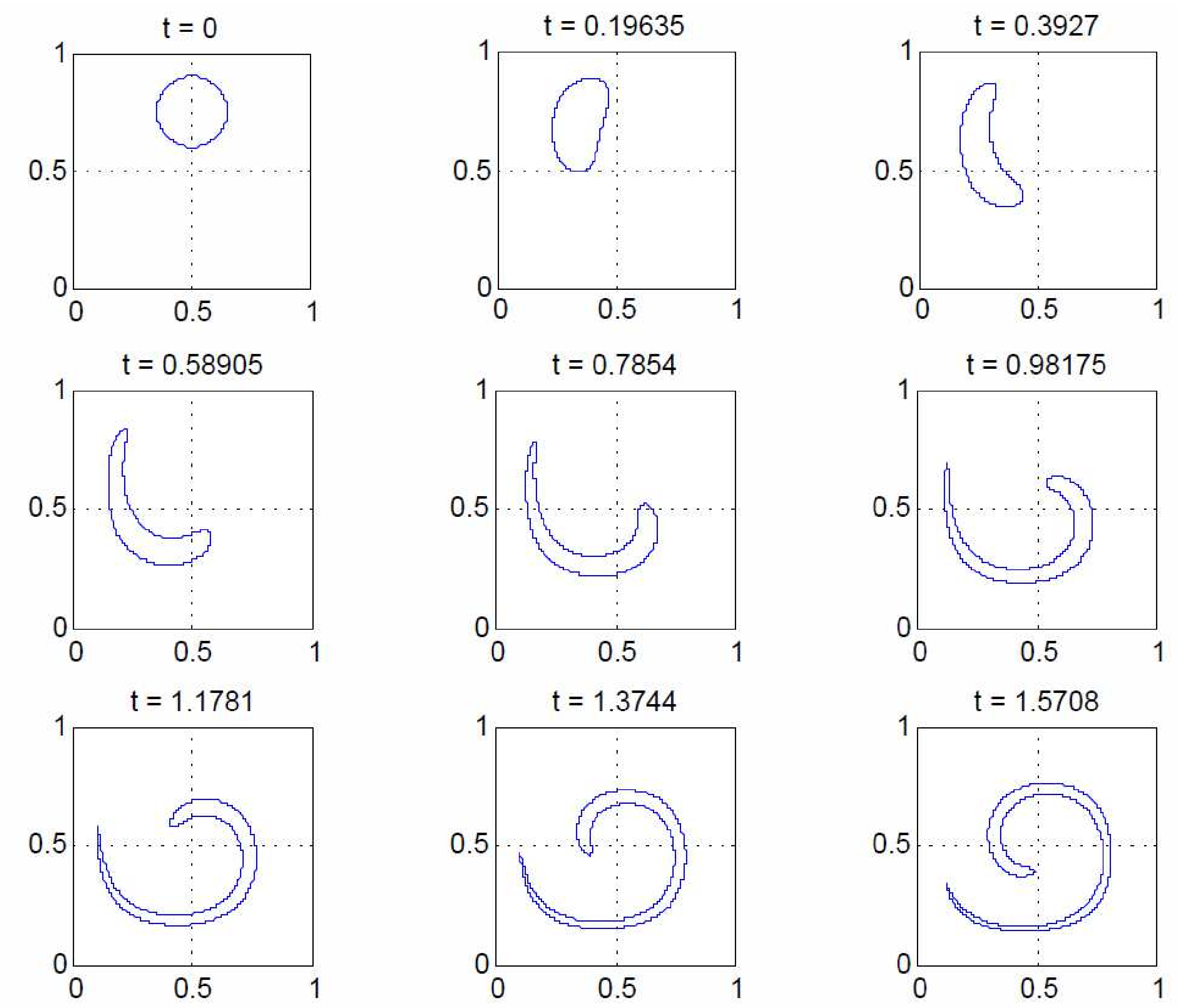


velocity and streamlines

- capturing interfaces in applications

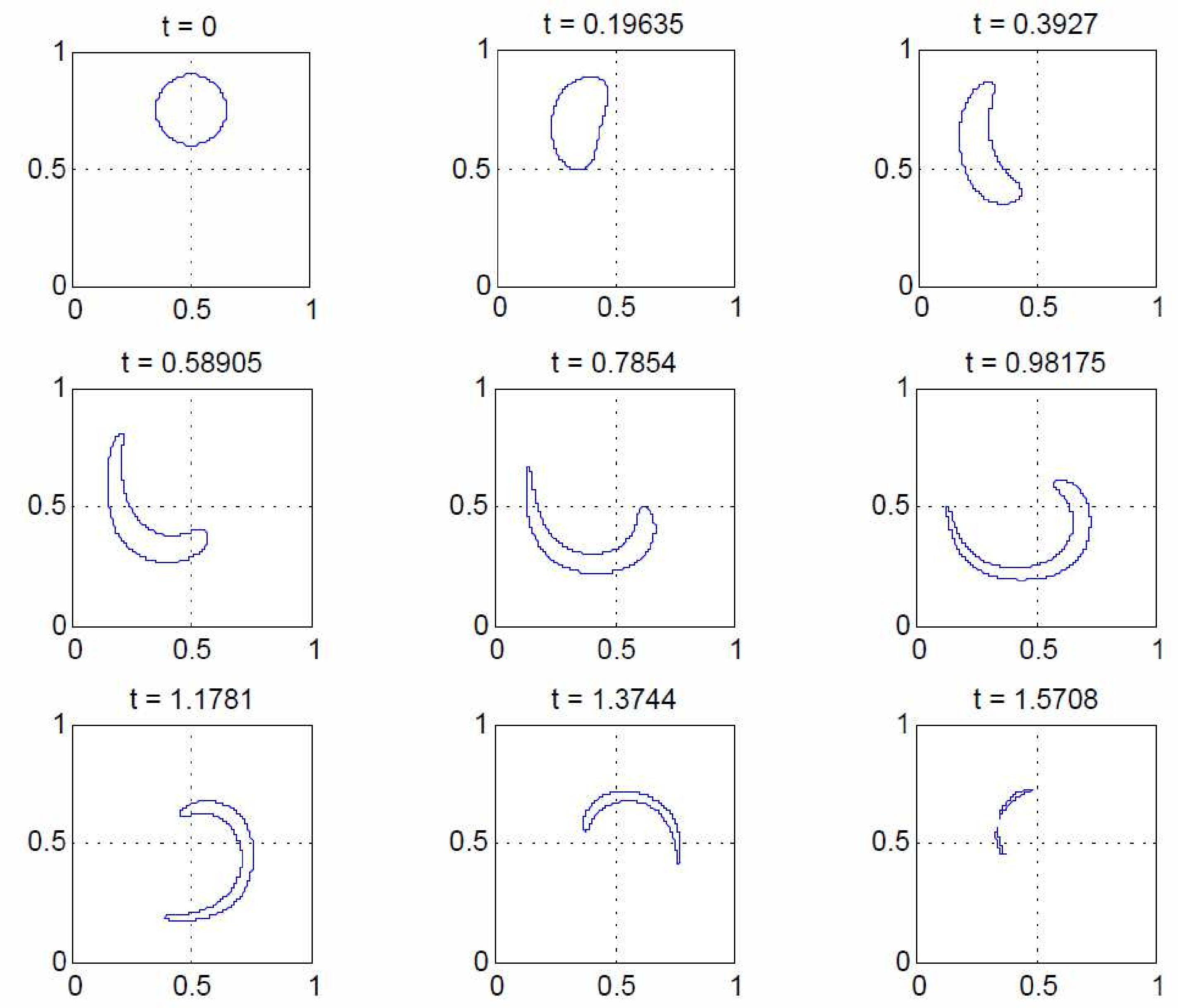
P. Frolkovič, K.Mikula: *High-resolution flux-based level set method*. SIAM J. Sci. Comp. 2007

Explicit schemes



2nd order accurate explicit upwind, done by Ch. Wehner

Explicit schemes



1^{st} order accurate explicit upwind on the same grid

Explicit schemes

Advantage

- good resolution for pure advection

Disadvantage

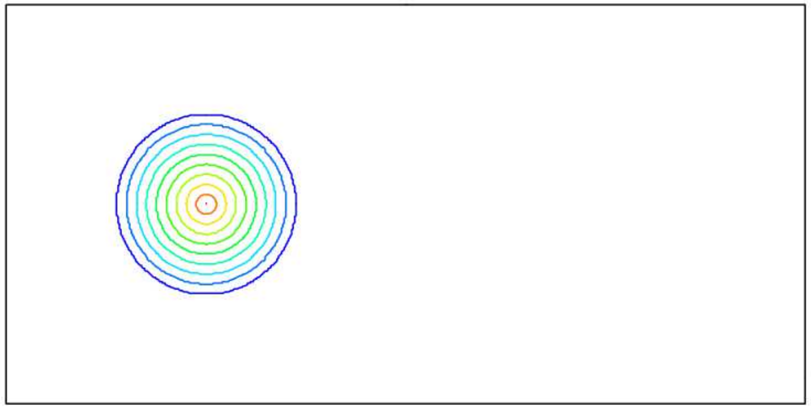
- decoupled from other terms

Explicit schemes

Time splitting errors

$$R_1 \partial_t c_1 + \partial_x c_1 + R_1 \lambda_1 c_1 = \qquad \dots, \quad R_1 = 1$$

$$R_2 \partial_t c_2 + \partial_x c_2 + R_2 \lambda_2 c_2 = R_1 \lambda_1 c_1 + \dots, \quad R_2 = 4$$



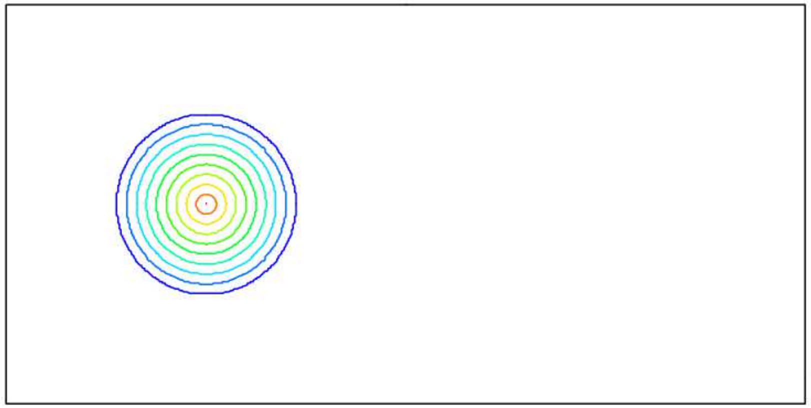
concentrations at t=0 …

Explicit schemes

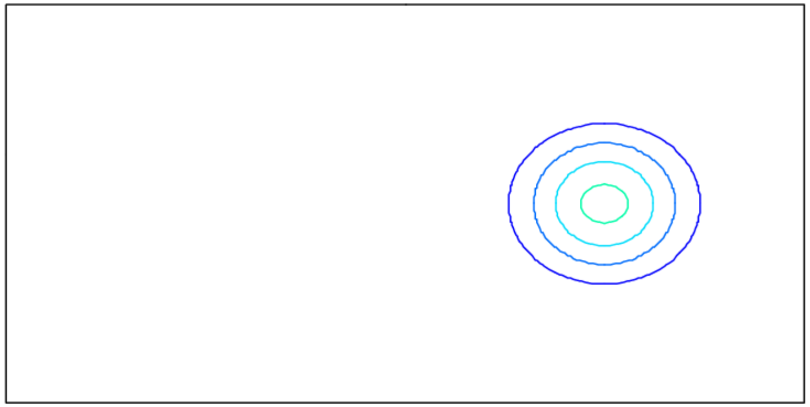
Time splitting errors

$$R_1 \partial_t c_1 + \partial_x c_1 + R_1 \lambda_1 c_1 = \qquad \dots, \quad R_1 = 1$$

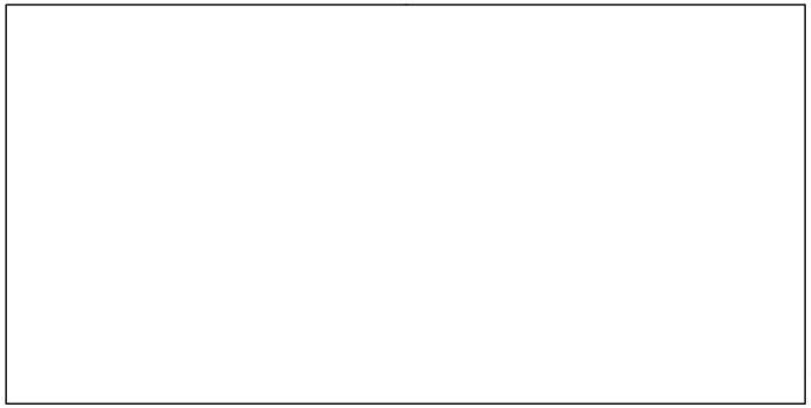
$$R_2 \partial_t c_2 + \partial_x c_2 + R_2 \lambda_2 c_2 = R_1 \lambda_1 c_1 + \dots, \quad R_2 = 4$$

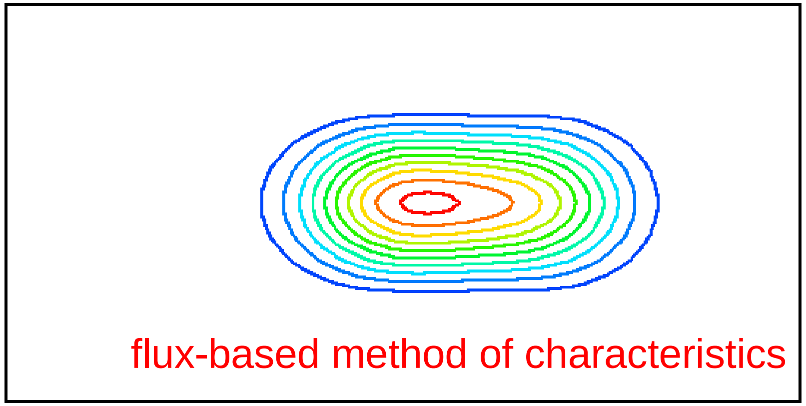


concentrations at t=0 …



… and after 2 large time steps





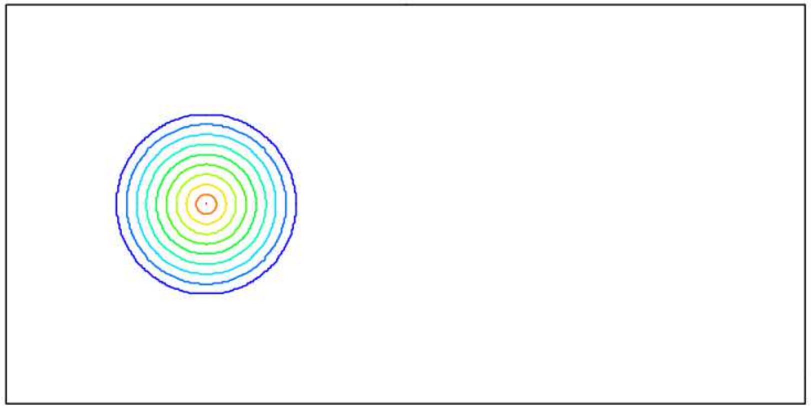
flux-based method of characteristics

Explicit schemes

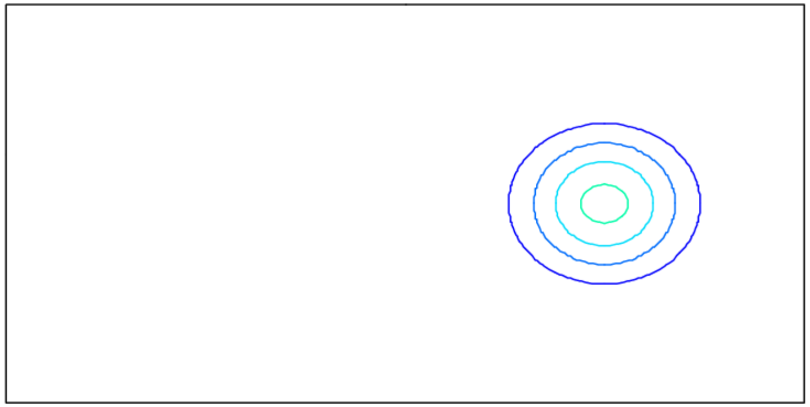
Time splitting errors

$$R_1 \partial_t c_1 + \partial_x c_1 + R_1 \lambda_1 c_1 = \qquad\qquad \ldots\,, \qquad R_1 = 1$$

$$R_2 \partial_t c_2 + \partial_x c_2 + R_2 \lambda_2 c_2 = R_1 \lambda_1 c_1 + \ldots\,, \qquad R_2 = 4$$



concentrations at t=0 …



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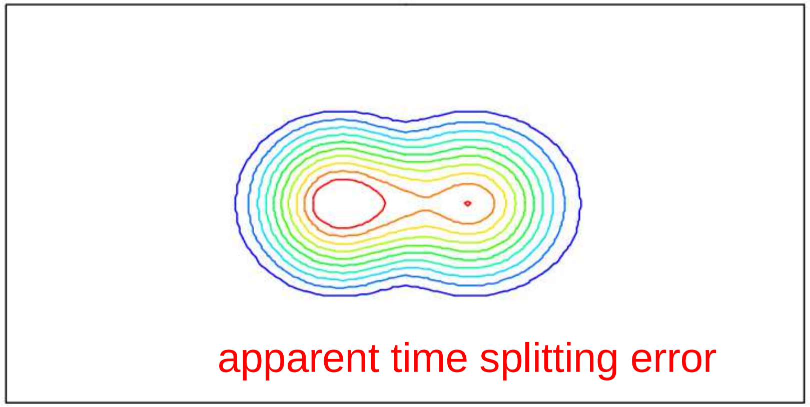


Semi-implicit schemes

Inflow Implicit / Outflow Explicit

Note that $V > 0$

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- origin idea

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1} - c_i^{n-1}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n} - c_i^{n}\right) = c_i^{n-1}$$

K.Mikula, M.Ohlberger: *Inflow-Implicit/Outflow-Explicit Scheme for Solving Advection Equations*, FVCA, 2011

Semi-implicit schemes

Inflow Implicit / Outflow Explicit Note that $V > 0$

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2}\right) = c_i^{n-1}$$

- origin idea

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1} - c_i^{n-1}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n} - c_i^{n}\right) = c_i^{n-1}$$

- upwind method with finite Taylor series

$$c_{i-\frac{1}{2}}^{n-1/2} - c_i^{n-1/2} = c_{i-1}^n - c_i^n + \frac{\Delta x}{2}\frac{c_i^n - c_{i-2}^n}{2\Delta x}$$

$$c_{i+\frac{1}{2}}^{n-1/2} - c_i^{n-1/2} = \frac{\Delta x}{2}\frac{c_{i+1}^{n-1} - c_{i-1}^{n-1}}{2\Delta x}$$

P. Frolkovič, K. Mikula, J. Urbán: *Semi-implicit finite volume level set method for advective motion of interfaces in normal direction*. Appl. Num. Math., 2014

Semi-implicit schemes

Inflow Implicit / Outflow Explicit

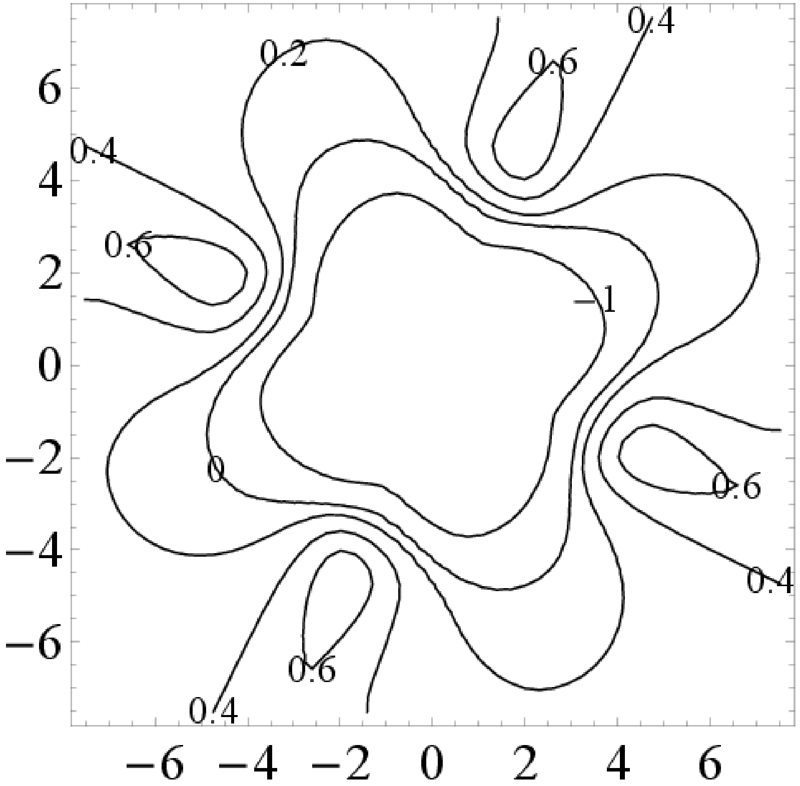
$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(c_{i+\frac{1}{2}}^{n-1} - c_i^{n-1}\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-\frac{1}{2}}^{n} - c_i^{n}\right) = c_i^{n-1}$$

- non-conservative in general
  - they can be rewritten to a conservative form
- second order accurate
- oscillatory in general
  - standard limiter techniques can be used
- linear system with matrices of special structures
  - special solvers can be used
    - fast sweeping and fast marching methods

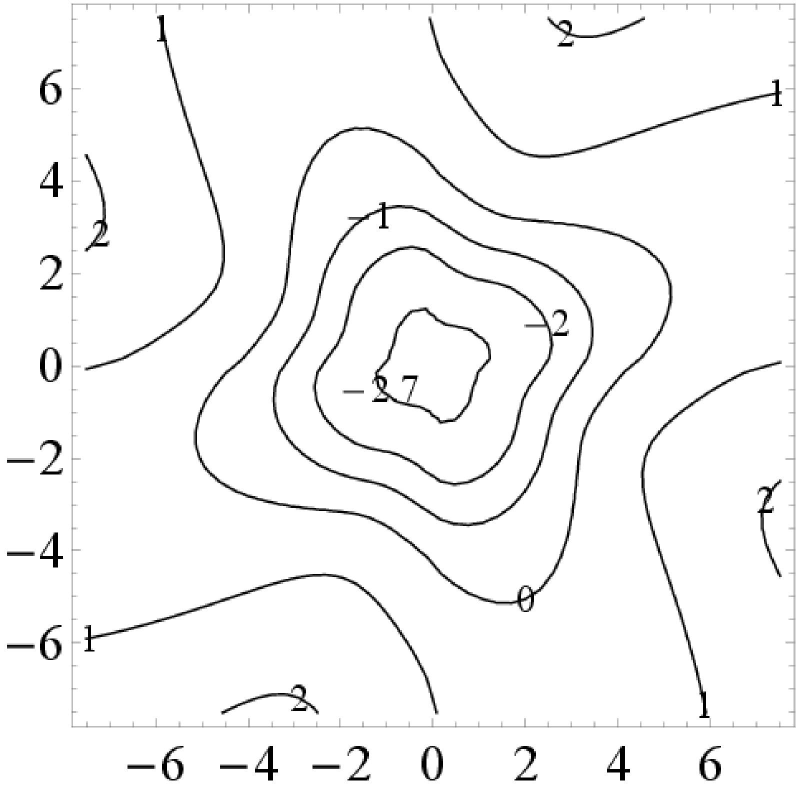
Semi-implicit schemes

Illustrative 2D example

- expansion in normal direction with variable speed



256 small ime steps



1 large time step

Semi-implicit schemes

Conservative form Note that $V > 0$

$$\bar{c}_i^n - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(\bar{c}_{i-\frac{1}{2}}^n - \bar{c}_i^n\right) = c_i^{n-1}$$

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(\bar{c}_{i+\frac{1}{2}}^n - \bar{c}_i^n\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(\bar{c}_{i-\frac{1}{2}}^n - \bar{c}_i^n\right) = c_i^{n-1}$$

Semi-implicit schemes

Conservative form Note that $V > 0$

$$\bar{c}_i^n - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(\bar{c}_{i-\frac{1}{2}}^n - \bar{c}_i^n\right) = c_i^{n-1}$$

$$c_i^n + \frac{\Delta t V_{i+\frac{1}{2}}}{\Delta x}\left(\bar{c}_{i+\frac{1}{2}}^n - \bar{c}_i^n\right) - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(\bar{c}_{i-\frac{1}{2}}^n - \bar{c}_i^n\right) = c_i^{n-1}$$

Limiter in implicit part

$$\bar{c}_i^n\left(1 + \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\right) = \bar{c}_{i-1}^n \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x} + \alpha_i^n\left(\bar{c}_i^n - \bar{c}_{i-2}^n\right)\frac{\Delta t V_{i-\frac{1}{2}}}{4\Delta x} + c_i^{n-1}$$

- choose α_i^n such that

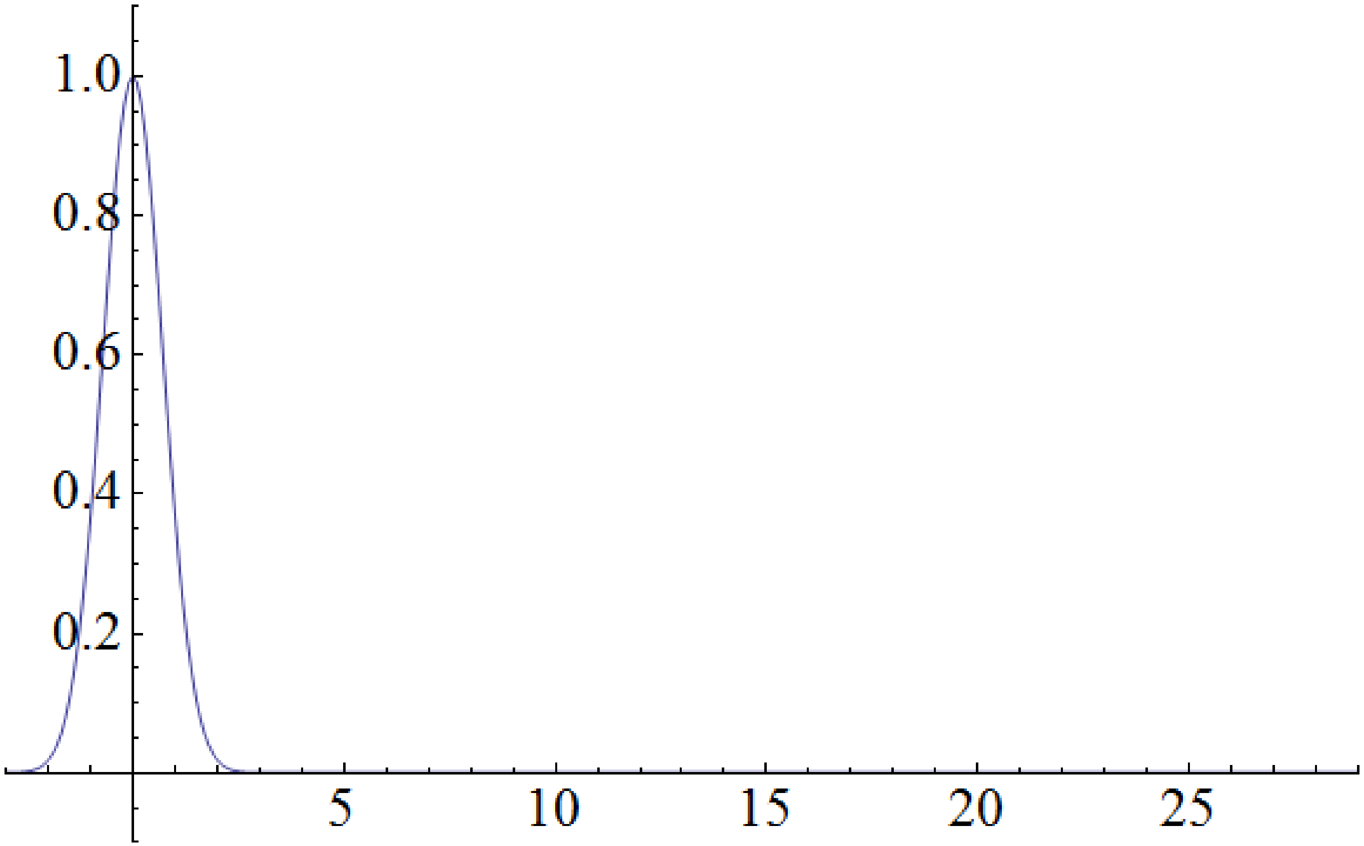
$$c^{\min} - c_i^{n-1} \leq \alpha_i^n\left(\bar{c}_i^n - \bar{c}_{i-2}^n\right)\frac{\Delta t V_{i-\frac{1}{2}}}{4\Delta x} \leq c^{\max} - c_i^{n-1}$$

Inflow Implicit/Outflow Explicit

Illustrative 1D transport equation, V=const

- 1^{st} order accurate fully implicit upwind

$$c_i^n - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-1}^n - c_i^n\right) = c_i^{n-1}$$



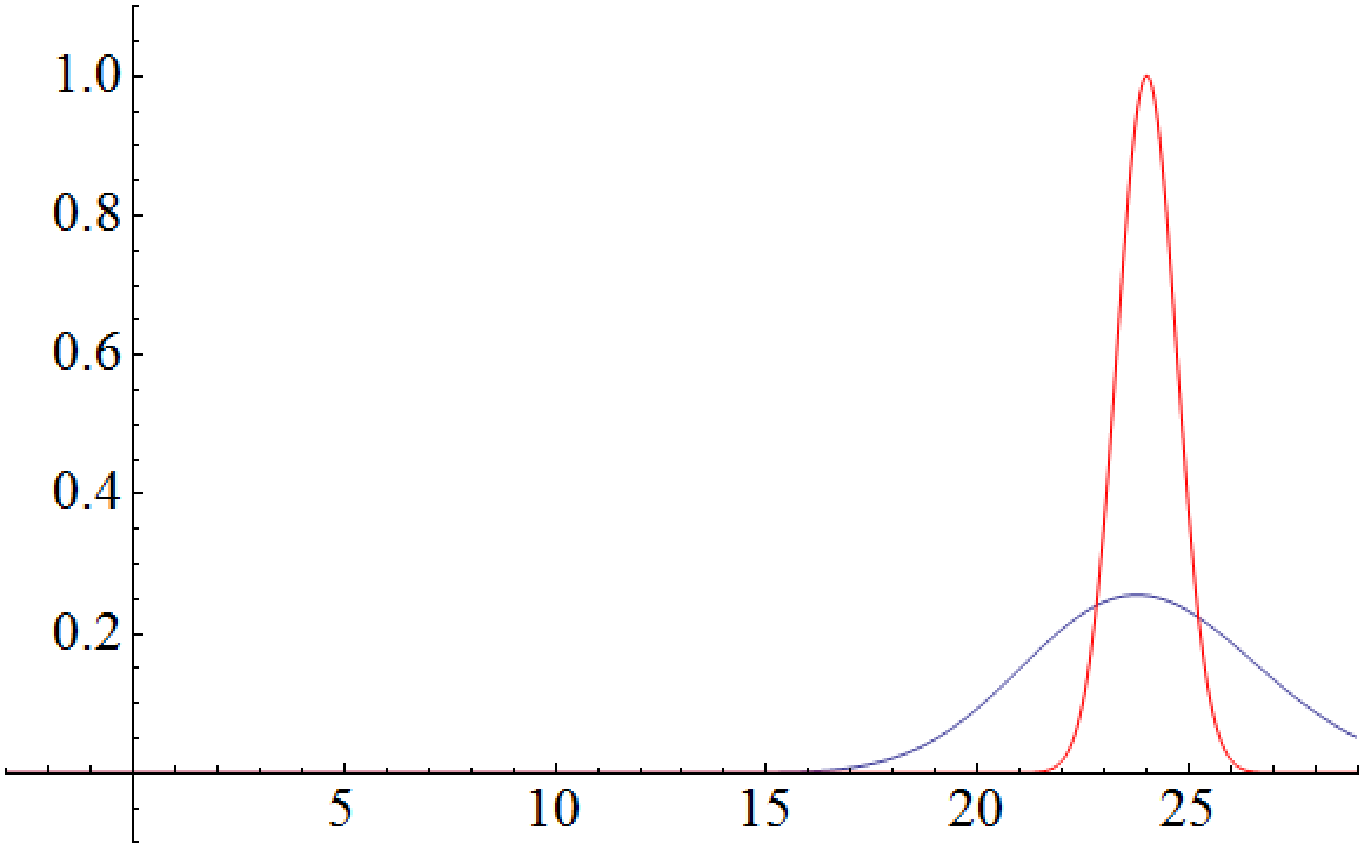
dx=0.1
CFL=1

Inflow Implicit/Outflow Explicit

Illustrative 1D transport equation, *V*=const

- 1st order accurate fully implicit upwind

$$c_i^n - \frac{\Delta t V_{i-\frac{1}{2}}}{\Delta x}\left(c_{i-1}^n - c_i^n\right) = c_i^{n-1}$$



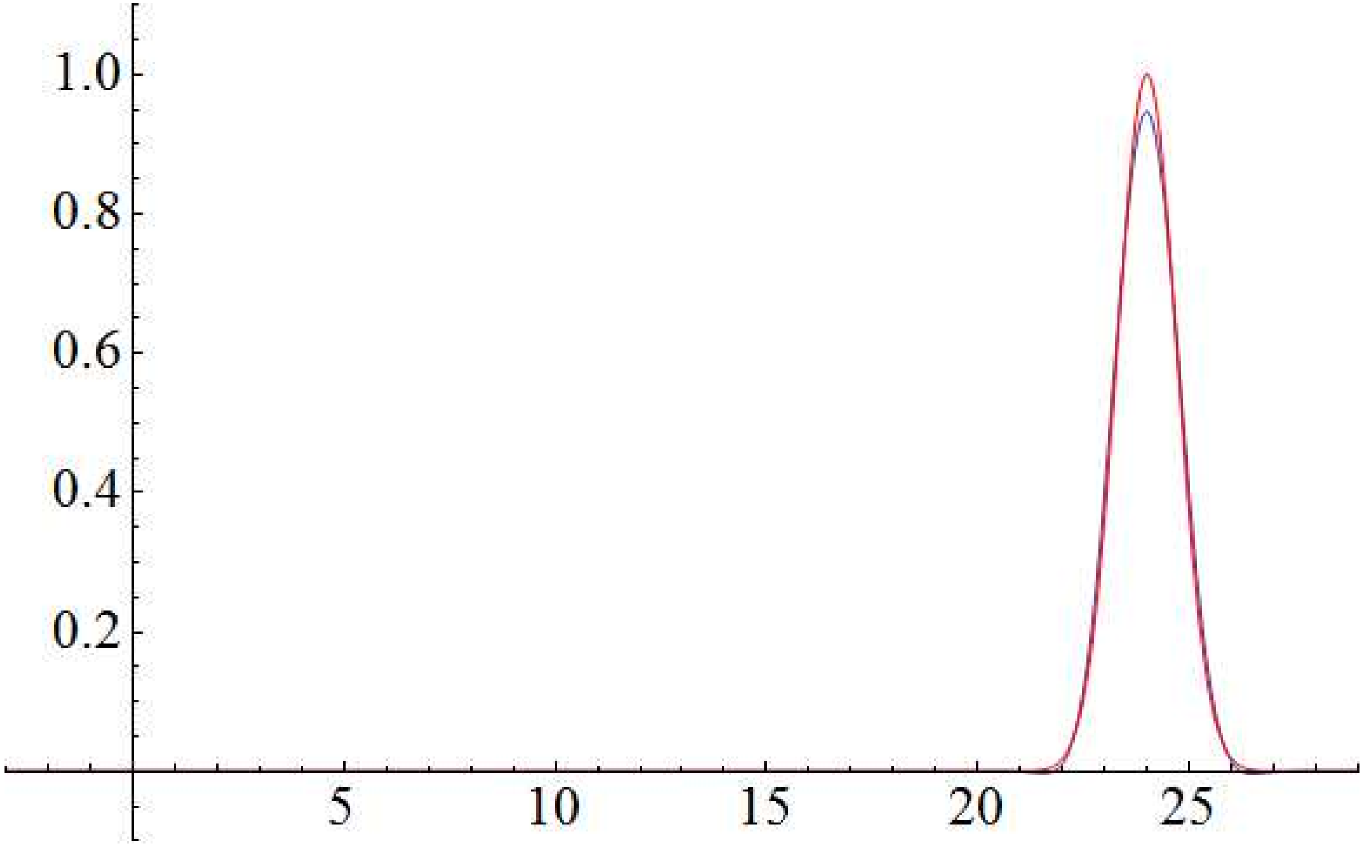
dx=0.1
CFL=1

Inflow Implicit/Outflow Explicit

Illustrative 1D transport equation, *V*=const

- 2nd order accurate semi-implicit upwind

$$c_i^n - \frac{\Delta t V_{i-1/2}}{4\Delta x}\left(-\bar{c}_{i-2}^n + 4\bar{c}_{i-1}^n - 3\bar{c}_i^n\right) = c_i^{n-1} - \frac{\Delta t V_{i+1/2}}{\Delta x}\left(\ldots\right.$$



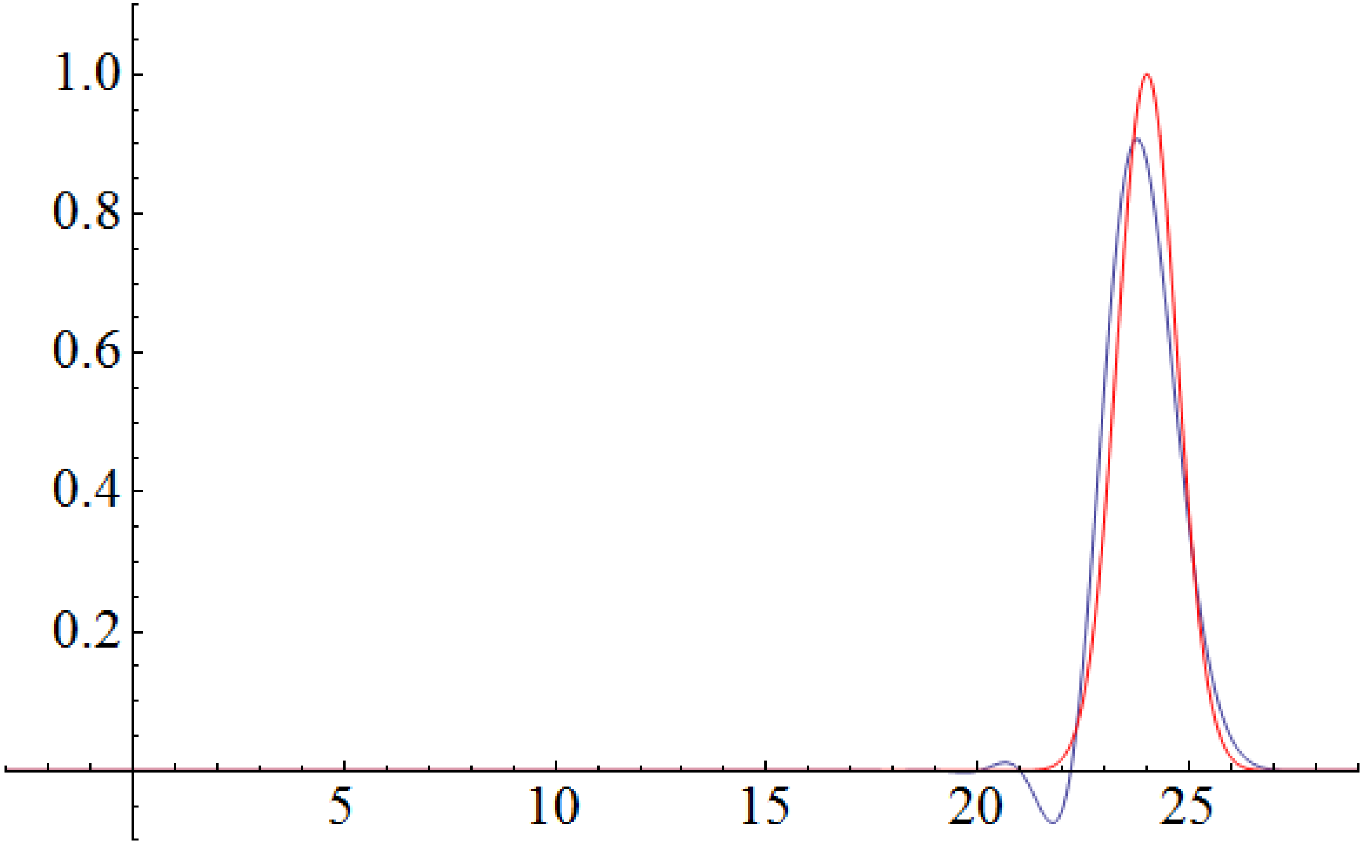
dx=0.1
CFL=1

Inflow Implicit/Outflow Explicit

Illustrative 1D transport equation, *V*=const

- 2^{nd} order accurate semi-implicit upwind

$$c_i^n - \frac{\Delta t V_{i-1/2}}{4\Delta x}\left(-\bar{c}_{i-2}^n + 4\bar{c}_{i-1}^n - 3\bar{c}_i^n\right) = c_i^{n-1} - \frac{\Delta t V_{i+1/2}}{\Delta x}\left(\ldots\right.$$



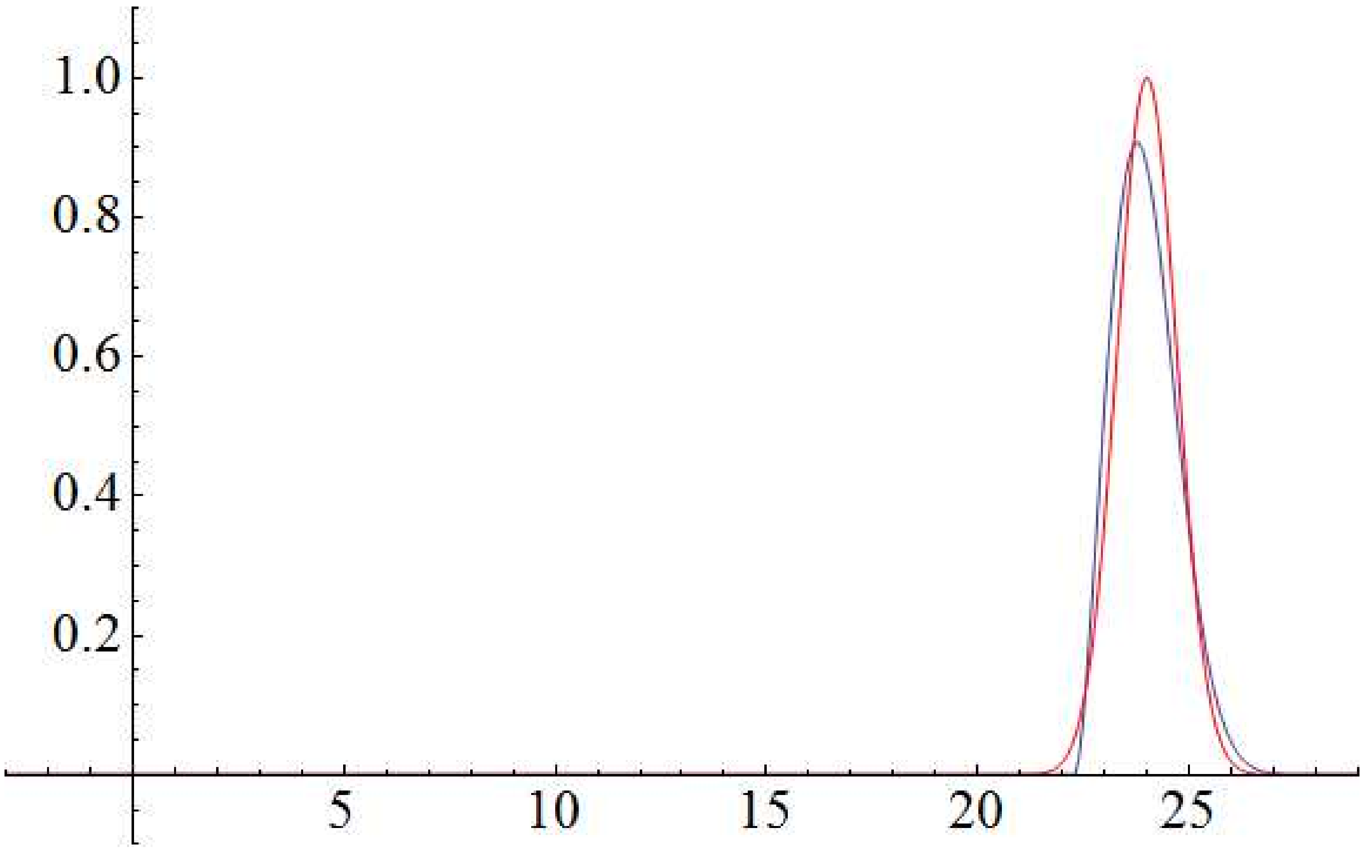
dx=0.1
CFL=2

Inflow Implicit/Outflow Explicit

Illustrative 1D transport equation, *V*=const

- 2nd order accurate method with limiter

$$c_i^n - \frac{\Delta t V_{i-1/2}}{4\Delta x}\left(4\bar{c}_{i-1}^n - 4\bar{c}_i^n + \alpha_i^n(\bar{c}_{i-2}^n - \bar{c}_i^n)\right) = c_i^{n-1} - \ldots$$



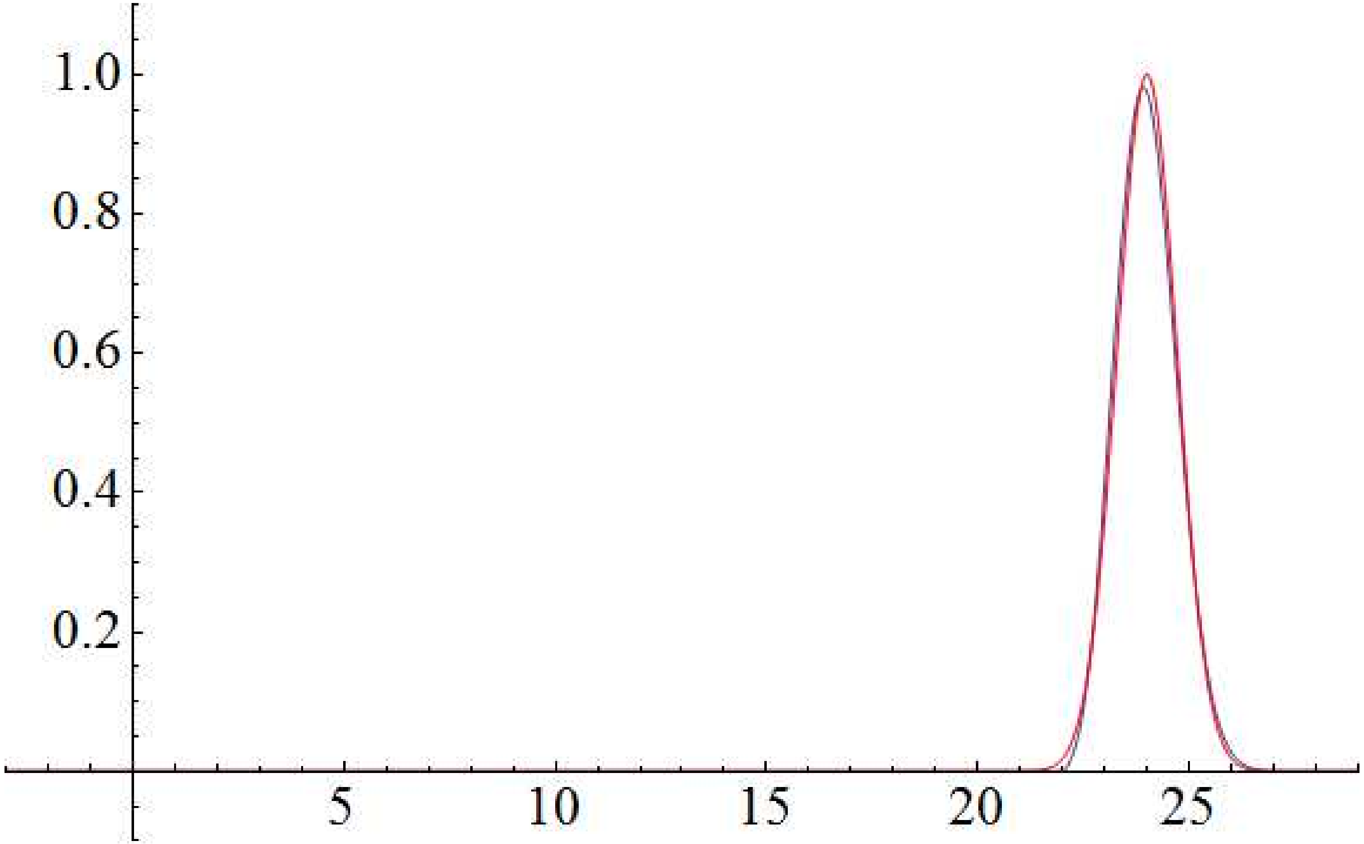
dx=0.1
CFL=2

Inflow Implicit/Outflow Explicit

Illustrative 1D transport equation, *V*=const

- 2nd order accurate method with limiter

$$c_i^n - \frac{\Delta t V_{i-1/2}}{4\Delta x}\left(4\bar{c}_{i-1}^n - 4\bar{c}_i^n + \alpha_i^n(\bar{c}_{i-2}^n - \bar{c}_i^n)\right) = c_i^{n-1} - \ldots$$



dx=0.05
CFL=2

Conclusion

- (semi-) implicit methods for advection dominated problems may be revisited