A General Point of View on Numerical Methods

Institut de Mécanique des Fluides et des Solides,
Strasbourg, France

ackerer@imfs.u-strasbg.fr

Who should be interested ?

Model developpers : some insight in new methods

Model users : you might understand why it sometimes does not work….

OUTLINE

1. Introduction

2. Solving advective dominant transport
   - 2.1. Eulerian methods: Finite Volumes, Finite Elements
   - 2.2. Eulerian-Lagrangian methods: Method of characteristics, ELLAM
   - 2.3. Lagrangian method: Random-walk

3. Solving dispersive dominant transport
   - 3.1. Mixed finite elements
   - 3.2. Multipoint flux approximation

4. Basic matrix algebra
   - 4.1. Matrix properties
   - 4.2. Solving linear systems

First known discretisation : Kepler (1571-1630), 360 segments to calculate Mars' trajectory.

John Napier, or Neper, (1550-1617) discovers the logarithms, which makes the calculations easier.

Baron Gaspard de Prony (1755 –1839) organised numerical calculations:

- a first group of mathematicians to develop the solutions,
- a second group to organize/simplify the calculations,
- a third group (about 60 persons) to do the job.

Charles Babbage (1792-1871) suggested to use machines to improve the calculation efficiency for the third group.

Richardson (1922) was first to apply FD to weather forecasting. It required 3 months CPU to predict the weather for next 24 hours.

Arithmomètre from Thomas de Colmar (1785-1870).

Mathematical models

Fluid mass balance :

$$S\frac{\partial h}{\partial t} + \nabla.\mathbf{q} = 0$$

Momentum conservation (Darcy's law) : $\mathbf{q} = -K\nabla h$

Solute mass balance :

$$\varepsilon\frac{\partial C}{\partial t} + \nabla.(\mathbf{q}C - \mathbf{D}\nabla C) = 0$$

q : specific discharge (Darcy velocity [L/T])
K : permeability tensor of the porous medium [L/T]
D : dispersion tensor defined by :

$$\mathbf{D} = D_m\mathbf{I} + (\alpha_L - \alpha_T)\mathbf{q}\mathbf{q}/|\mathbf{q}| + \alpha_T|\mathbf{q}|\ \mathbf{I}$$

D_m : molecular diffusion coefficient [L^2/T],
I : the unit tensor [-],
$\alpha_{L,}$ α_T : longitudinal and transversal dispersivity [L].

A family of well known partial differential equations (PDE)

Elliptic PDE : $\nabla.\left(b\nabla u\right)=0$

Parabolic PDE : $a\dfrac{\partial u}{\partial t}+\nabla.\left(b\nabla u\right)=0$

Hyperbolic PDE : $a\dfrac{\partial u}{\partial t}+\nabla.(bu)=0$

corresponding to many mathematical models used in Physics and Earth Sciences :

Heat transfer, solute diffusion, electricity, solid mechanics,

potential flow, magnetostatics, ... geology,...

Two main problems will be adressed:

Advective dominant transport (sharp fronts)

Eulerian methods: Finite Volumes, Finite Elements
Eulerian-Lagrangian methods: Method of characteristics, ELLAM
Lagrangian method: Random-walk

Discontinuous full tensor flux related parameter (K or D – diffusion type models)

Mixed finite elements
Multipoint flux approximation

$$\mathbf{div}\, K\,\mathbf{grad}\, u = f,\ (x,y,z) \in V\ ; \quad u(x,y,z) = 0,\ (x,y,z) \in \partial V$$

Flux Form: $\mathbf{div}\,\mathbf{W} = f\ ,\ \ \mathbf{W} = -K\,\mathbf{grad}\,u$

Flux Operator: $G\,u = -K\,\mathbf{grad}\,u\ \rightarrow\ \ \mathbf{div}\,\mathbf{W} = \mathbf{f}\ ,\ \ \mathbf{W} = \mathbf{G}\,\mathbf{u}$

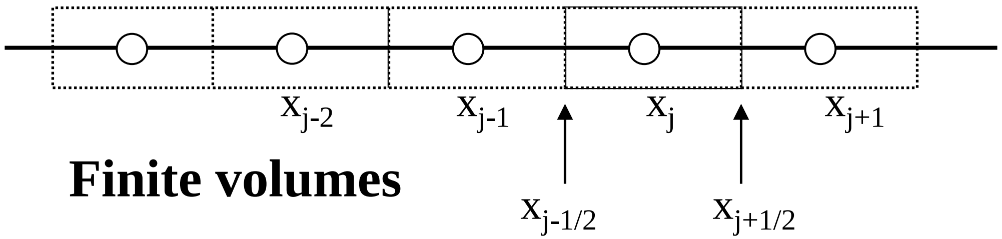
Integral Identity: $\int_V u\,\mathbf{div}\mathbf{W}\,dV - \int_V (K^{-1}\mathbf{W}, G\,u)\,dV = 0$

Inner Products and Adjointness of Divergence and Flux Operator:

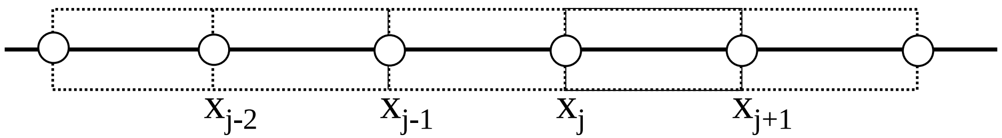
$$(u,\, v)_H = \int_V u\, v\, dV\ ;\ (\mathbf{A},\,\mathbf{B})_{\mathcal{H}} = \int_V (K^{-1}\,\mathbf{A},\,\mathbf{B})\,dV$$

$$(u,\,\mathbf{div}\,\mathbf{W})_H - (\mathbf{W},\, G\,u)_{\mathcal{H}} = 0;\ \rightarrow G = \mathbf{div}^*$$

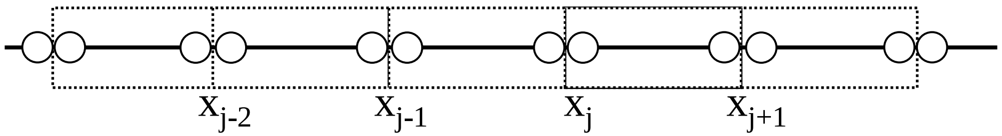
Conservation: $\int_V \mathbf{div}\mathbf{W}\,dV = \oint_{\partial V} (\mathbf{W}, \mathbf{n})\,dS = \int_V f\,dV$



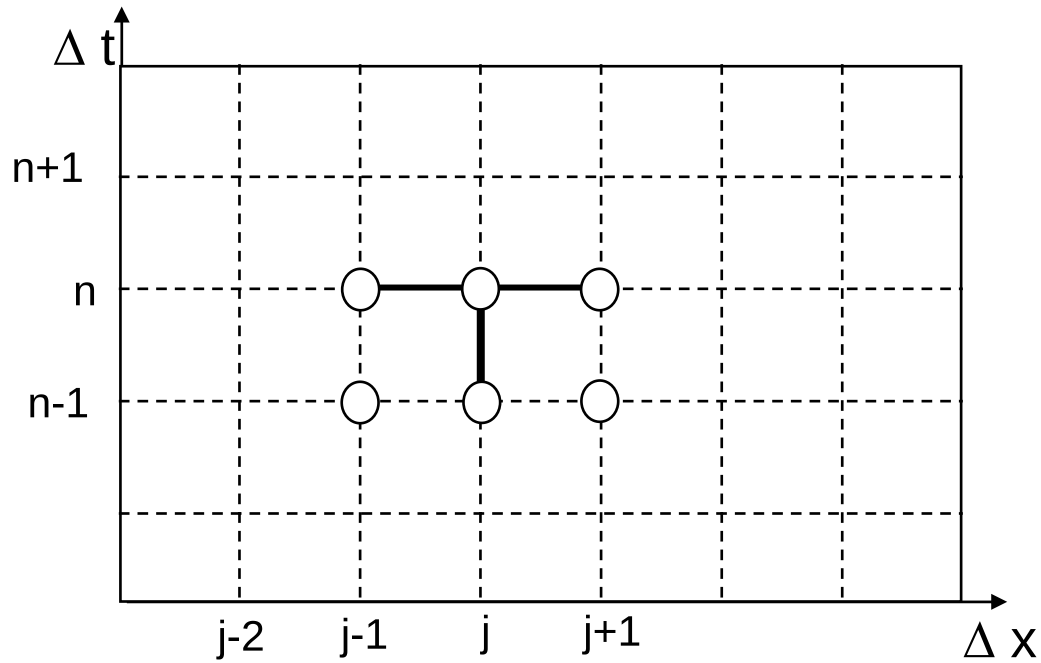
Finite volumes



Finite elements



Discontinuous finite elements



Space/time discretization

Finite differences method (FD):

Basic ideas:

1. Use Taylor's (1685-1731) series

$$f(x+\Delta x) = f(x) + \Delta x \frac{\partial f}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 f}{\partial x^2} + \ldots$$

$$f(x-\Delta x) = f(x) - \Delta x \frac{\partial f}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 f}{\partial x^2} + \ldots$$

$$\frac{\partial f}{\partial x} \simeq \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

$$\frac{\partial f}{\partial x} \simeq \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

$$\frac{\partial^2 f}{\partial x^2} \simeq \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2}$$

2. Replace the derivatives

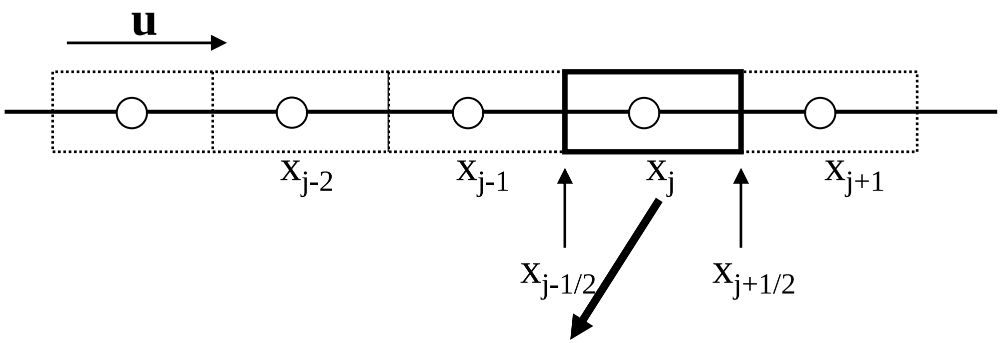
$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0$$

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{\left(C_j^{n*} - C_{j-1}^{n*}\right)}{\Delta x} = 0$$

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{\left(C_{j+1}^{n*} - C_{j-1}^{n*}\right)}{2\Delta x} = 0$$

Finite Volumes methods

FVM have a very strong physical meaning



$$\Delta x \frac{C_j^{n+1} - C_j^n}{\Delta t} = u\left(C_{j-1/2}^{n*} - C_{j+1/2}^{n*}\right)$$

$$C_{j+1/2} = C_j$$

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{\left(C_j^{n*} - C_{j-1}^{n*}\right)}{\Delta x} = 0$$

$$C_{j+1/2} = \frac{1}{2}\left(C_j + C_{j+1}\right)$$

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{\left(C_{j+1}^{n*} - C_{j-1}^{n*}\right)}{2\Delta x} = 0$$

Some key numbers (1D)

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = 0$$

$$\Delta x \frac{C_j^{n+1} - C_j^n}{\Delta t} = u\left(C_{j-1}^n - C_j^n\right)$$

$$C(x+\Delta x) = C(x) + \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2} + \ldots$$

$$\frac{\partial C}{\partial x} \simeq \frac{C(x+\Delta x) - C(x)}{\Delta x} - \frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2}$$

$$C_j^{n+1} = C_j^n\left(1 - \frac{u\Delta t}{\Delta x}\right) + C_{j-1}^n$$

$$\frac{\partial C}{\partial t} + u\frac{C(x+\Delta x) - C(x)}{\Delta x} - \left(D + u\frac{\Delta x}{2}\right)\frac{\partial^2 C}{\partial x^2} = 0$$

To avoid oscillation for this scheme

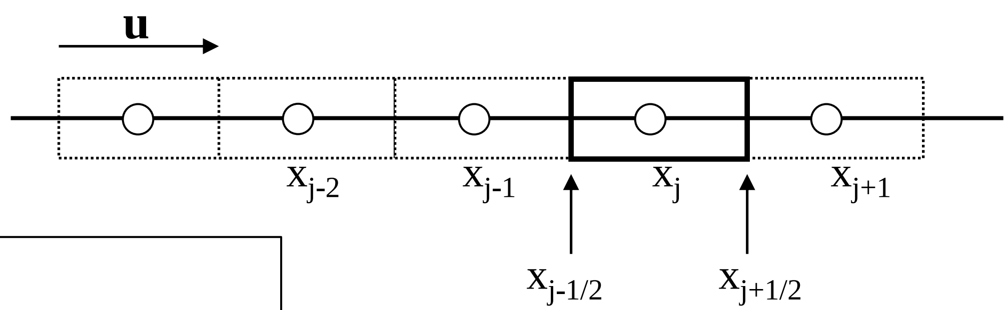
$$CFL = \frac{u\Delta t}{\Delta x} < 1$$

(R. Courant, K. Friedrichs & H. Lewy ,1924)

To reduce numerical diffusion

$$\frac{u\Delta x}{2} \ll D \quad \text{or}$$

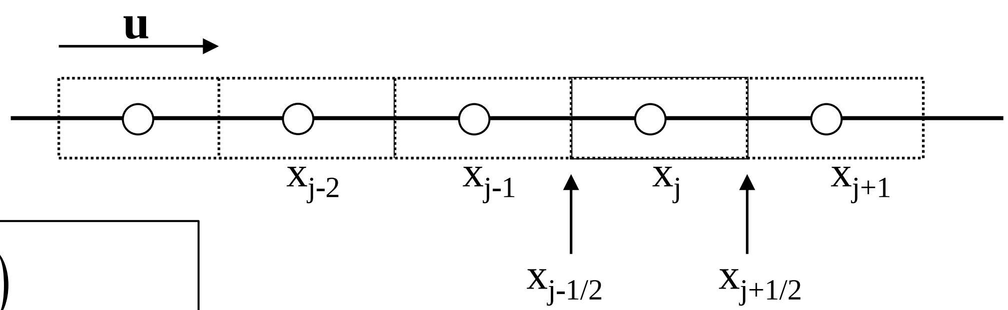
$$\text{Grid Peclet number} = \frac{u\Delta x}{D} \ll 2$$



General FV formulation

$$\frac{1}{\Delta t}\left(aC_j^{n+1} + (1-2a)C_j^n + (a-1)C_j^{n-1}\right) + u\left\{\frac{\theta}{\Delta x}\left(C_{j+1/2}^{n+1} - C_{j-1/2}^{n+1}\right) + \frac{1-\theta}{\Delta x}\left(C_{j+1/2}^{n} - C_{j-1/2}^{n}\right)\right\} = 0$$

For a = 1 and θ =0, explicit scheme
For a = 1 and θ =1, implicit scheme
For a = 1 and θ =1/2, Crank-Nicholson scheme
For a = 1/2 and θ =0, Leap-Frog scheme
For a = 5/6 and θ =1/3, third order scheme
For a = 3/2 and θ =1, first order BDF
....



$$C_{j+1/2} = \frac{1}{2}\left(\left(-\beta\right)C_{j-1} + \left(1+2\beta\right)C_j + \left(1-\beta\right)C_{j+1}\right)$$

For β = 0, centered scheme

$$C_{j+1/2} = \frac{1}{2}\left(C_j + C_{j+1}\right)$$

For β = 1/3, third order upwind scheme

$$C_{j+1/2} = \frac{1}{2}\left(-\frac{1}{3}C_{j-1} + \frac{5}{3}C_j + \frac{2}{3}C_{j+1}\right)$$

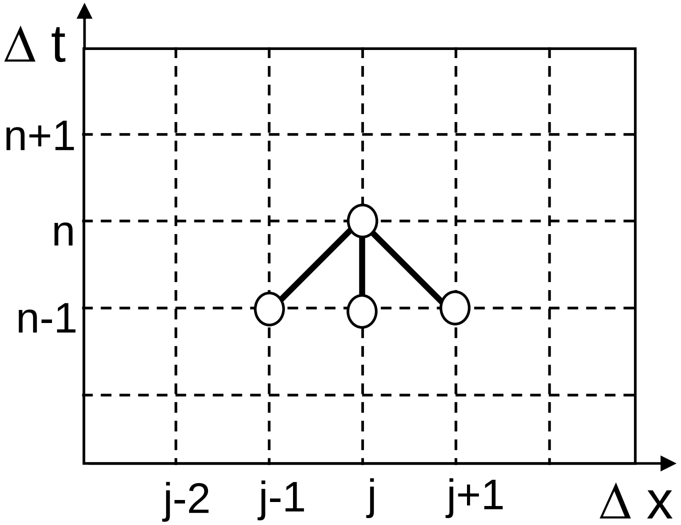
For β = 1, fully upwind scheme

$$C_{j+1/2} = \frac{1}{2}\left(-C_{j-1} + 3C_j\right)$$

Explicit scheme : a = 1, θ =0

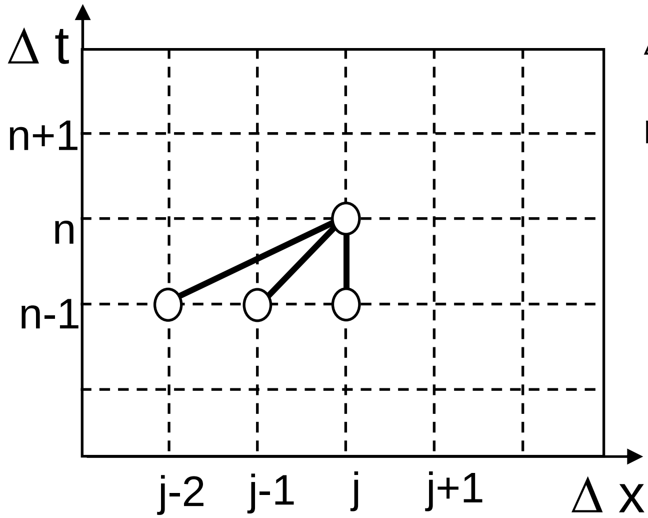
For β = 0, centered scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(C_{j+1} - C_{j-1}\right)$$



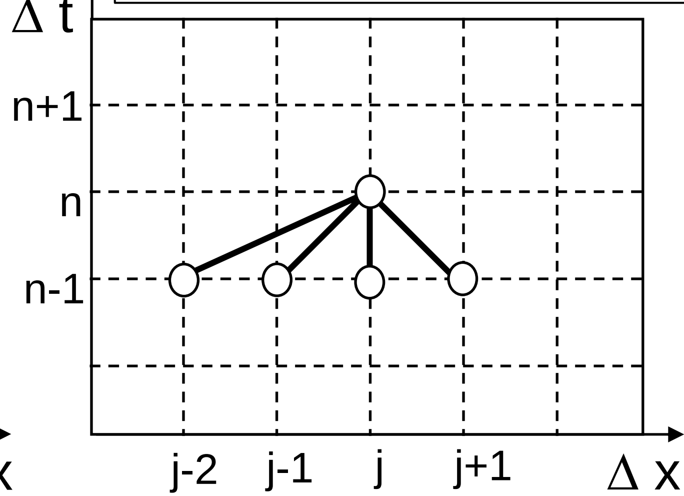
For β = 1, fully upwind scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(C_{j-2} - 4C_{j-1} + 3C_{j}\right)$$



β = 1/3: 3rd upwind scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(\frac{1}{3}C_{j-2} - 2C_{j-1} + C_{j} + \frac{2}{3}C_{j+1}\right)$$



Implicit scheme : a = 1, θ =1

For β = 0, centered scheme

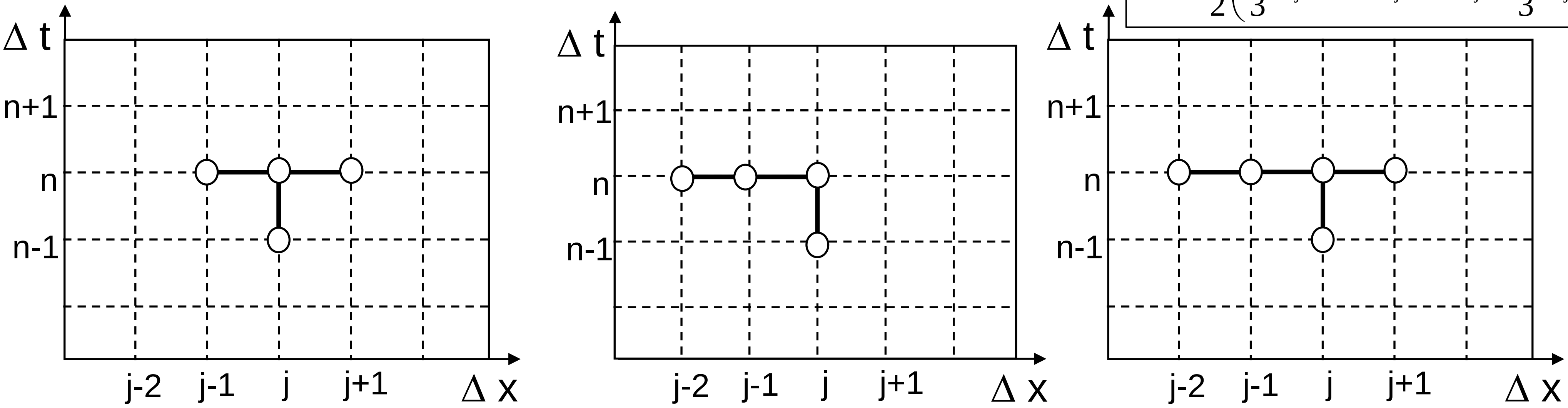
$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(C_{j+1} - C_{j-1}\right)$$

For β = 1, fully upwind scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(C_{j-2} - 4C_{j-1} + 3C_{j}\right)$$

β = 1/3: 3rd upwind scheme

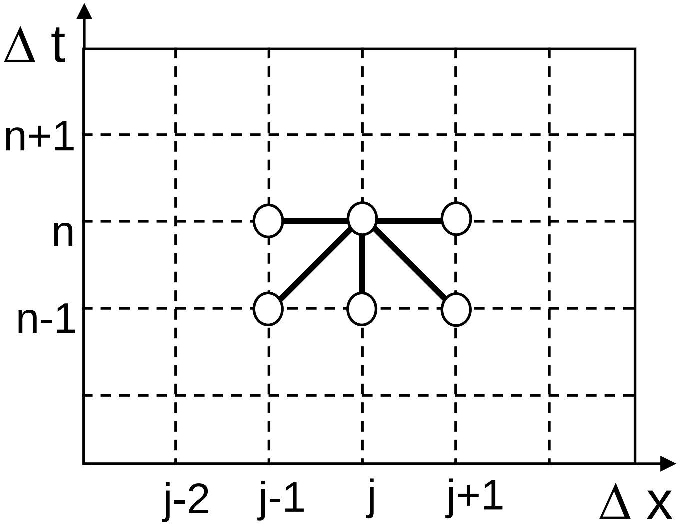
$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(\frac{1}{3}C_{j-2} - 2C_{j-1} + C_{j} + \frac{2}{3}C_{j+1}\right)$$



Crank-Nicholson scheme : a = 1, θ =1/2

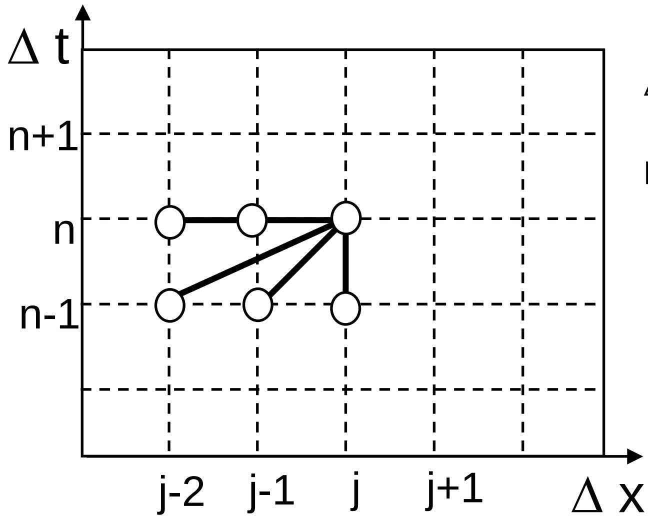
For β = 0, centered scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(C_{j+1} - C_{j-1}\right)$$



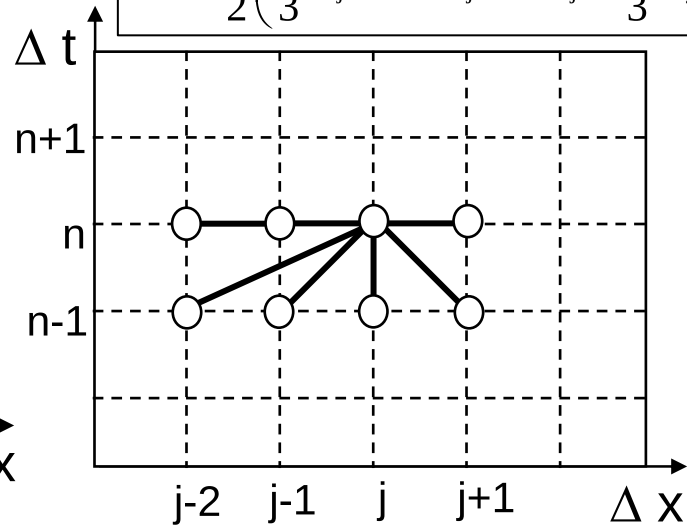
For β = 1, fully upwind scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(C_{j-2} - 4C_{j-1} + 3C_{j}\right)$$



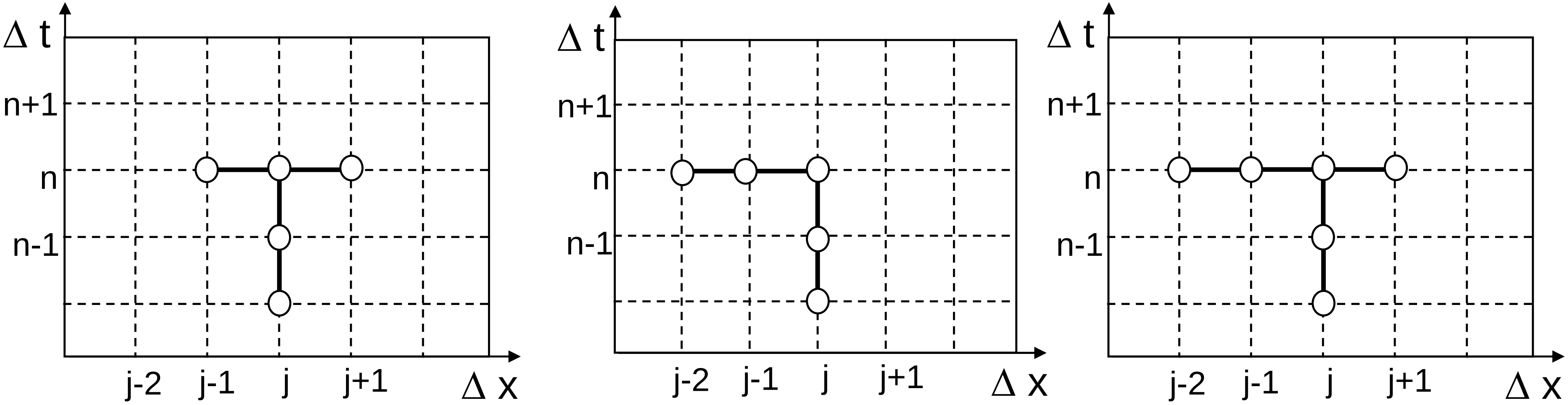
β = 1/3: 3rd upwind scheme

$$C_{j+1/2} - C_{j-1/2} = \frac{1}{2}\left(\frac{1}{3}C_{j-2} - 2C_{j-1} + C_{j} + \frac{2}{3}C_{j+1}\right)$$



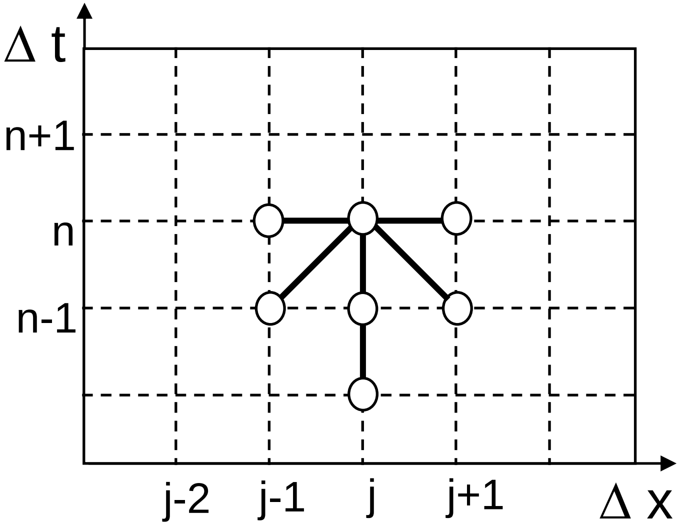
First order BDF : a = 3/2 θ =1

For β = 0, centered scheme   For β = 1, fully upwind scheme β = 1/3: 3rd order upwind scheme

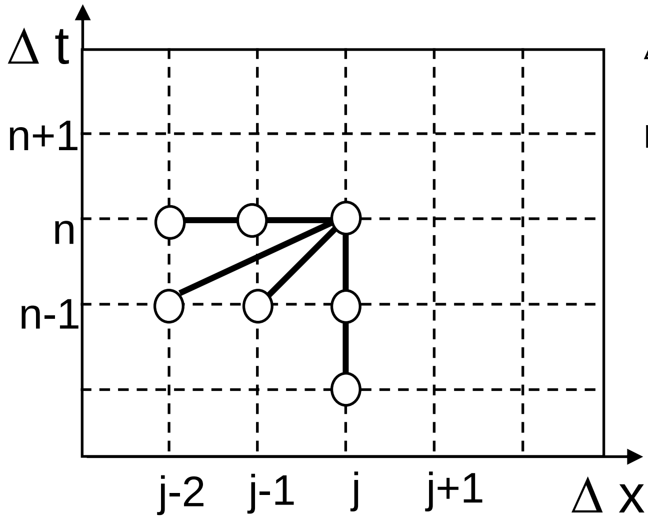


Third order : a = 5/6 θ =1/3

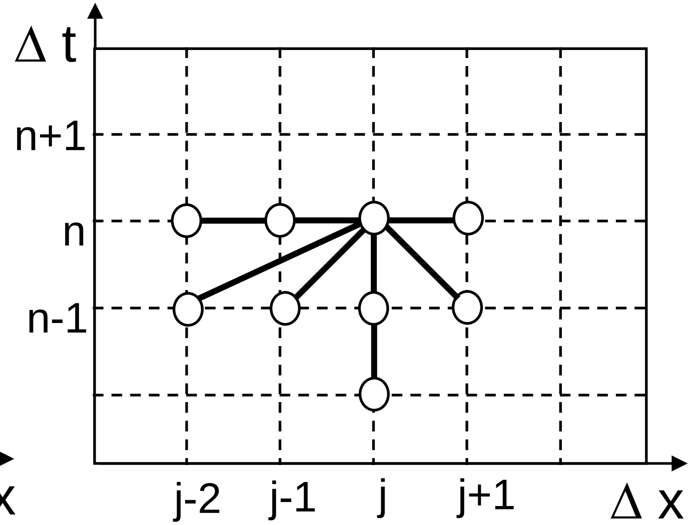
For β = 0, centered scheme



For β = 1, fully upwind scheme



β = 1/3: 3rd order upwind scheme

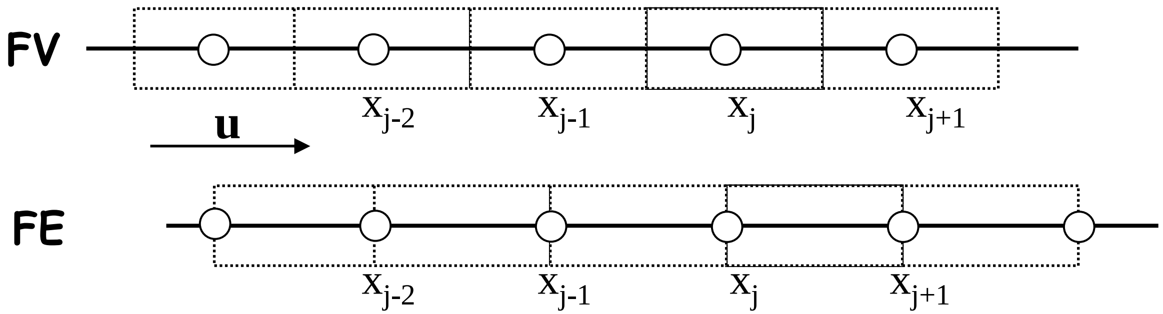


Flux discretisation

Time discretization

	1rd order Upwind	Centered	3rd order Upwind
Implicit	CFL=1 CFL=5	CFL=1 CFL=5	CFL=1 CFL=5
Crank-Nicholson	CFL=1 CFL=5	CFL=1 CFL=5	CFL=1 CFL=5
1rd order BDF	CFL=1 CFL=5	CFL=1 CFL=5	CFL=1 CFL=5

Galerkin Finite Elements method



$$L(C) = \frac{\partial C}{\partial t} + \nabla \cdot \left(uC - D\nabla C \right) = 0$$

Basic ideas:

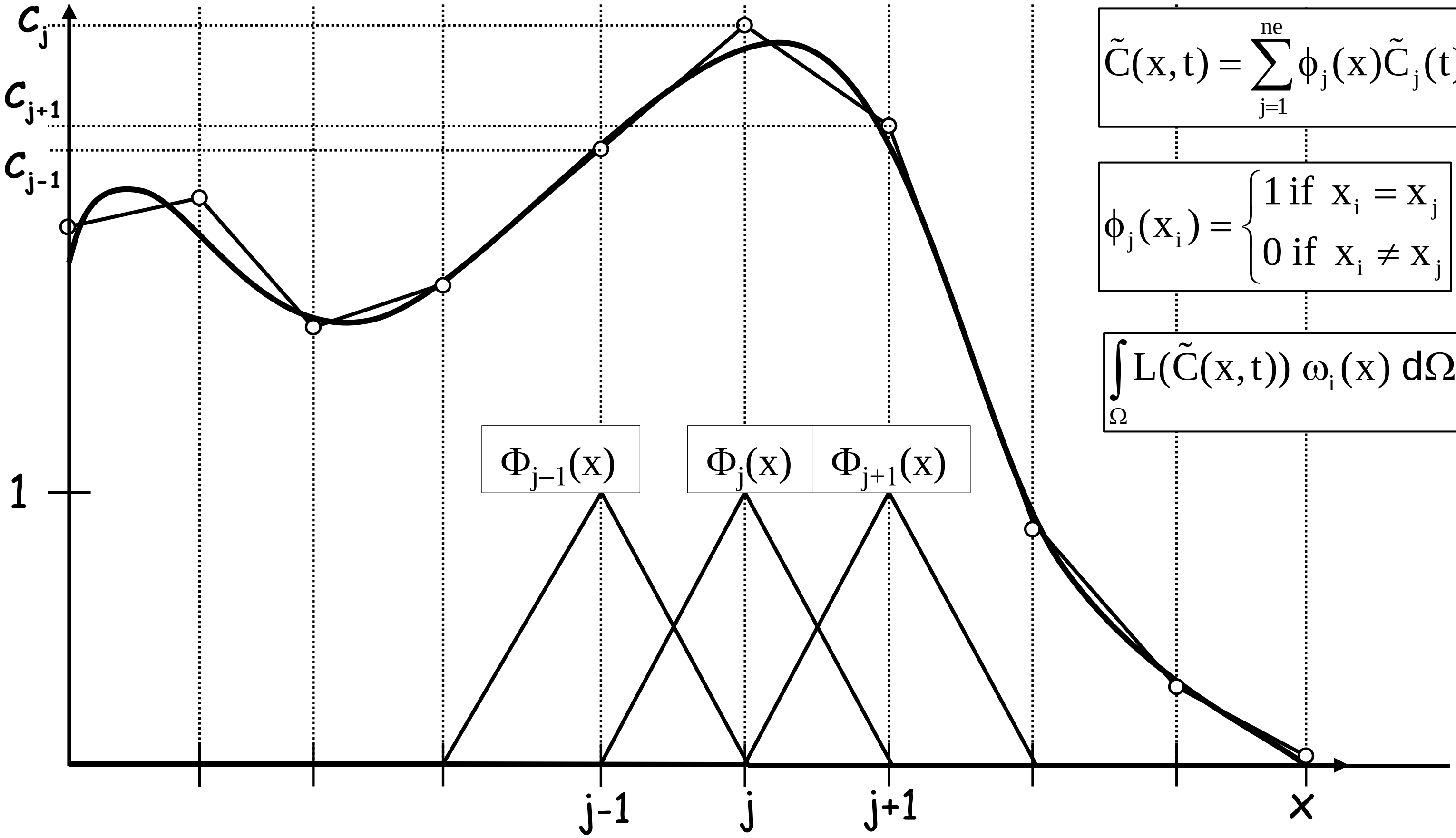
1. Approximate the unknown function by a sum of 'simple' functions

$$\tilde{C}(x,t) = \sum_{j=1}^{ne} \phi_j(x)\tilde{C}_j(t)$$ with $$\phi_j(x_i) = \begin{cases} 1 \text{ if } x_i = x_j \\ 0 \text{ if } x_i \neq x_j \end{cases}$$ so that $$\tilde{C}(x_j,t) = \tilde{C}_j(t)$$

2. The numerical solution should be as close as possible to the exact solution over the domain

$$\int_\Omega L(\tilde{C}(x,t))\ \omega(x)\ d\Omega = 0$$ for any $$\omega(x)$$

$$\int_\Omega L(\tilde{C}(x,t))\ \omega_i(x)\ d\Omega = 0$$ with i=1 to ne,which leads to ne equations with ne unknowns



$$\tilde{C}(x,t) = \sum_{j=1}^{ne} \phi_j(x)\tilde{C}_j(t)$$

$$\phi_j(x_i) = \begin{cases} 1 \text{ if } x_i = x_j \\ 0 \text{ if } x_i \neq x_j \end{cases}$$

$$\int_\Omega L(\tilde{C}(x,t))\ \omega_i(x)\ d\Omega = 0$$

Nodal interpolation

Basic ideas:

3. Choose $\omega_i(x) = \phi_i(x)$

$$\int_\Omega \left(\frac{\partial C}{\partial t} + \nabla \cdot \left(uC - D\nabla C \right) \right) \phi_i \; d\Omega = 0$$

leads to

$$\int_\Omega \left[\frac{\partial \sum_j \left(\tilde{C}_j \phi_j \right)}{\partial t} + \nabla \cdot \left(u \sum_j \left(\tilde{C}_j \phi_j \right) - D\nabla \sum_j \left(\tilde{C}_j \phi_j \right) \right) \right] \phi_i \; d\Omega = 0$$

4. Standard Euler/implicit scheme for time discretization, for example

$$\int_\Omega \left[\frac{\sum_j \left(\tilde{C}_j^{n+1} \phi_j \right) - \sum_j \left(\tilde{C}_j^{n} \phi_j \right)}{\Delta t} + \nabla \cdot \left(u \sum_j \left(\tilde{C}_j^{n+1} \phi_j \right) - D\nabla \sum_j \left(\tilde{C}_j^{n+1} \phi_j \right) \right) \right] \phi_i \; d\Omega = 0$$

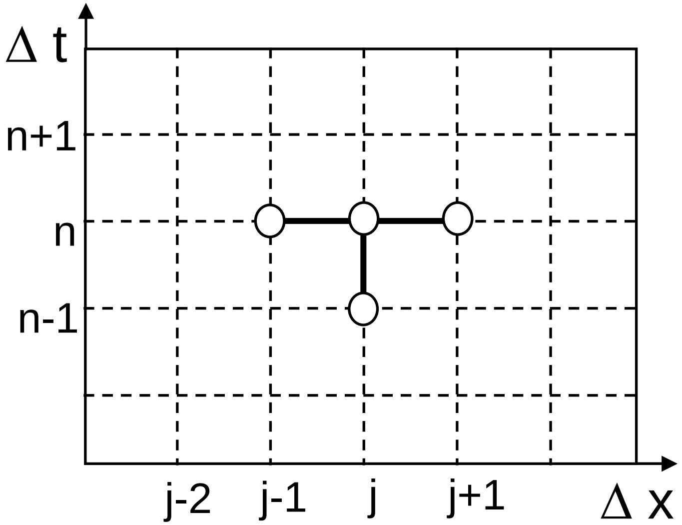
written for i=1 to ne.

The next steps are more or less easy mathematics ...

Example :

1D simulation with $\phi(x)=ax+b$, constant velocity and dispersion

$$
\begin{cases}
\displaystyle\int_\Omega \left[\left(\frac{\sum_j\left(\tilde{C}_j^{n+1}\phi_j\right)-\sum_j\left(\tilde{C}_j^{n}\phi_j\right)}{\Delta t}\right)\right]\phi_i\ d\Omega=\frac{1}{6\Delta t}\left(\tilde{C}_{j-1}^{n+1}-\tilde{C}_{j-1}^{n}\right)+\frac{1}{3\Delta t}\left(\tilde{C}_{j}^{n+1}-\tilde{C}_{j}^{n}\right)+\frac{1}{6\Delta t}\left(\tilde{C}_{j+1}^{n+1}-\tilde{C}_{j+1}^{n}\right) \\
\displaystyle\int_\Omega \left[\nabla\cdot\left(u\sum_j\left(\tilde{C}_j^{n+1}\phi_j\right)-D\nabla\sum_j\left(\tilde{C}_j^{n+1}\phi_j\right)\right)\right]\phi_i\ d\Omega=\frac{u}{2\Delta x}\left(\tilde{C}_{j+1}^{n+1}-\tilde{C}_{j-1}^{n+1}\right)-\frac{D}{\Delta x^2}\left(\tilde{C}_{j-1}^{n+1}-2\tilde{C}_{j1}^{n+1}+\tilde{C}_{j+1}^{n+1}\right)
\end{cases}
$$



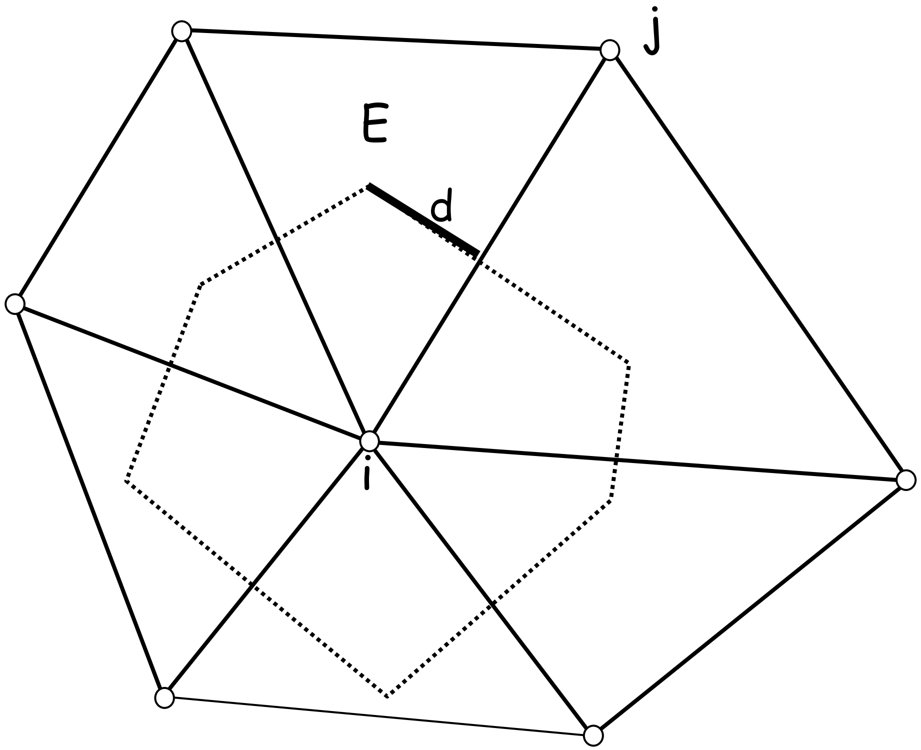
CFL=1

CFL=5

In 2D/3D :

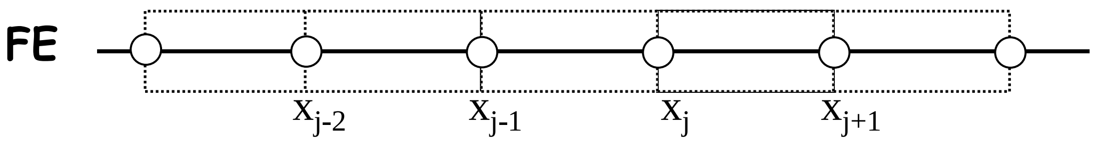
$$\int_{\Omega}\left(\frac{\partial C}{\partial t}+\nabla\cdot\left(uC-D\nabla C\right)\right)\phi_i \; d\Omega=0$$

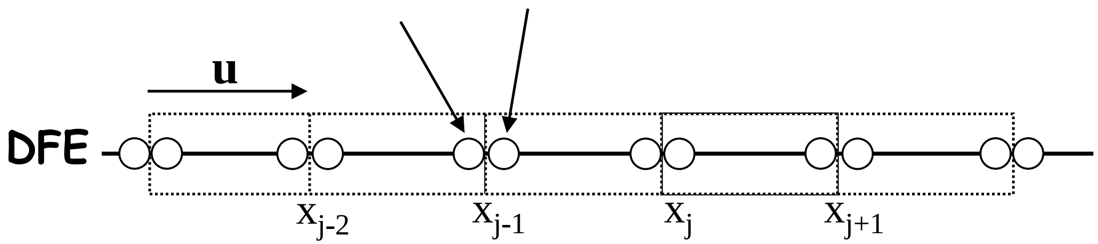
It is also a mass balance over a given patch:



$$q^E_{i,j}=\left[u^E\left(\frac{C_i+C_j}{2}\right)-D^E\frac{C_j-C_i}{l_{i,j}}\right]d$$

Galerkin Discontinuous Finite elements method





Basic ideas:

1. Approximate the unknown function by a sum of 'simple' functions INSIDE an element E

$$\tilde{C}(x,t) = \sum_{j=1}^{E} \phi_j(x)\tilde{C}_j(t)$$

2. Defining on node/edge/face A inside of E and

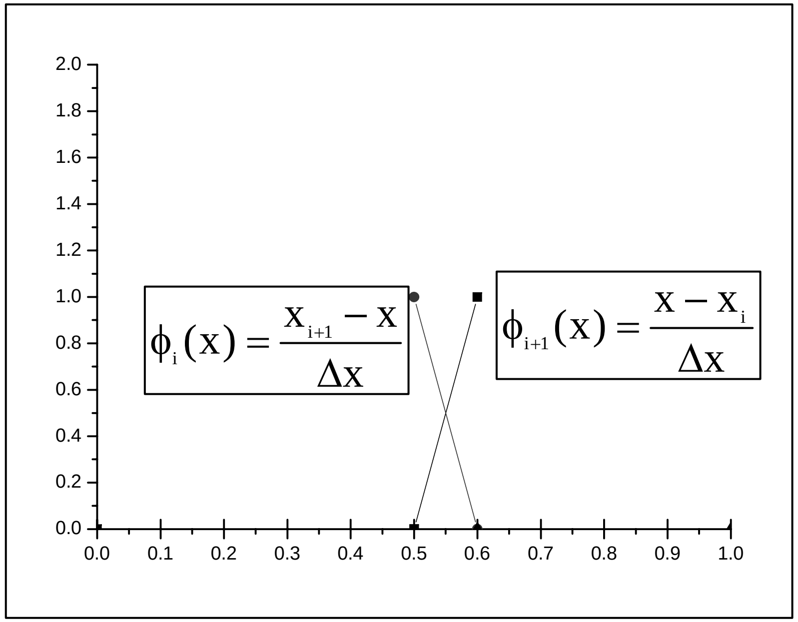
on edge/face A outside of E

Hyperbolic 1D

$$\frac{\partial C}{\partial t} = -\nabla \cdot (uC)$$

Linear approximation

$$C(x,t) = \phi_i(x)C_i(t) + \phi_{i+1}(x)C_{i+1}(t)$$



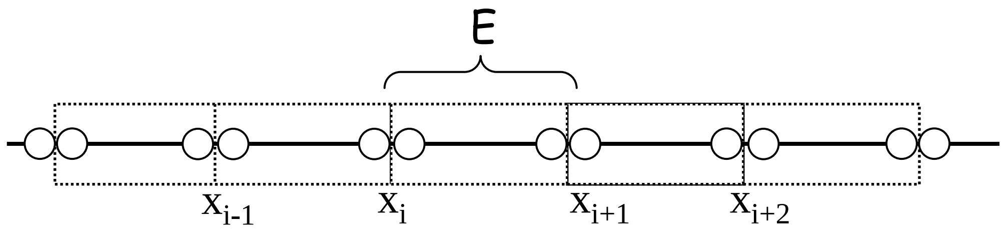
Variational form

$$\int_E \frac{\partial C}{\partial t} w_i dx = -\int_E \nabla.(uC) w_i dx$$

$$\int_E \frac{\partial C}{\partial t} w_i dx = \int_E uC\nabla w_i dx \ - u(C_{i+1} w_i(x_{i+1}) - C_i w_i(x_i))$$

Galerkin formulation

$$w_i(x) = \phi_i(x)$$



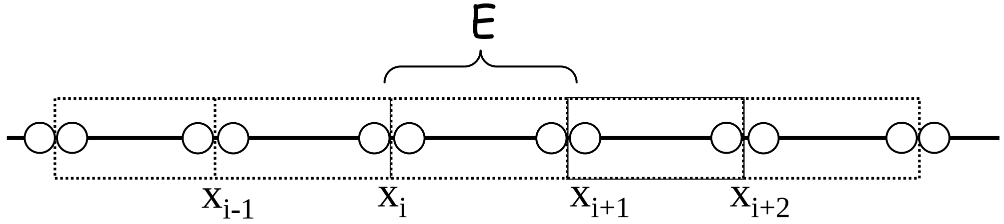
Discretization

$$\begin{cases} \int_E \frac{\partial C}{\partial t} w_i \, dx = \int_E uC\nabla w_i dx + uC_i^* \\ \int_E \frac{\partial C}{\partial t} w_{i+1} dx = \int_E uC\nabla w_{i+1} dx - uC_{i+1}^* \end{cases}$$

Explicit formulation leads to a local system:

$$\begin{cases} 2\tilde{C}_i^{n+1} + \tilde{C}_{i+1}^{n+1} = C_i^n \left(2 - 3\frac{u\Delta t}{\Delta x}\right) + C_{i+1}^n \left(1 - 3\frac{u\Delta t}{\Delta x}\right) + u\frac{6\Delta t}{\Delta x} C_i^{*,n} \\ \tilde{C}_i^{n+1} + 2\tilde{C}_{i+1}^{n+1} = C_i^n \left(1 + 3\frac{u\Delta t}{\Delta x}\right) + C_{i+1}^n \left(2 + 3\frac{u\Delta t}{\Delta x}\right) - u\frac{6\Delta t}{\Delta x} C_{i+1}^{*,n} \end{cases}$$

DGFE : 1D discretization



Step 1: $t \in \left[t, t + \Delta t/2\right]$

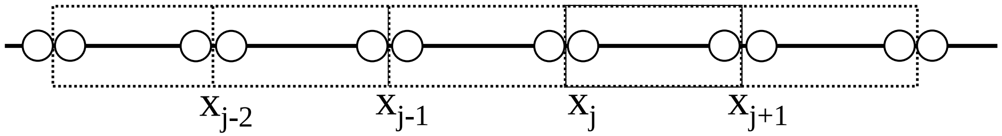
$$\begin{cases} 2C_i^{n+1/2} + C_{i+1}^{n+1/2} = C_i^n\left(2 - 3\dfrac{u\Delta t/2}{\Delta x}\right) + C_{i+1}^n\left(1 - 3\dfrac{u\Delta t/2}{\Delta x}\right) + u\dfrac{6\Delta t/2}{\Delta x}C_i^n \\ C_i^{n+1/2} + 2C_{i+1}^{n+1/2} = C_i^n\left(1 + 3\dfrac{u\Delta t/2}{\Delta x}\right) + C_{i+1}^n\left(2 + 3\dfrac{u\Delta t/2}{\Delta x}\right) - u\dfrac{6\Delta t/2}{\Delta x}C_{i+1}^n \end{cases}$$

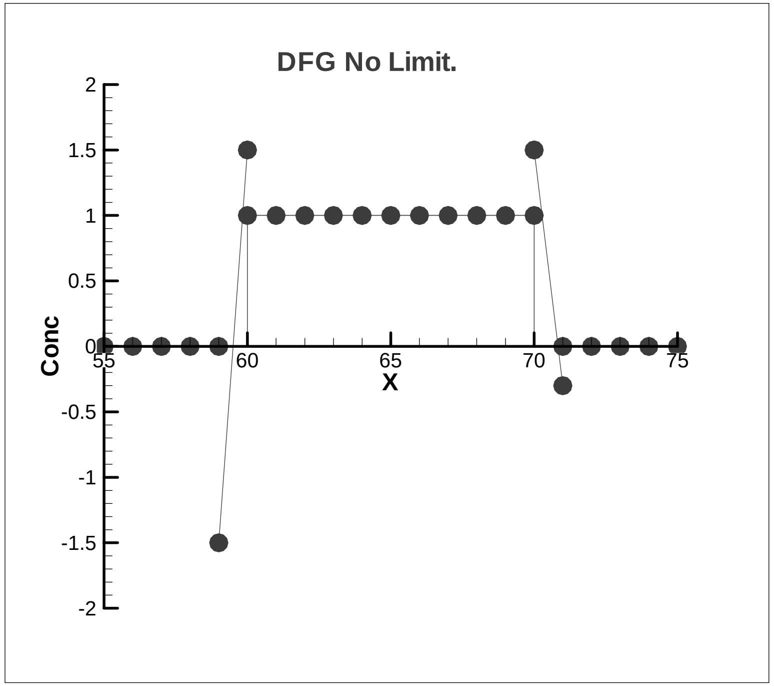
Step 2: $t \in \left[t, t + \Delta t\right]$

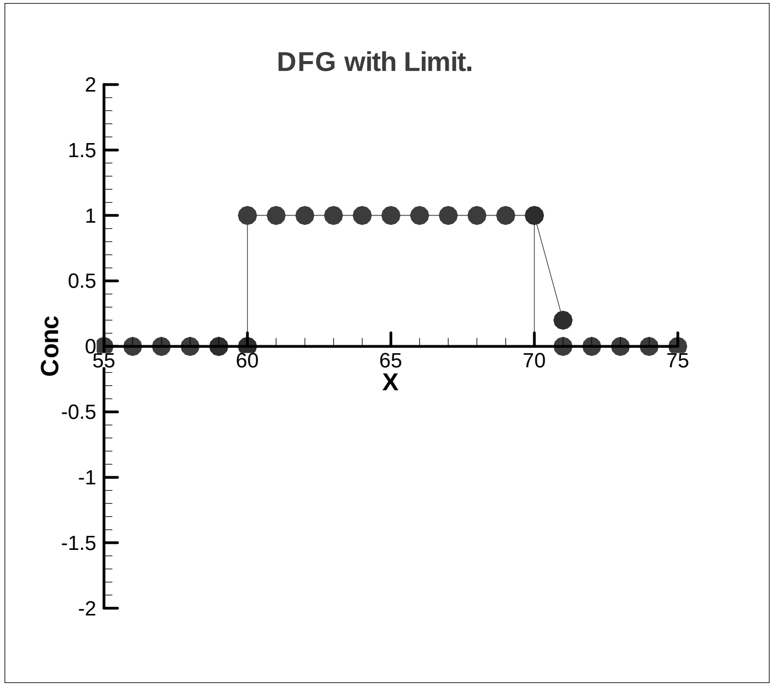
$$\begin{cases} 2\tilde{C}_i^{n+1} + \tilde{C}_{i+1}^{n+1} = C_i^{n+1/2}\left(2 - 3\dfrac{u\Delta t}{\Delta x}\right) + C_{i+1}^{n+1/2}\left(1 - 3\dfrac{u\Delta t}{\Delta x}\right) + u\dfrac{6\Delta t}{\Delta x}C_i^{n+1/2,\text{in or out}} \\ \tilde{C}_i^{n+1} + 2\tilde{C}_{i+1}^{n+1} = C_i^{n+1/2}\left(1 + 3\dfrac{u\Delta t}{\Delta x}\right) + C_{i+1}^{n+1/2}\left(2 + 3\dfrac{u\Delta t}{\Delta x}\right) - u\dfrac{6\Delta t}{\Delta x}C_{i+1}^{n+1/2,\text{in or out}} \end{cases}$$

Basic ideas:

Oscillations avoided by slope limitation

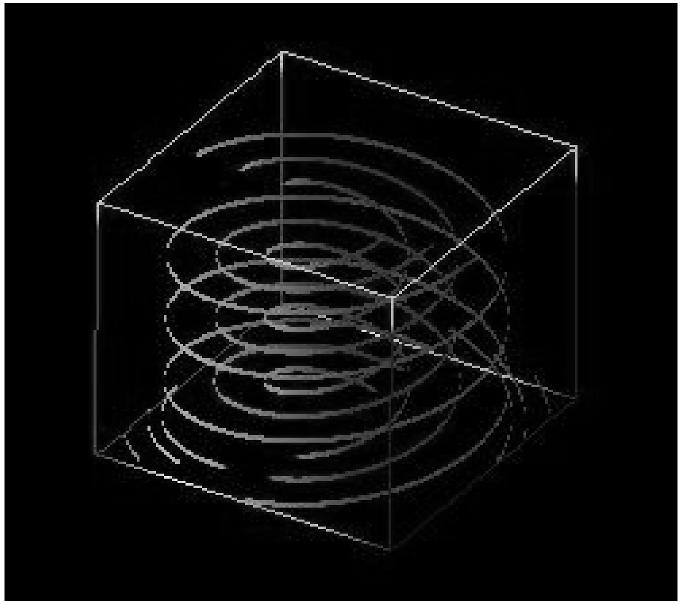


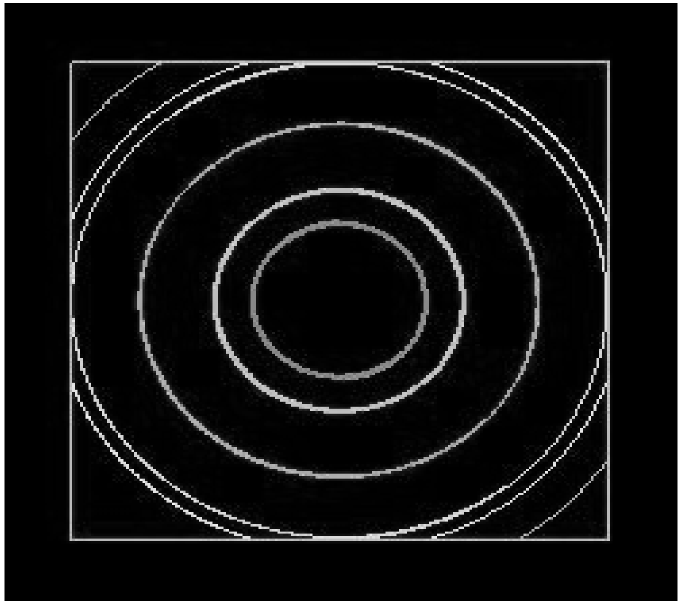




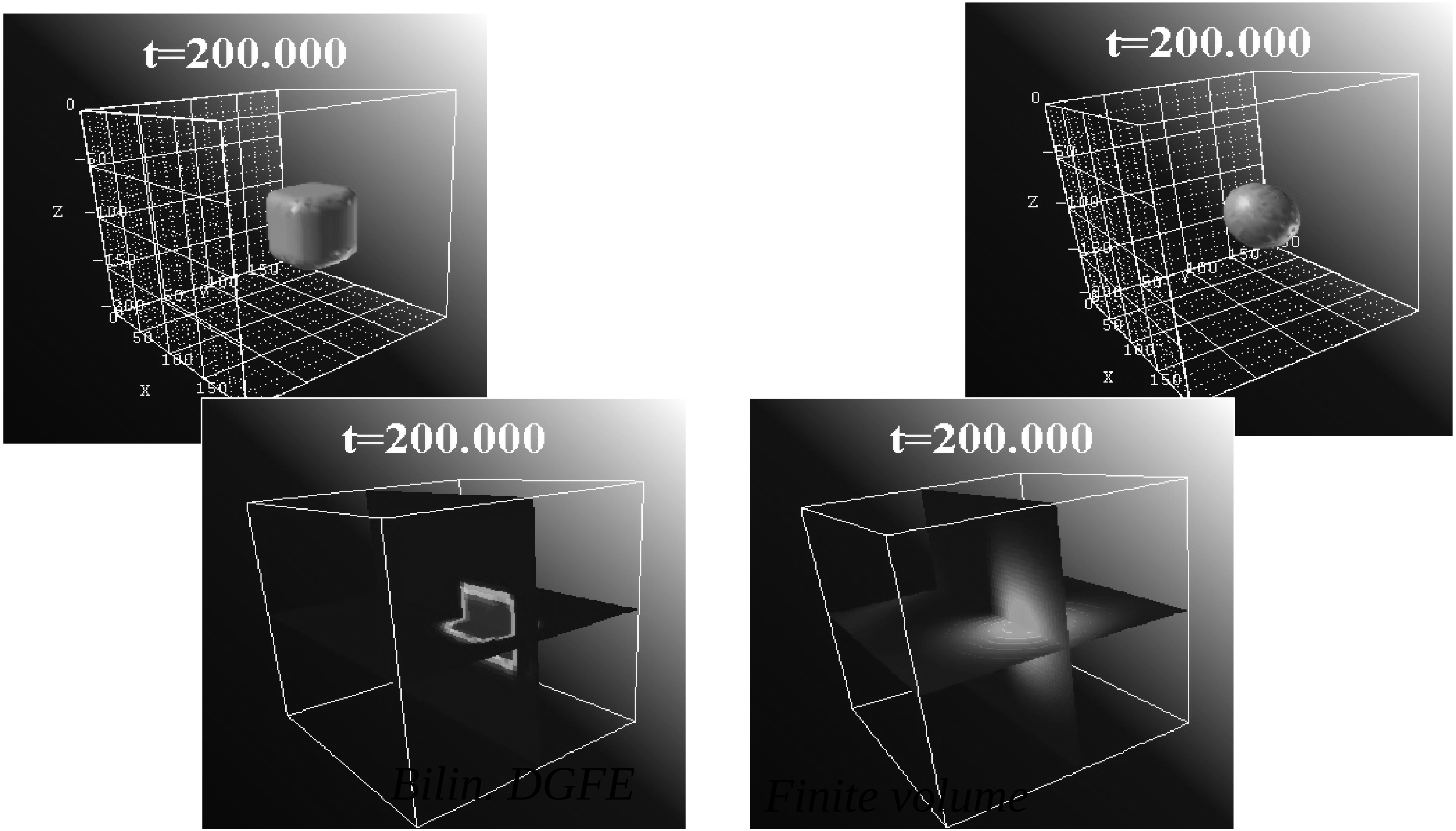
CFL=1

3D Benchmarks





Velocity field $\mathbf{v} = \begin{bmatrix} -\alpha y & \alpha x & 1 \end{bmatrix}^T$


t=200.000
t=200.000
t=200.000
t=200.000
Bilin. DGFE
Finite volume

Eulerian- Lagrangian method

Basic ideas:

Split the transport equation in two:
- Convective part solved by particle tracking along characteristics
- Dispersive part solved by an eulerian scheme

Most popular approaches:

MOC: method of characteristics (Garder et al., 1964)

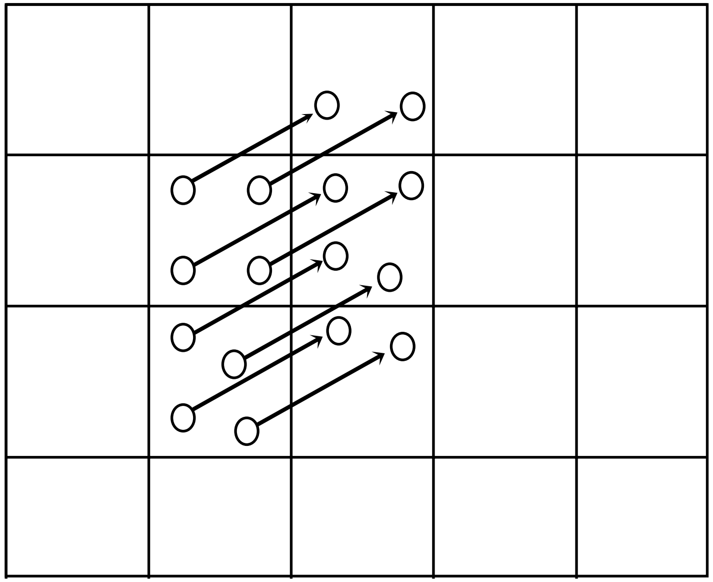
MMOC: modified method of characteristics (Russel & Wheeler, 1983)

HMOC: hybrid of characteristics (Neuman, 1984)

An alternative

ELLAM: Eulerian-Lagrangian Localized Adjoint Method (Celia et al., 1990)

MOC in a few steps:



1. Move particles from X(t) to X(t+Δt) along a characteristic

2. Concentration in cell j is given by $C_j^{n*} = \frac{1}{Np}\sum_{p=1}^{Np} C_p^n$

3. Calculation of dispersion by an eulerian method with

$$\frac{C_j^{n+1} - C_j^{n,adv}}{\Delta t} + \nabla.(-\mathbf{D}\nabla C) = 0$$

$$C_j^{n,ad} = \omega C_j^{n*} + (1-\omega)C_j^n$$

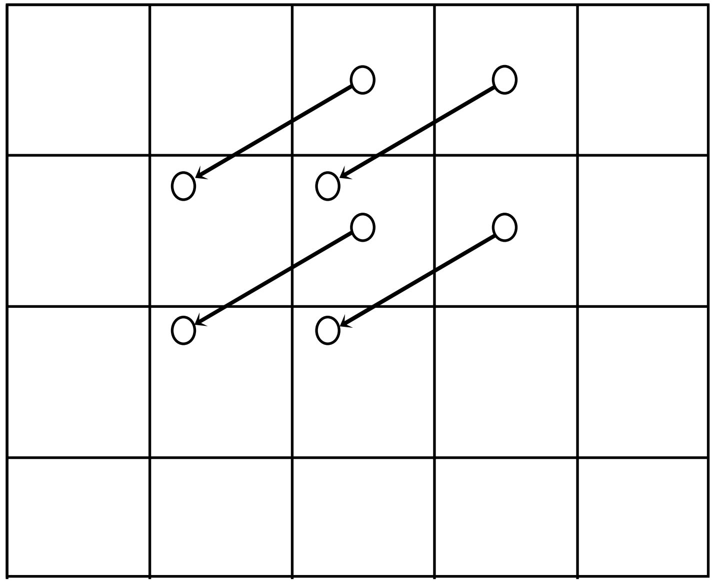
4. Calculation of the concentration at t+Δt for each particle by interpolation of C_j

MMOC :

The first step is modified

- One particle is settled in the center of the cell at $t+\Delta t$.

- Its concentration is obtained by backtracking along a characteristic.

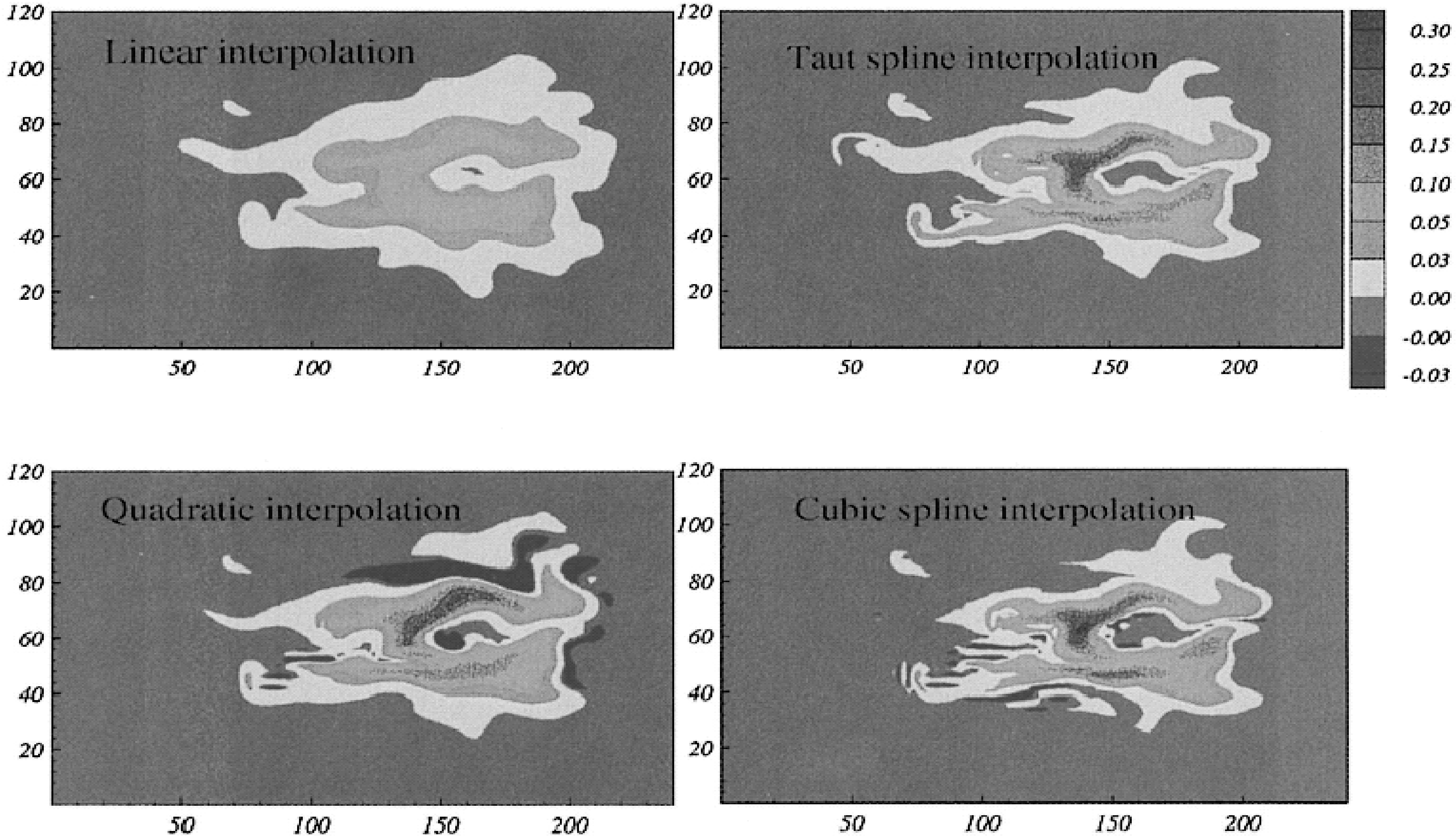


HMOC :

Mixing of MOC at sharp fronts and MMOC elsewhere

NOTICE

Interpolations lead to numerical diffusion/oscillation and mass conservation problems.



(Ruan, McLaughlin, WRR, 1999)

ELLAM: Eulerian-Lagrangian Localized Adjoint Method

$$\frac{\partial C}{\partial t}+\frac{\partial\left(uC\right)}{\partial x}-\frac{\partial}{\partial x}\left(D\,\frac{\partial C}{\partial x}\right)=0$$

Basic ideas:

1. Define test functions such as:

$$\omega=\begin{cases}\omega\left(x,t\right) & t\in\left[t^{n},t^{n+1}\right]\\ 0 & \text{else}\end{cases}$$

2. Write the transport equation in a weak formulation

$$\int_0^T\int_\Omega\left[\frac{\partial C}{\partial t}\omega+\frac{\partial\left(uC\right)}{\partial x}\omega-\frac{\partial}{\partial x}\left(D\,\frac{\partial C}{\partial x}\right)\omega\right]dxdt=0$$

3. Integration by part leads to

$$\int_0^T\int_\Omega\frac{\partial(\omega C)}{\partial t}dxdt-\int_0^T\int_\Omega C\left[\frac{\partial\omega}{\partial t}+u\frac{\partial\omega}{\partial x}\right]dxdt+\int_0^T\int_{\partial\Omega}\frac{\partial}{\partial x}\left[\left(uC-D\frac{\partial C}{\partial x}\right)\omega\right]dxdt+\int_0^T\int_\Omega D\frac{\partial C}{\partial x}\frac{\partial\omega}{\partial x}dxdt=0$$

4. For , the test function $\omega(x,t)$ is defined by $\frac{\partial\omega}{\partial t}+u\frac{\partial\omega}{\partial x}=0$

$$\int_0^T\int_\Omega \frac{\partial(\omega C)}{\partial t}dxdt-\int_0^T\int_\Omega C\left[\frac{\partial\omega}{\partial t}+u\frac{\partial\omega}{\partial x}\right]dxdt+\int_0^T\int_{\partial\Omega}\frac{\partial}{\partial x}\left[\left(uC-D\frac{\partial C}{\partial x}\right)\omega\right]dxdt+\int_0^T\int_\Omega D\frac{\partial C}{\partial x}\frac{\partial\omega}{\partial x}dxdt=0$$

which leads to (Russel & Celia, 2002)

$$\int_\Omega C^{n+1}\omega^{n+1}dx+\int_0^T\int_\Omega(D.\nabla C).\nabla\omega dxdt+\int_0^T\int_{\partial\Omega}\left[(uC-D.\nabla C)\omega\right]dxdt=\int_\Omega C^n\omega^n(x)dx$$

With Dirichlet C=0 boundaries,

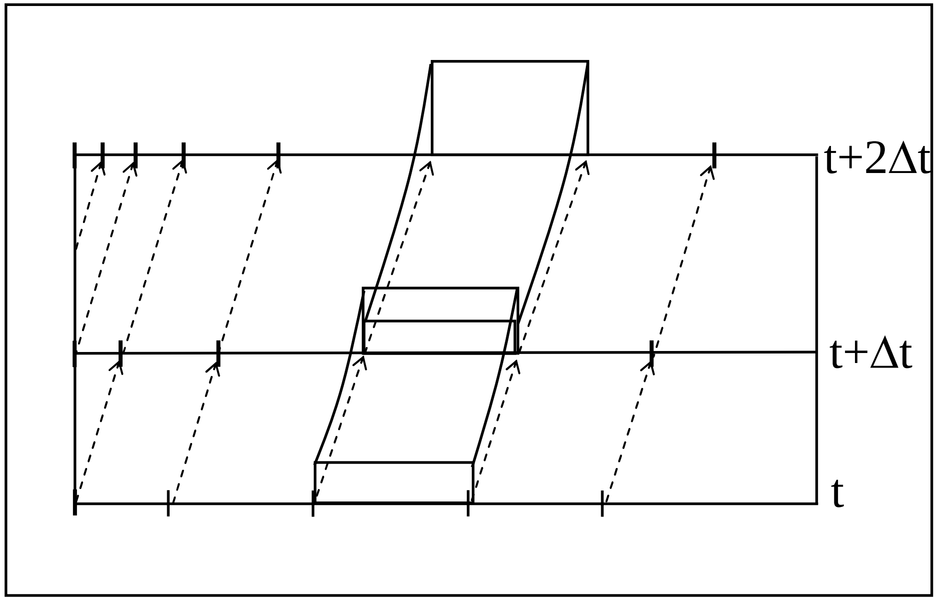
$$\int_{x_{i-1}}^{x_{i+1}}\omega_i^{n+1}C^{n+1}dx+\Delta t^{n+1*}\int_\Omega D\frac{\partial C^{n+1}}{\partial x}\frac{\partial\omega_i^{n+1}}{\partial x}dx=\int_{x_{i-1}^*}^{x_{i+1}^*}\omega_i^n C^n dx$$

5. Calculation of each integral by choosing ω and an approximation of C

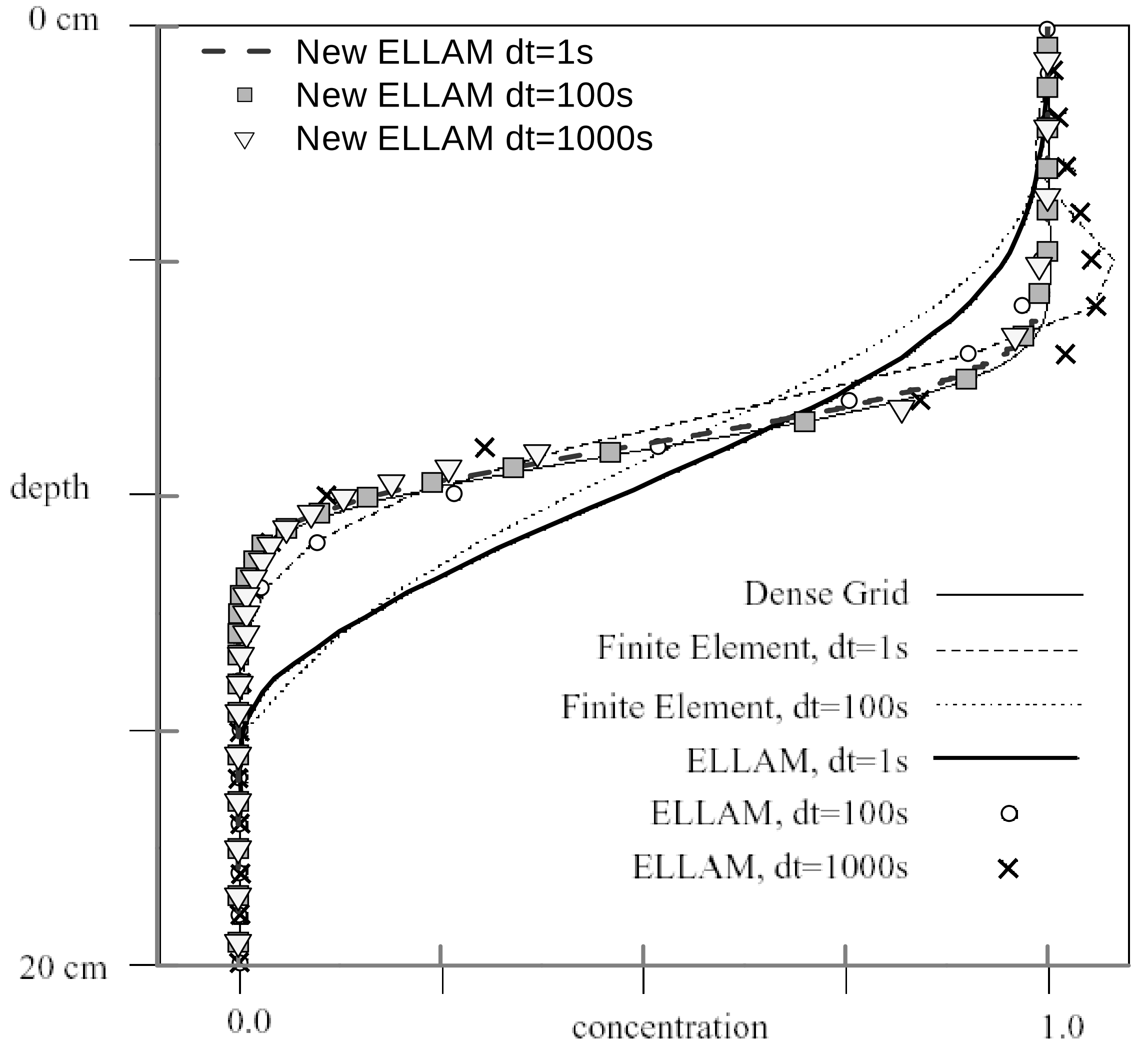
For example $\tilde{C}(x,t)=\sum_{j=1}^{ne}\phi_j(x)\tilde{C}_j(t)$ with $\phi_j(x_i)=\begin{cases}1 \text{ if } x_i=x_j\\ 0 \text{ if } x_i\neq x_j\end{cases}$ and $\omega(x,t^{n+1})=\phi_j(x_i)$

An alternative approach: moving the mesh (Younès, 2004)

1. Each node moves with the fluid velocity
2. At the inflow, new nodes are created
3. At the outflow, nodes are deleted



Concentration distribution at t = 1000s

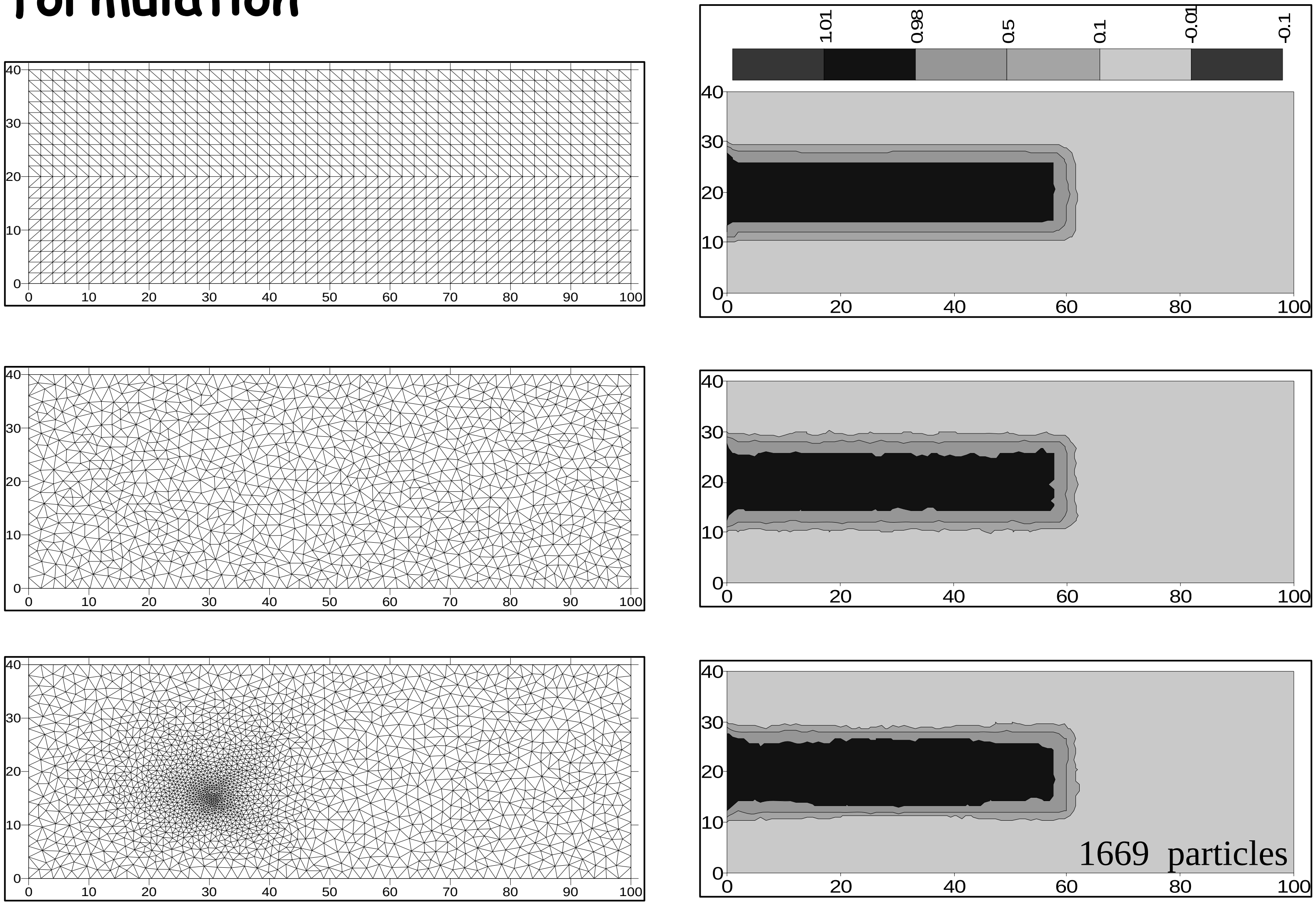


$$CPU^{EFS}_{(\Delta t=0.1s)} = 44s$$

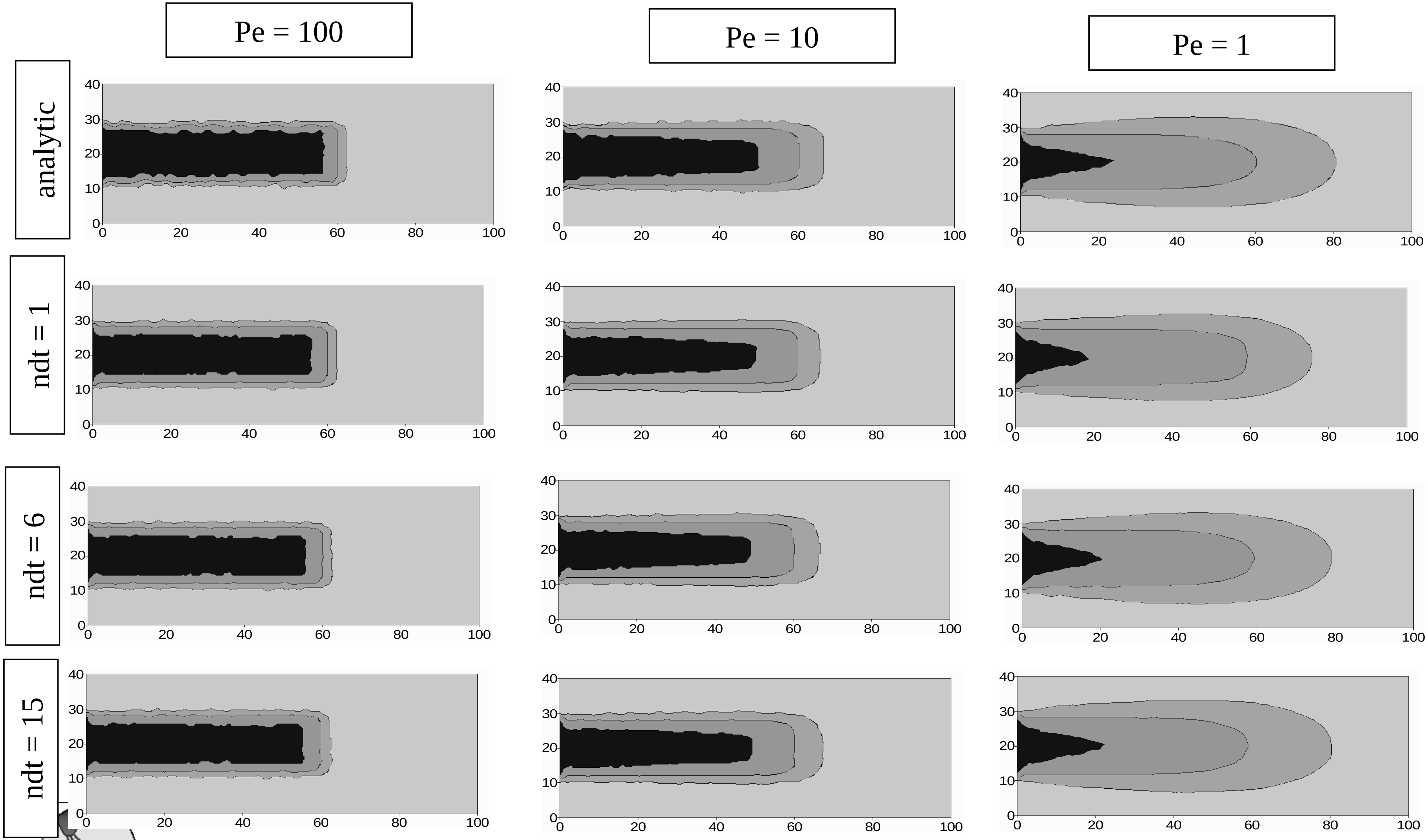
$$CPU^{ELLAM}_{(\Delta t=1s)} = 17s$$

$$CPU^{ELLAM}_{(\Delta t=1000s)} = 0.14s$$

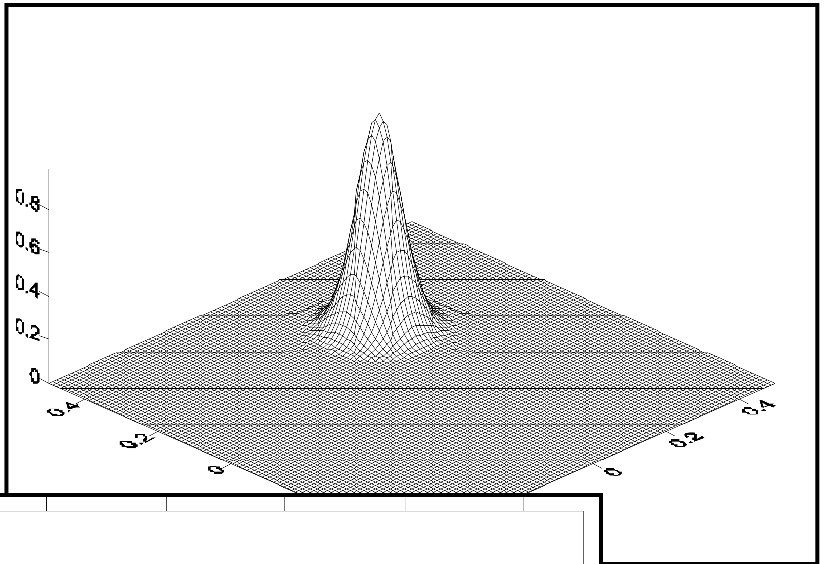
New formulation

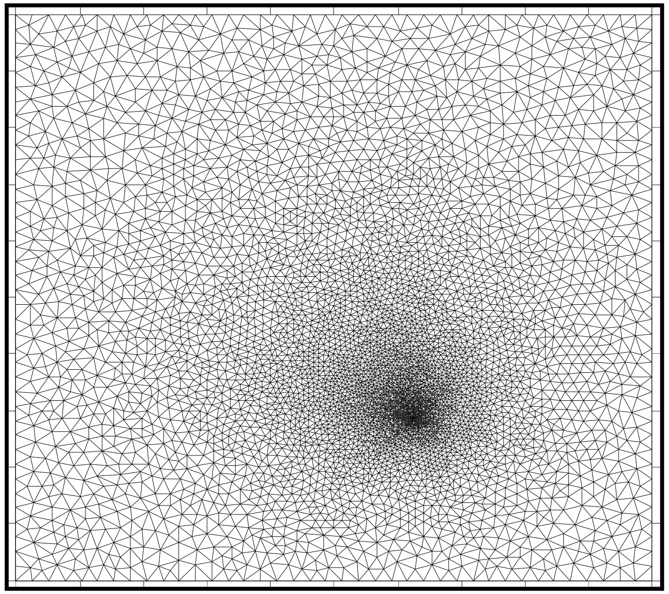


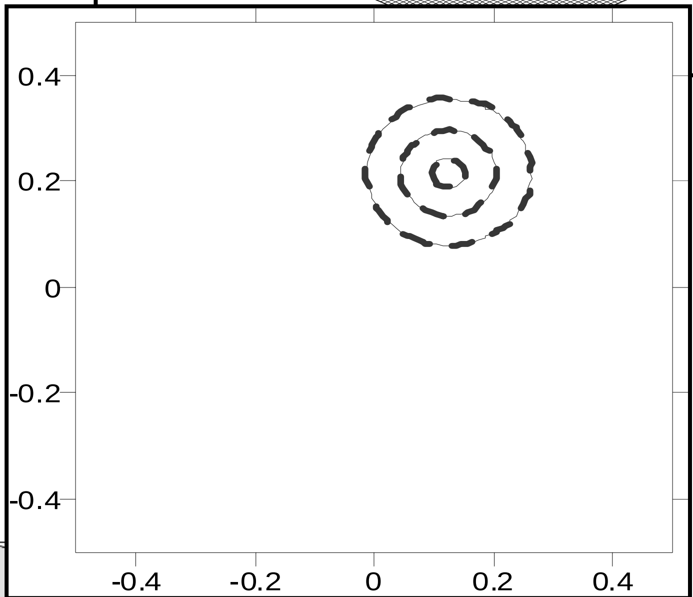
Advective dominant transport: Eulerian- Lagrangian method



➢Rotating Gaussian pulse







	Max C.	RMSE Error	CPU (s)
Std. ELLAM	1.12	$2.7\ 10^{-3}$	99.0
DGFEM	0.88	$5.0\ 10^{-3}$	284.5
New ELLAM	0.999	$1.4\ 10^{-3}$	1.4

Reactive transport

Transport of 2 substances (oxygène + organic subs) with bio-degradation.

$$\begin{cases} \dfrac{\partial C_1}{\partial t} + \dfrac{\partial \left(q_1(x,t) C_1 \right)}{\partial x} - \dfrac{\partial}{\partial x}\left(D_1(x,t) \dfrac{\partial C_1}{\partial x} \right) + K_1\left(C_1, C_B\right) C_1 = f_1\left(C_2, C_B\right) \\ \dfrac{\partial C_2}{\partial t} + \dfrac{\partial \left(q_2(x,t) C_2 \right)}{\partial x} - \dfrac{\partial}{\partial x}\left(D_2(x,t) \dfrac{\partial C_2}{\partial x} \right) + K_2\left(C_2, C_B\right) C_2 = f_2\left(C_1, C_B\right) \end{cases}$$

$$K_1 = \left(\frac{\mu_1 C_B}{K_h^1 + C_1} \right)$$

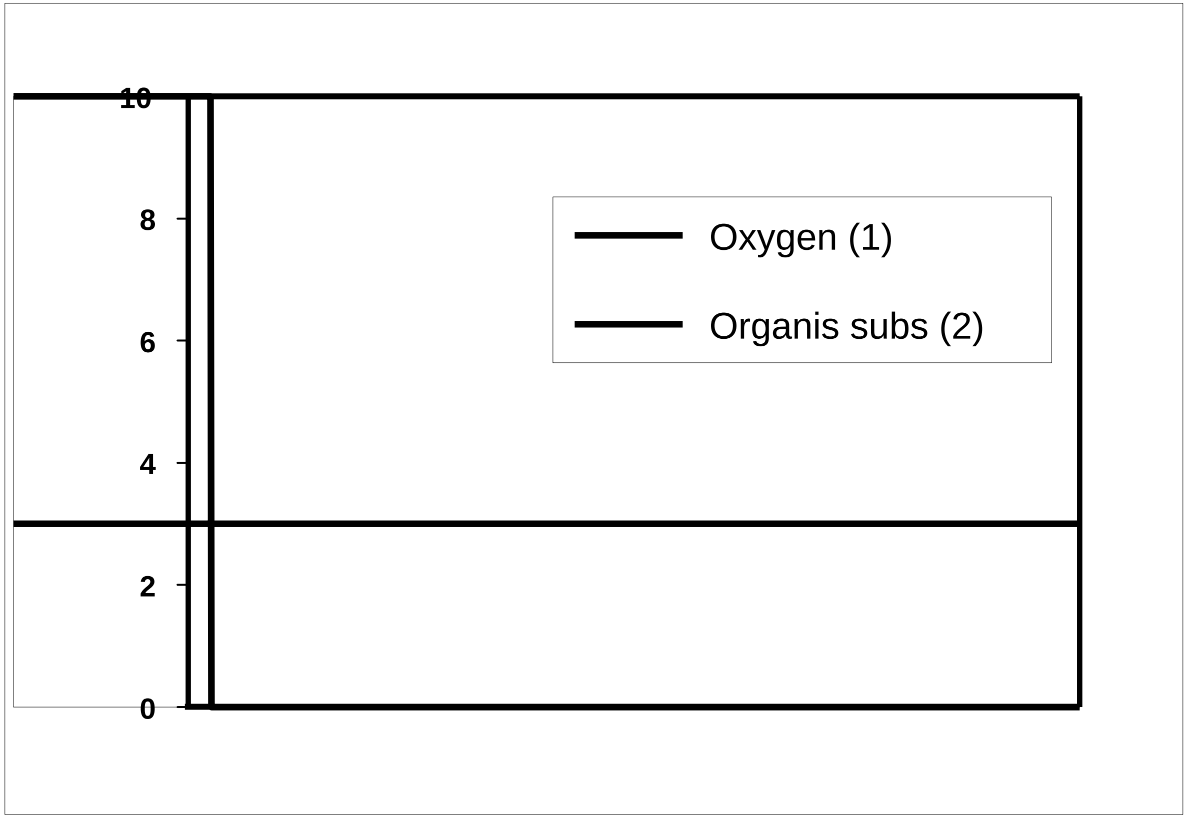
$$f_1 = -\kappa_{12} \left(\frac{\mu_2 C_B}{K_h^2 + C_2} \right) C_2$$

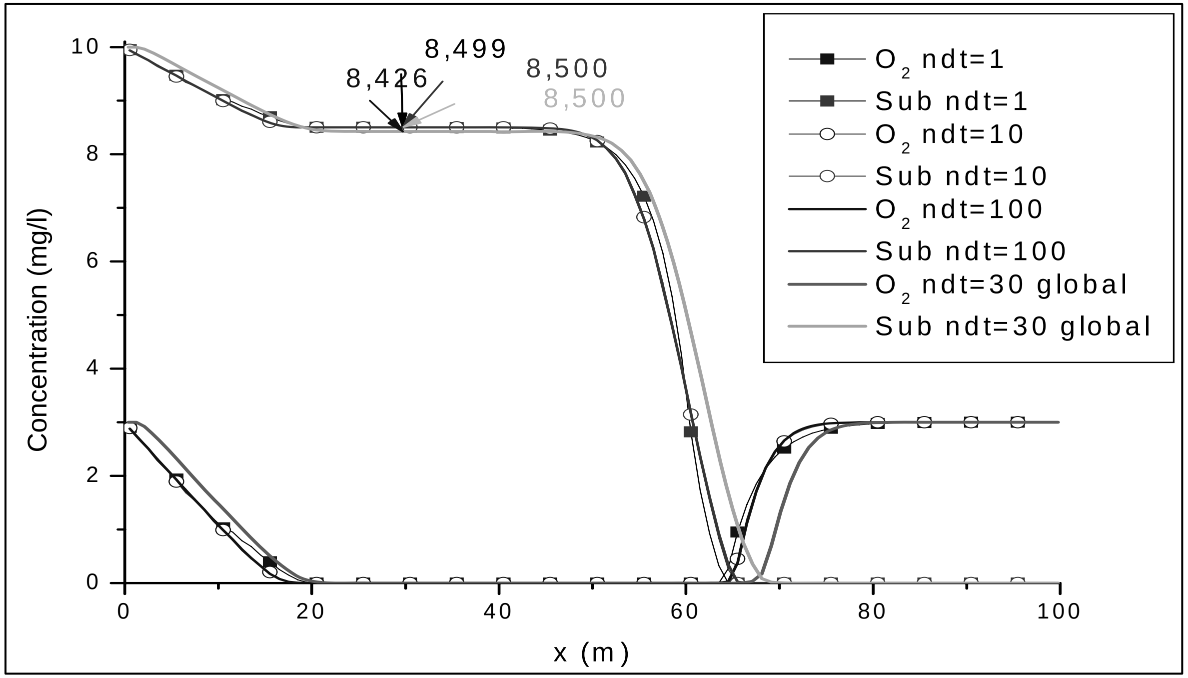
$$K_2 = \left(\frac{\mu_2 C_B}{K_h^2 + C_2} \right)$$

$$f_2 = -\kappa_{21} \left(\frac{\mu_1 C_B}{K_h^1 + C_1} \right) C_1$$

Initial conditions: $C_1(x,0) = 3.0\, mg/L$ $C_2(x,0) = 0$ $C_B(x,t) = 0.2\, mg/L$

Boundary conditions: $C_1(0,t) = 3.0\, mg/L$ $C_2(0,t) = 10.0\, mg/L$



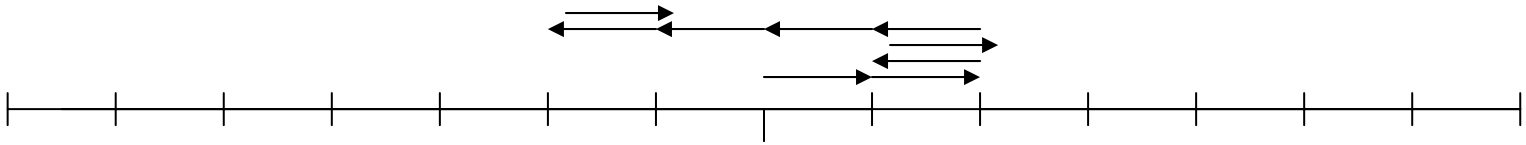


Globale			Séparation d'opérateurs		
ndt = 20	ndt = 40	ndt = 400	ndt = 100	ndt = 10	ndt = 1
8.342	8.443	8.498	8.5	8.5	8.499

Random-Walk method

Basic ideas: Use particles for advection and dispersion

Underlying theory



Defining :

l, the length of a step

x = ml

For large n, it is possible to make a description of the problem through the equation

$$\frac{\partial W}{\partial t} = \beta \frac{\partial W}{\partial x} + D \frac{\partial^2 W}{\partial x^2}$$

$$\beta = -n\langle x \rangle, \ D = \frac{1}{2} n \langle x^2 \rangle$$

which is not strictly equivalent to the transport equation:

$$\frac{\partial C}{\partial t} = u \frac{\partial C}{\partial x} + \frac{\partial}{\partial x}(D \ \frac{\partial C}{\partial x})$$

Displacement for homogeneous dispersion

$$x(t^{n+1}) = x(t^n) + u(x(t^n))\Delta t + Z\sqrt{2D(x(t^n))\Delta t}$$

Driving force

Random fluctation with

```
do k=1,nt                          ! Loop over the time steps
    do i=1,nb                      ! Loop over the particles
      call RANDOM_NUMBER(rx)
      rx=2.00*(rx-0.5)
      xp(i)=xp(i)+u*dt+rx*SQRT(24.0*al*u*dt)

      call RANDOM_NUMBER(ry)
      ry=2.00*(ry-0.5)
      yp(i)=yp(i)+ry*SQRT(24.0*at*u*dt)
   end do
end do
```

Particles

Concentration

SUMMARY

Eulerian methods (Finite Volumes, Finite Elements):

Generate oscillation/dispersion if Courant and Peclet criteria are not fullfilled,

Higher order scheme or discontinuous FE reduces dispersion but are explicit (small Δt)

Eulerian-Lagrangian methods (Method of characteristics, ELLAM):

Difficult particles handling. Can generate oscillation/dispersion/mass balance problems. Unstructured meshes ?

ELLAM has a more rigourous theoretical framework and can be applied on unstructured meshes (Younès et al., 2005).

Lagrangian method (Random-walk):

Free of dispersion (in theory), generates oscillations.

Non linear transport ?

Discontinuous full tensor flux related parameter

Focus on the following equations :

$$\nabla.\mathbf{q} = f$$

with (Darcy's law, Fick's law, …) : $\mathbf{q} = -K\nabla h$

K may be strongly discontinuous with a strong anisotropy ratio and arbitrary principal directions.

The grid directions are not aligned with the principal directions of K.

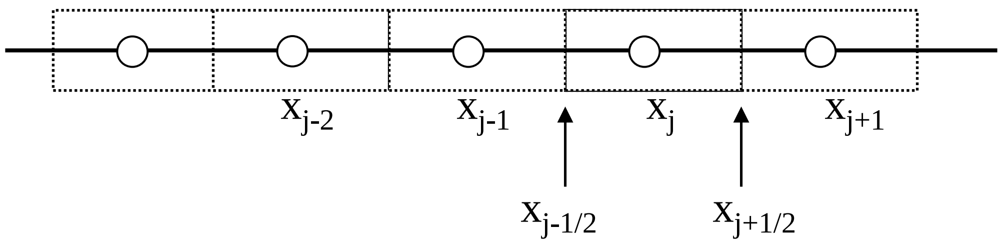
The discretization should be locally conservative with explicit flux.

The discretization must yield convergence for both h and q.

Basic ideas:

1. Continuity of the state variable and the related fluxes at element edges
2. Linear variation of the state variable inside the element

1 dimension

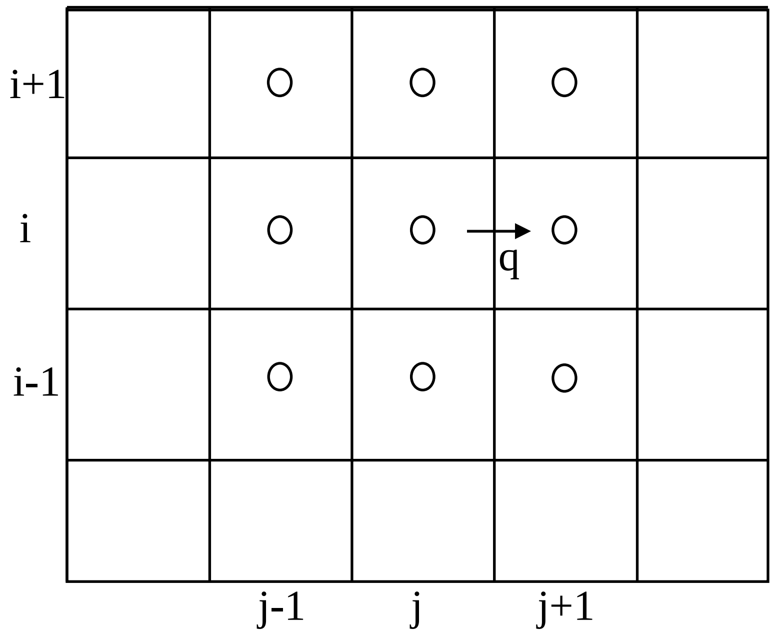


$$q_{j+1/2} = -K_j \frac{h_{j+1/2} - h_j}{\Delta x_j / 2} = -K_{j+1} \frac{h_{j+1} - h_{j+1/2}}{\Delta x_{j+1} / 2}$$

$$q_{j+1/2} = -\bar{K}_j \frac{h_{j+1} - h_j}{\Delta x_j / 2 + \Delta x_{j+1} / 2}$$

with $$\frac{\Delta x_j + \Delta x_{j+1}}{\bar{K}} = \frac{\Delta x_j}{K_j} + \frac{\Delta x_{j+1}}{K_{j+1}}$$

2 dimensions

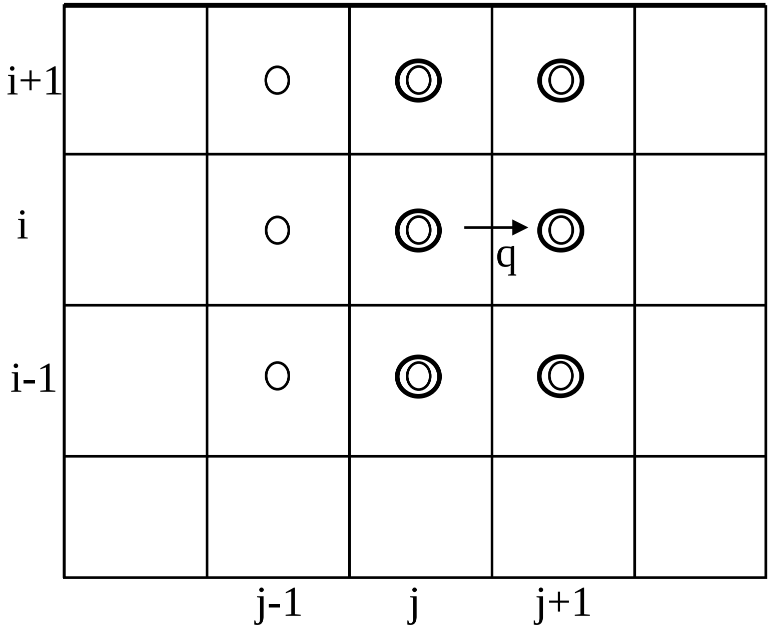


$$q_{j+1/2,i} = -\left[K_{xx} \frac{\partial h}{\partial x} + K_{xy} \frac{\partial h}{\partial y} \right] = ?\bar{K},\ ?\frac{\partial h}{\partial x},\ ?\frac{\partial h}{\partial y}$$

Finite difference approximation

$$\frac{\partial h}{\partial x} \simeq \frac{h_{j+1,i} - h_{j,i}}{\Delta x}$$

$$\frac{\partial h}{\partial y} \simeq \frac{1}{2}\left[\left(\frac{h_{j+1,i+1} - h_{j+1,i-1}}{2\Delta x}\right) + \left(\frac{h_{j,i+1} - h_{j,i-1}}{2\Delta x}\right)\right]$$



$$\frac{\Delta x_j + \Delta x_{j+1}}{\bar{\bar{K}}} = \frac{\Delta x_j}{K_j} + \frac{\Delta x_{j+1}}{K_{j+1}}$$

$$\bar{D} \simeq f(u_{j+1/2,i}, \alpha_j, \alpha_{j+1})$$

Mixed Finite Elements method

Basic ideas:

1. Apply the same idea than FE, but for velocity

$$\vec{q} = \sum_{i=1}^{3} Q_i^A \vec{\omega}_i^A$$

with $\int_{A_j} \vec{\omega}_i^A \vec{n}_j^A \, dA_j = \begin{cases} = 1 \text{ if } i = j \\ = 0 \text{ if } i \neq j \end{cases}$ for a triangle $\vec{\omega}_i^A = \frac{1}{2|A|}\begin{pmatrix} x - x_i^A \\ y - y_i^A \end{pmatrix}, \quad i = 1,2,3$

2. Write both conservation equation and Darcy's law in a variational form

$$\int_\Omega \left(c\frac{\partial h}{\partial t} + \nabla.\vec{q} - f\right) d\Omega = 0$$

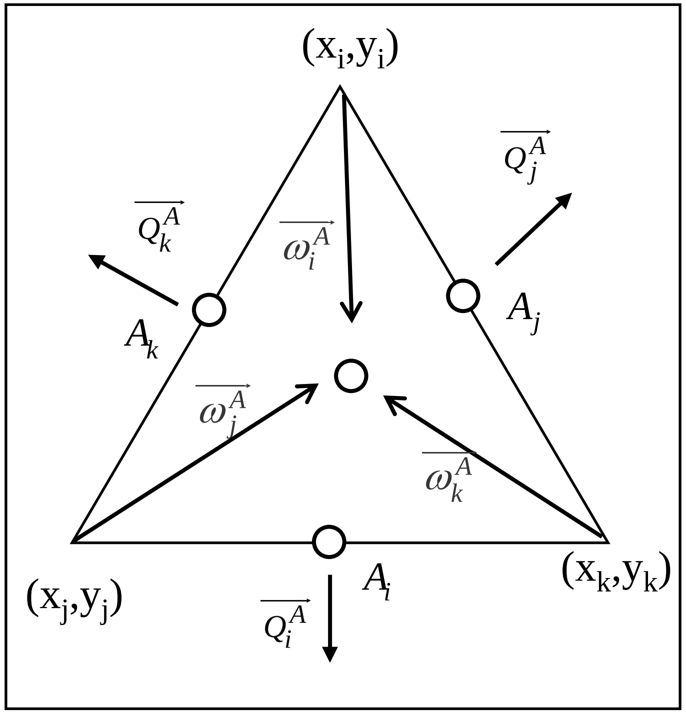
$$\int_A \vec{q}_A \vec{\omega}_i^A = -K^A \int_A \nabla h \vec{\omega}_i^A$$

Variational formulation of Darcy's law

$$\int_A \vec{q}_A \vec{\omega}_i^A = -K^A \int_A \nabla h \vec{\omega}_i^A$$

$$Q_i^A = a \sum_{j=1}^{3} B_{ij}^{-1} \left(h^A - Th_j^A \right)$$

$$B_{ij} = \int_A \vec{\omega}_i^A \vec{\omega}_j^A$$



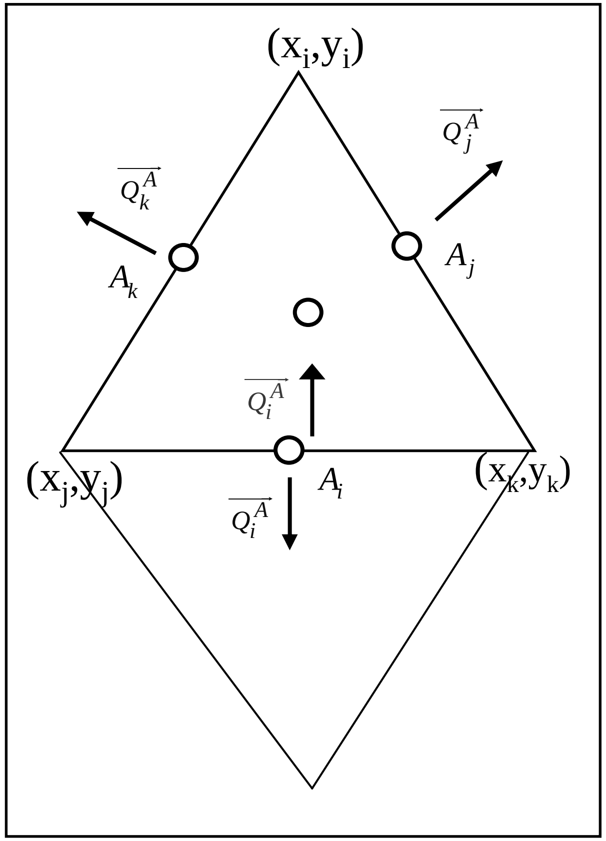
where, after some calculations ….

$$B^{-1} = \frac{1}{|A|} \begin{bmatrix} \mathbf{r}_{jk}\mathbf{r}_{jk} & \mathbf{r}_{jk}\mathbf{r}_{ki} & \mathbf{r}_{jk}\mathbf{r}_{ij} \\ \mathbf{r}_{jk}\mathbf{r}_{ki} & \mathbf{r}_{ki}\mathbf{r}_{ki} & \mathbf{r}_{ij}\mathbf{r}_{ki} \\ \mathbf{r}_{jk}\mathbf{r}_{ij} & \mathbf{r}_{ij}\mathbf{r}_{ki} & \mathbf{r}_{ij}\mathbf{r}_{ij} \end{bmatrix} + \frac{1}{3\ell} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

$$\ell = \sum_{j=1}^{3} B_{ij} = \frac{\ell_{ij} + \ell_{ik} + \ell_{jk}}{48|A|} \geq \sqrt{3}/12$$

Implicit FV for the mass balance equation

$$\frac{c|A|}{\Delta t}\left(h^{A,n+1}-h^{A,n}\right)+\sum_{j=1}^{3}Q_j^{A,n+1}=|A|f_A=Q_s^A$$



Hybridation

$$h^{A,n+1}=\frac{a}{\beta}\sum_{i=1}^{3}\alpha_i Th_i^{A,n+1}+\frac{\lambda}{\beta}h^{A,n}+\frac{Q_s^A}{\beta}$$

From mass bal. eq.

$$Q_i^{A,n+1}=a\left[\frac{a\alpha_i}{\beta}\sum_{j=1}^{3}\alpha_j Th_j^{A,n+1}-\sum_{j=1}^{3}B_{ij}^{-1}Th_j^{A,n+1}+\frac{\lambda\alpha_i}{\beta}h^{A,n}+\frac{\alpha_i Q_s^A}{\beta}\right]$$

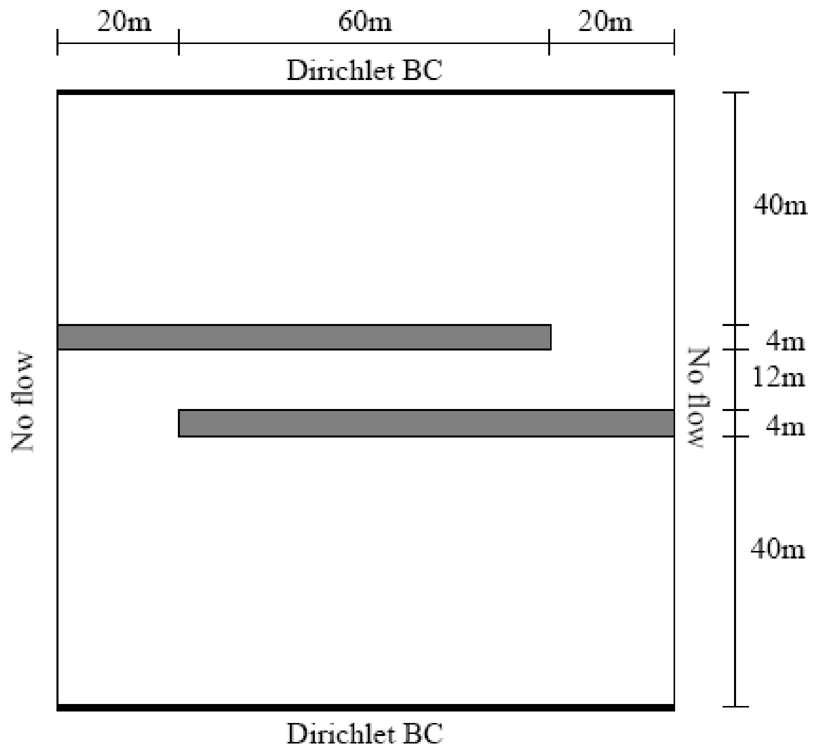
From Darcy eq.

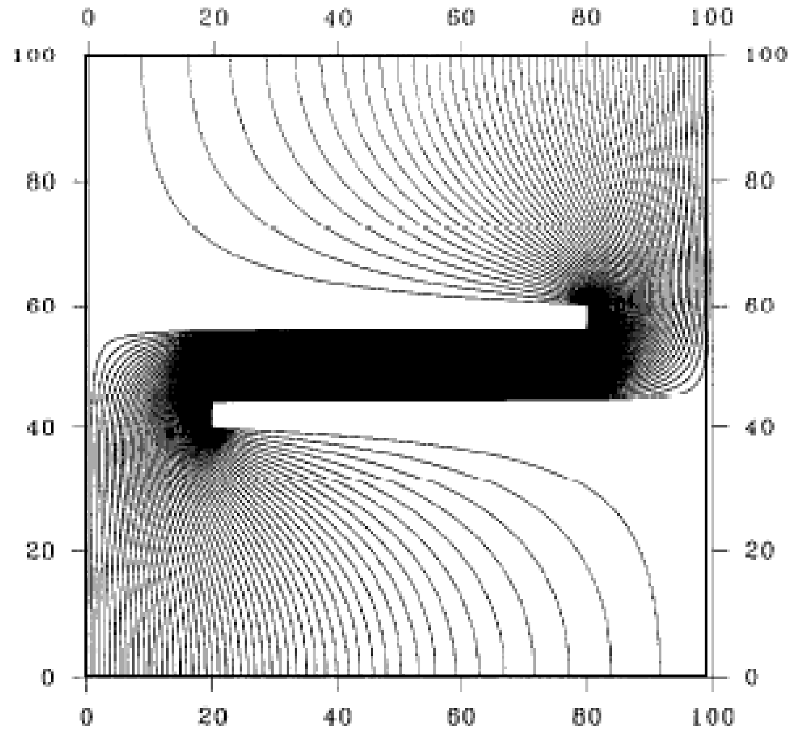
Continuity of pressure and flux between two adjacent elements A & B:

$$Th_i^A=Th_i^B \qquad Q_i^{A,n+1}+Q_i^{B,n+1}=0$$

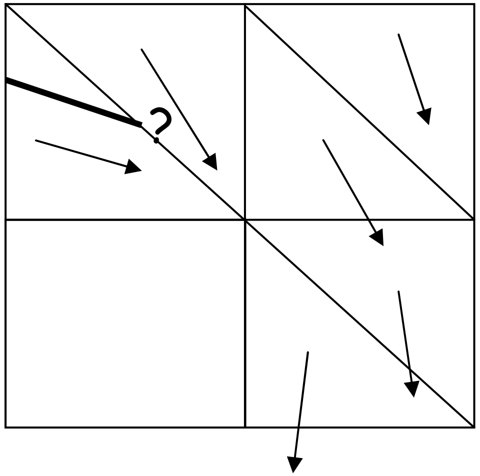
⇒ An equation per element edge

Dispersive dominant transport: Mixed Finite Elements

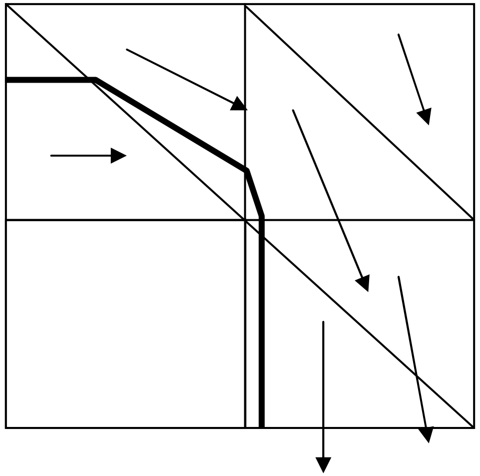




$$\text{Error} = \sum_i \left| x(i)_{start} - \left(100 - x(n-i+1)_{end}\right) \right|$$



Standard finite element

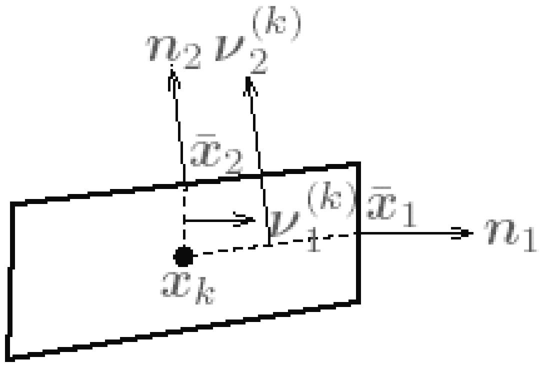


Mixed finite element

Mesh size	25 x 25	50 x 50	100 x 100	200 x 200
		Standard finite element		
Nb unknowns	624	2 499	9 999	39 999
Error, m	100	50	23	12
CPU, s	0.7	4.0	28.2	208
		Mixed finite element		
Nb unknowns	1 875	7 500	30000	120 000
Error, m	0	0	0	0
CPU, s	2.5	17.1	131.4	1 047

Multipoint flux approximation (MPFA) method

Flux expression in each cell

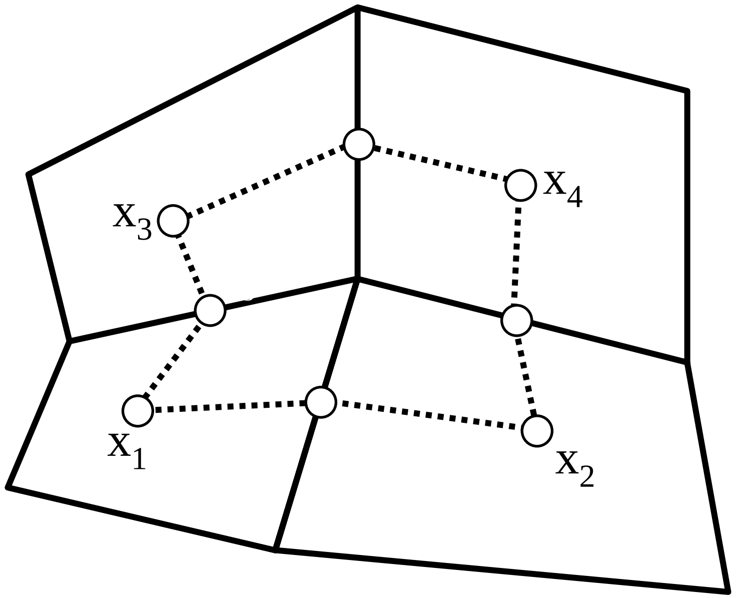


$$
\begin{bmatrix} q_1^{(k)} \\ q_2^{(k)} \end{bmatrix} = -\boldsymbol{G}_k \begin{bmatrix} \bar{u}_1 - u_k \\ \bar{u}_2 - u_k \end{bmatrix}, \qquad \boldsymbol{G}_k = \frac{1}{2F_k} \begin{bmatrix} \Gamma_1 \boldsymbol{n}_1^{\mathrm{T}} \boldsymbol{K}_k \boldsymbol{\nu}_1^{(k)} & \Gamma_1 \boldsymbol{n}_1^{\mathrm{T}} \boldsymbol{K}_k \boldsymbol{\nu}_2^{(k)} \\ \Gamma_2 \boldsymbol{n}_2^{\mathrm{T}} \boldsymbol{K}_k \boldsymbol{\nu}_1^{(k)} & \Gamma_2 \boldsymbol{n}_2^{\mathrm{T}} \boldsymbol{K}_k \boldsymbol{\nu}_2^{(k)} \end{bmatrix}
$$

(from Aavatsmark et al., IMA Workshop, 2004)

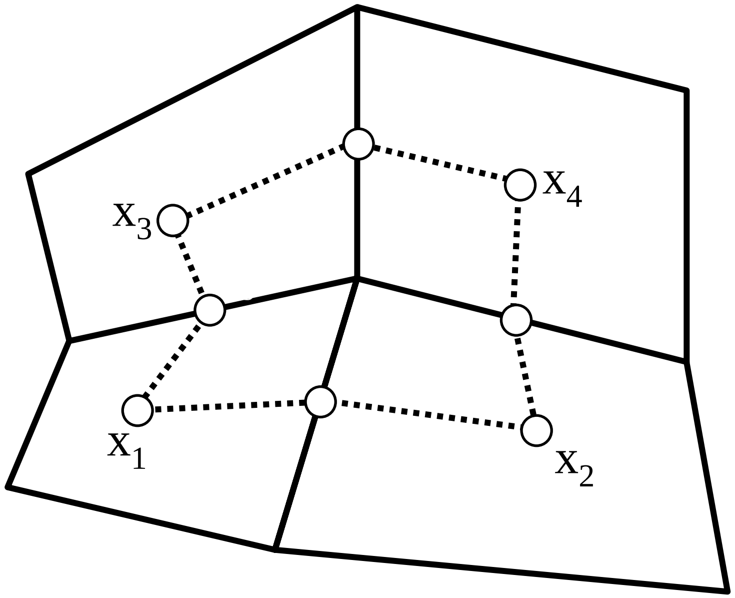
Basic ideas:

1. The flux is calculated trough the half edge of an element
2. Linear variation of the state variable inside the sub-element
3. Continuity of fluxes and state variable



$$q_1 = -g_{1,1}^{(1)}(\bar{h}_1 - h_1) - g_{1,2}^{(1)}(\bar{h}_3 - h_1)$$
$$= -g_{1,1}^{(2)}(\bar{h}_1 - h_2) - g_{1,2}^{(2)}(\bar{h}_4 - h_2)$$

$$q_2 = -g_{1,1}^{(4)}(\bar{h}_2 - h_4) - g_{1,2}^{(4)}(\bar{h}_4 - h_4)$$
$$= -g_{1,1}^{(3)}(\bar{h}_2 - h_3) - g_{1,2}^{(3)}(\bar{h}_3 - h_3)$$



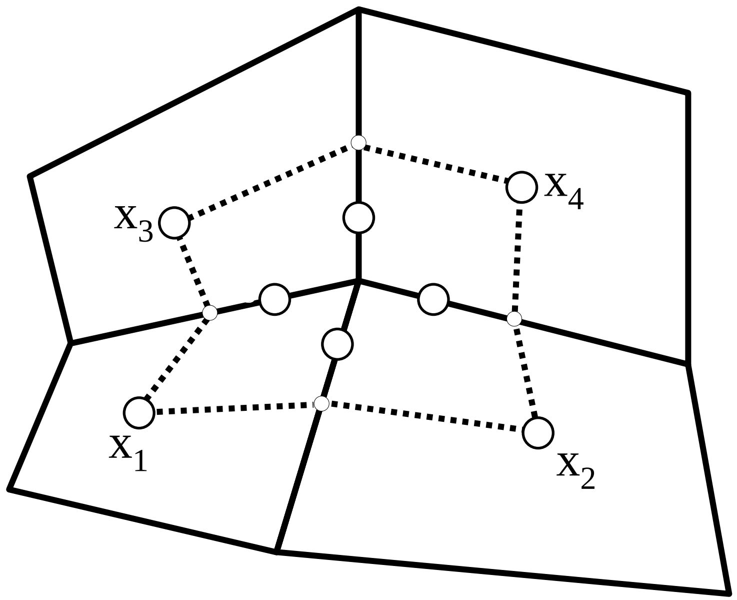
$$q_1 = -g_{1,1}^{(1)}(\bar{h}_1 - h_1) - g_{1,2}^{(1)}(\bar{h}_3 - h_1)$$
$$= -g_{1,1}^{(2)}(\bar{h}_1 - h_2) - g_{1,2}^{(2)}(\bar{h}_4 - h_2)$$

$$\mathbf{q} = [q_1, q_2, q_3, q_4]^T$$
$$\mathbf{h} = [h_1, h_2, h_3, h_4]^T$$
$$\bar{\mathbf{h}} = [\bar{h}_1, \bar{h}_2, \bar{h}_3, \bar{h}_4]^T$$

Using continuity of fluxes and state variable

$$\left.\begin{aligned} \mathbf{q} &= \mathbf{A}\mathbf{h} + \mathbf{B}\bar{\mathbf{h}} \\ \mathbf{M}\bar{\mathbf{h}} &= \mathbf{N}\mathbf{h} \end{aligned}\right\} \qquad \mathbf{q} = \left(\mathbf{A} + \mathbf{B}\mathbf{M}^{-1}\mathbf{N}\right)\mathbf{h}$$

Related scheme :Edwards & Roger



SUMMARY

MFEM,

- the pressure head and the velocity are approximated simultaneously
- The mass is conserved locally
- The method can be applied to general elements and general coefficients (no additionnal assumptions)
- Unknowns are one value per edge/face.

MPFA,

- Additionnal assumption (consistent scheme ?)
- The mesh should not be too skewed
- One unknown per element + local system to solve

Basic matrix algebra

Eulerian and ELLAM schemes lead to a system matrix of the form:

$$\mathbf{Ax=b}$$

The properties of matrix **A** are important in the selection of an appropriate solver.

A is *diagonally dominant* $\sum_{j=1, j\neq i}^{N} \left|\mathbf{A}_{ij}\right| < \left|\mathbf{A}_{ii}\right|$

A is *sparse* (i.e. contains many zero elements).

A may (all saturated groundwater flow problems) or may not (many solute transport problems) be *symmetrical*.

A may or may not be *positive definite* i.e. $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0 \text{ for all } \mathbf{x} \in \mathbb{R}^N$
or all eigenvalues are positive

A may or may not be a *M-matrix* i.e. $A_{ii} > 0, A_{ij} \leq 0$

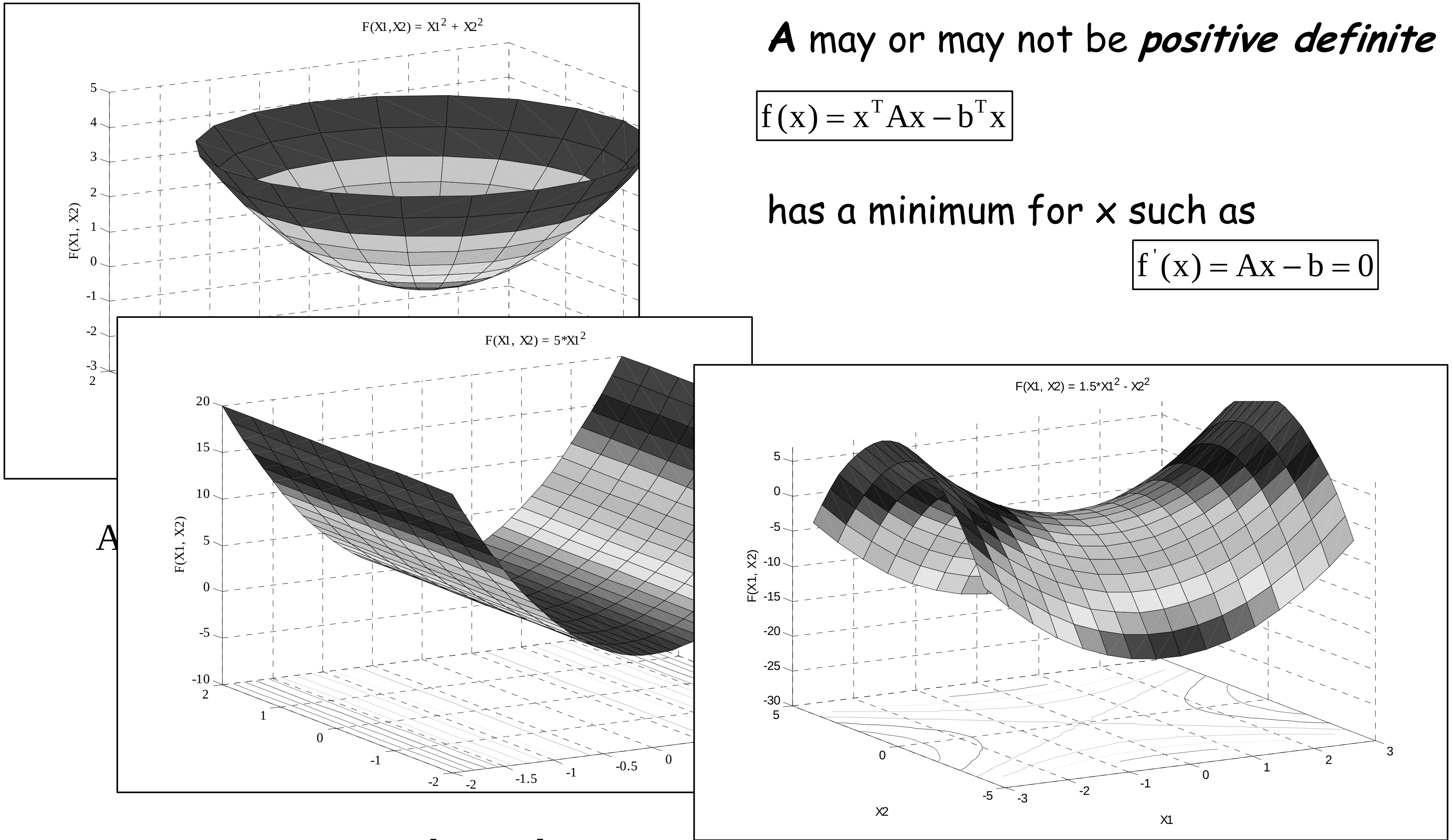
The condition number of **A** can be defined by cond(*A*) = $\lambda_{max}(A) / \lambda_{min}(A)$ where λ are the eigenvalues.

Cond<1 the problem is well-conditioned

Cond>>1 the problem is ill-conditioned

The relative error estimate is given by:

$$\frac{\|x - \bar{x}\|}{\|x\|} \leq \text{cond}(\mathbf{A}) \frac{\|\mathbf{A}x - b\|}{\|b\|}$$



A may or may not be ***positive definite***

$$f(x) = x^T A x - b^T x$$

has a minimum for x such as

$$f'(x) = Ax - b = 0$$

One eigenvalue is close to 0.

One eigenvalue is positive, and another is negative.

The dream

The matrix is sparse:

small storage because only non-zero values are stored

The matrix is symmetric:

reduced number of operation for the solver

small storage half of the matrix is stored

The matrix is definite positive:

efficient iterative solver can be used

The matrix is a M-matrix:

respects the maximum principle: no local minimum or maximum,

i.e. no oscillations

Iterative Methods:

methods which asymptotically approach the true solution as the number of steps increases.

Direct Methods :

methods that yield the theoretically exact result in a fixed number of steps. (Assuming an infinitely precise computing engine.)

Typical iterative methods:

1. Jacobi method
2. Gauss-Seidel method
3. Successive Over-Relaxation (SOR), or LSOR
4. Alternative Direction Implicit (ADI) method
5. Conjugate Gradient Methods
6. Biconjugate Gradients and CGSTAB
7. Multigrid Methods

If the matrix A is diagonally dominant
then the Jacobi iteration converges to $\mathbf{x}$ for any initial guess

If A is symmetric and positive definite,
then the Gauss-Seidel iteration converges to x for any initial guess

For Conjugate Gradient methods, without roundoff error, if A has m distinct eigenvalues, converges in m iterations, but often less!

Typical direct methods:

1. Elimination Methods
   - Gauss Elimination
   - Gauss-Jordan Elimination
   - Cholesky Factorization (Numerically Symmetric)
   - LU or LDU factorization,(Crout, Doolittle, Banachiewicz)

$$\begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ m_{n1} & m_{n2} & \cdots & m_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & \cdots & u_{1n} \\ 0 & 1 & \cdots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

2. Frontal/multifrontal methods

SUMMARY

Iterative Methods

Need few RAM

Can be very efficient if the initial guess is close to the solution (transient)

Require specific matrix properties to converge

Elimination Methods

No convergence criteria .

Factors can be used repeatedly.

Factors can be ‘easily’ modified to accommodate matrix/network changes.

Need RAM and CPU time

AND THE FUTURE .....

Advective dominant transport: ELLAM should be more popular

Coupled systems: reactive transport

Non-matching space and time discretization

A posteriori error estimate with grid refinment

....

Merci pour votre attention