Numerical Simulation Methods in Geophysics, Part 12: Advection problems and the Finite Volume Method

1. MGPY+MGIN

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Recap

1. The Finite Difference (FD) method
   - elliptic: Poisson equation in 1D, look into 2D/3D
   - parabolic: diffusion equation in 1D, time-stepping
   - hyperbolic: acoustic wave equation in 1D
2. The Finite Element (FE) method
   - Poisson equation in 1D & 2D
   - complex Helmholtz equation in 2D for EM problems
   - solving EM problems and computational aspects

Boundary conditions

Neumann (implicitly by choice of shape functions)

$$\frac{\partial u}{\partial n} = 0 \Rightarrow \mathbf{n} \times \boldsymbol{\nabla} \times \mathbf{E} = 0 \Rightarrow \mathbf{n} \times \mathbf{B} = 0$$

Dirichlet

$$u = 0 \Rightarrow \mathbf{n} \times \mathbf{E} = 0 \Rightarrow \mathbf{n} \cdot \mathbf{B} = 0$$

Mixed boundary conditions

So far…

- Dirichlet Boundary conditions $u = u_0$
- Neumann Boundary conditions $\frac{\partial u}{\partial n} = g_B$

vectorial problems: $\mathbf{n} \cdot \mathbf{E} = 0$ (Neumann) or $\boldsymbol{\nabla} \times \mathbf{E} = 0$ (Dirichlet)

In general mixed, also called Robin (or impedance convective) BC

$$au + b\frac{\partial u}{\partial n} = c$$

Example DC resistivity with point source

$$\boldsymbol{\nabla} \cdot \sigma \boldsymbol{\nabla} u = \boldsymbol{\nabla} \cdot \mathbf{j} = I\delta(\mathbf{r} - \mathbf{r}_s)$$

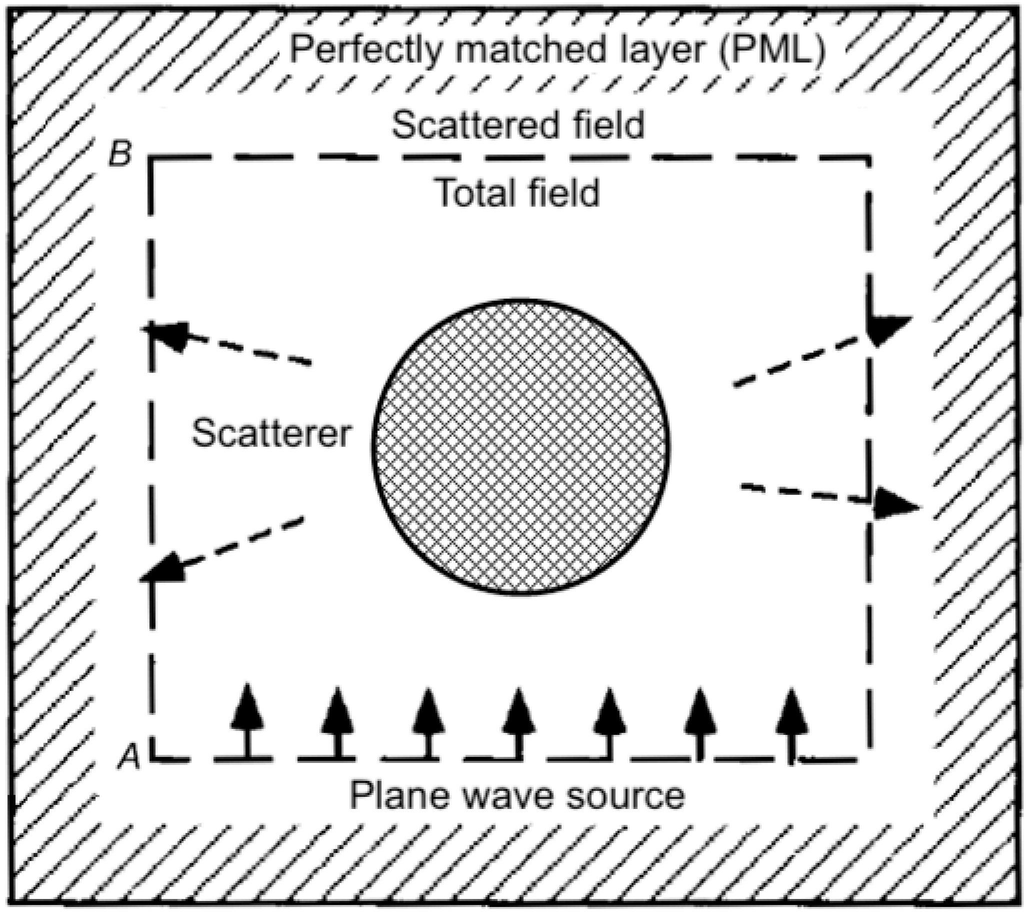
solution for homogeneous σ on surface: $u = \frac{I}{2\pi\sigma} \frac{1}{|\mathbf{r}-\mathbf{r}_s|}$

E-field $\mathbf{E} = -\frac{I}{2\pi\sigma} \frac{\mathbf{r}-\mathbf{r}_s}{|\mathbf{r}-\mathbf{r}_s|^3}$

normal direction $\mathbf{E} \cdot \mathbf{n} = -\frac{u}{|\mathbf{r}-\mathbf{r}_s|} \cos\phi$ purely geometric

$$\frac{\partial u}{\partial n} + \frac{\cos\phi}{|\mathbf{r} - \mathbf{r}_s|} = 0$$

Perfectly matched layers



$$\frac{\partial}{\partial x} \to \frac{1}{1 + i\sigma/\omega} \frac{\partial}{\partial x}$$

$$x \to x + \frac{i}{\omega} \int^{x} \sigma(x')\mathrm{d}x'$$

Absorbing boundary conditions

wave equation (e.g. in 2D)

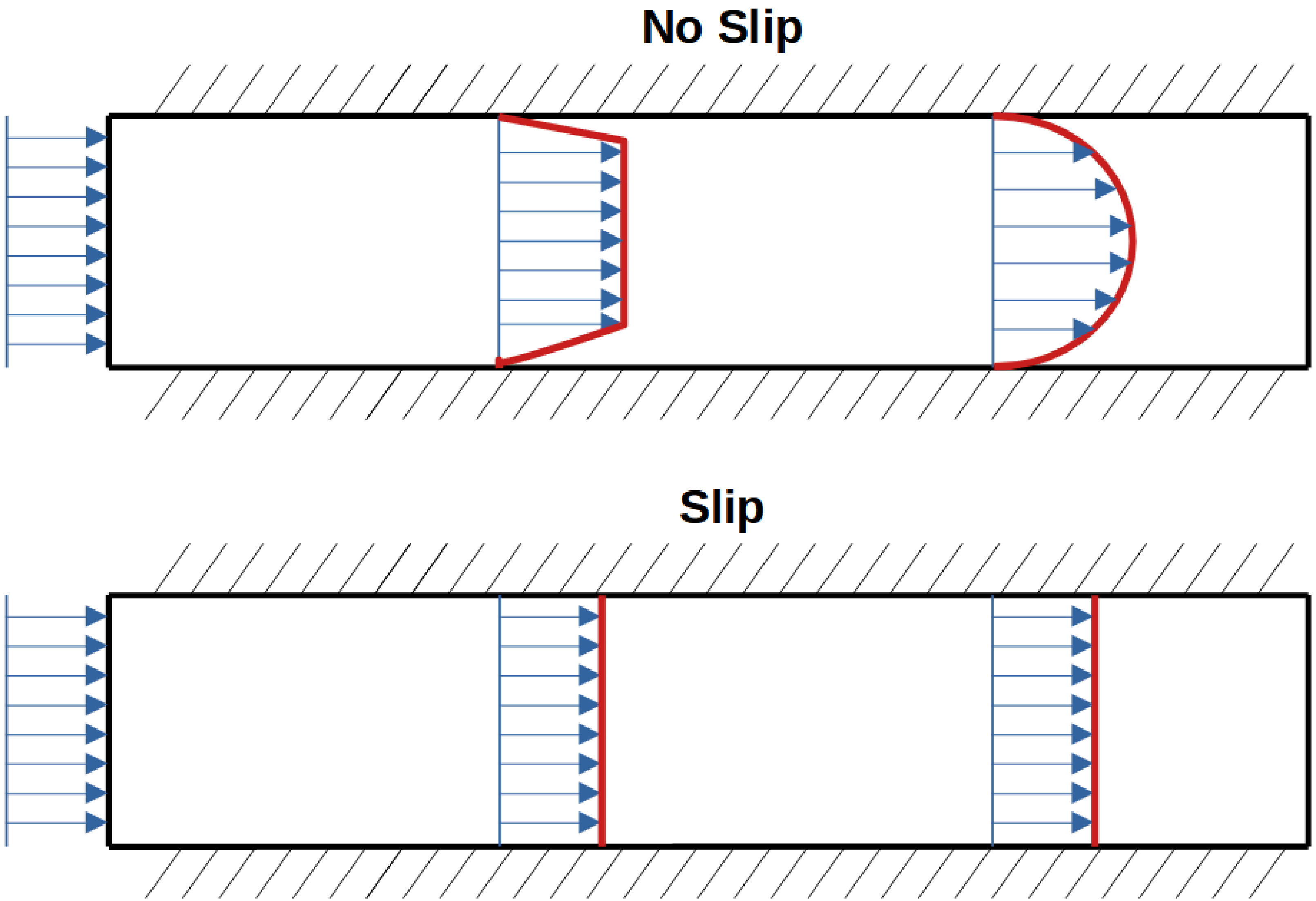
$$\frac{\partial^2 u}{\partial t^2} - v^2 \nabla^2 u = 0$$

Fourier transform in t and y (boundary direction) $\Rightarrow \omega, k$

$$\omega^2 \hat{u} - v^2 \frac{\partial^2 \hat{u}}{\partial x^2} + v^2 k^2 \hat{u} = 0$$

ordinary DE with solution $\hat{u} = \sum a_i e^{\lambda x}$ with $\lambda^2 = k^2 - \omega^2 / v^2$

No-slip boundary condition



Time-domain EM

- Fourier transform excitation $\Rightarrow$ solve in FD $\Rightarrow$ backtransform
- solve with Time-Stepping: Governing equation

$$\boldsymbol{\nabla} \times \mu^{-1} \boldsymbol{\nabla} \times \mathbf{e} + \sigma \frac{\partial \mathbf{e}}{\partial t} = - \frac{\partial \mathbf{j}_s}{\partial t}$$

$$\mathbf{K}\mathbf{u}(t) + \mathbf{M}\partial_t \mathbf{u}(t) = \mathbf{s}(t)$$

Implicit time stepping

$$\mathbf{K}\mathbf{u}^{n+1} + \mathbf{M}\frac{\mathbf{u}^{n+1} - \mathbf{u}^{n}}{\Delta t} = \mathbf{s}(t)$$

$$(\Delta t\mathbf{K} + \mathbf{M})\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^{n} + \Delta t\mathbf{s}^{n+1}$$

second-order

$$(2\Delta t\mathbf{K} + 3\mathrm{M})\mathbf{u}^{n+2} = \mathbf{M}(4\mathbf{u}^{n+1} - \mathbf{u}^{n}) - 2\Delta t\mathbf{s}^{n+2}$$

Solution in pyGIMLi

step by step

```
import pygimli.solver as ps
A = ps.createStiffnessMatrix(mesh, a)
M = ps.createMassMatrix(mesh, b)
f = ps.createLoadVector(mesh, f)
ps.assembleNeumannBC(b, boundaries)
ps.assembleDirichletBC(A, b)
ps.assembleRobinBC(A, boundaries, b)
u = ps.linSolve(A, b)
```

or shortly

```
from pygimli.physics.seismics import solve
bc = {'Dirichlet': {4: 1.0, 3: 0.0},
      'Neumann': {2: 1.0}}
u = ps.solveFiniteElements(mesh, a, b, f,
                           bc=bc, t=times,
u = solvePressureWave(mesh, velocities, ti
                      sourcePos, uSource)
```

$$c\frac{\partial u}{\partial t} = \boldsymbol{\nabla}\cdot(a\boldsymbol{\nabla}u) + bu + f(\mathbf{r},t)$$

Advection problems

Volume elements move with velocity $\mathbf{v}$ and take (advectio=move with)

$$\frac{\partial T}{\partial t} \Rightarrow \frac{\partial T}{\partial t} + \frac{\mathrm{d}z}{\mathrm{d}t}\frac{\partial T}{\partial z}$$

in 3D $\mathbf{v} \cdot \boldsymbol{\nabla} T \Rightarrow$ advection-dispersion equation

$$\frac{\partial T}{\partial t} - \boldsymbol{\nabla} \cdot a \boldsymbol{\nabla} T + \mathbf{v} \cdot \boldsymbol{\nabla} T = \boldsymbol{\nabla} \cdot q_s$$

Continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V u(\mathbf{r},t)\mathrm{d}V = \int_V \frac{\partial u(\mathbf{r},t)}{\partial t} + \int_V \mathbf{v}\cdot\boldsymbol{\nabla} u(\mathbf{r},t)\mathrm{d}V$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V u(\mathbf{r},t)\mathrm{d}V = \int_V \frac{\partial u(\mathbf{r},t)}{\partial t} + \int_{\partial V} u(\mathbf{r},t)\mathbf{v}\cdot\mathbf{n}$$

Conservation of mass (u=ϱ) $\Rightarrow$ divergence of flux $u\mathbf{v}$

$$\frac{\partial u}{\partial t} + \boldsymbol{\nabla}\cdot(u\mathbf{v}) = 0$$

can also be conservation of impuls or energy

Advection-dispersion equation (general)

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} u - \boldsymbol{\nabla} \cdot (a \boldsymbol{\nabla} u) = bu + f(\mathbf{r}, t)$$

flux $\mathbf{v} \cdot \boldsymbol{\nabla} u$ (Advection), stiffness $-\boldsymbol{\nabla} \cdot (a \boldsymbol{\nabla} u)$ (Dispersion=Diffusion)

arising in *Computational Fluid Dynamics*

Solve, e.g., by `pyGIMLi.solver.solveFiniteVolume` (Link)

```
bc = dict(Dirichlet={4: 1.0, 3: 0.0}, Neumann={2: 1.0})
u = ps.solveFiniteVolume(mesh, a, b, f, bc=bc, t=times, c)
```

Computational magnetohydrodynamics

Magnetohydrodynamic induction equation

$$\frac{\partial \mathbf{B}}{\partial t} = \boldsymbol{\nabla} \times \frac{1}{\mu\sigma} \boldsymbol{\nabla} \times \mathbf{B} + \boldsymbol{\nabla} \times (\mathbf{v} \times \mathbf{B})$$

Forces on fluid (induction, Coriolis, pressure, gravity, Lorentz)

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \boldsymbol{\nabla})\mathbf{v} + \boldsymbol{\nabla} p = -2\omega \times \mathbf{v} + \alpha T \mathbf{g} + \mathbf{j} \times \mathbf{B}/\rho$$

FE solution can bear instabilities

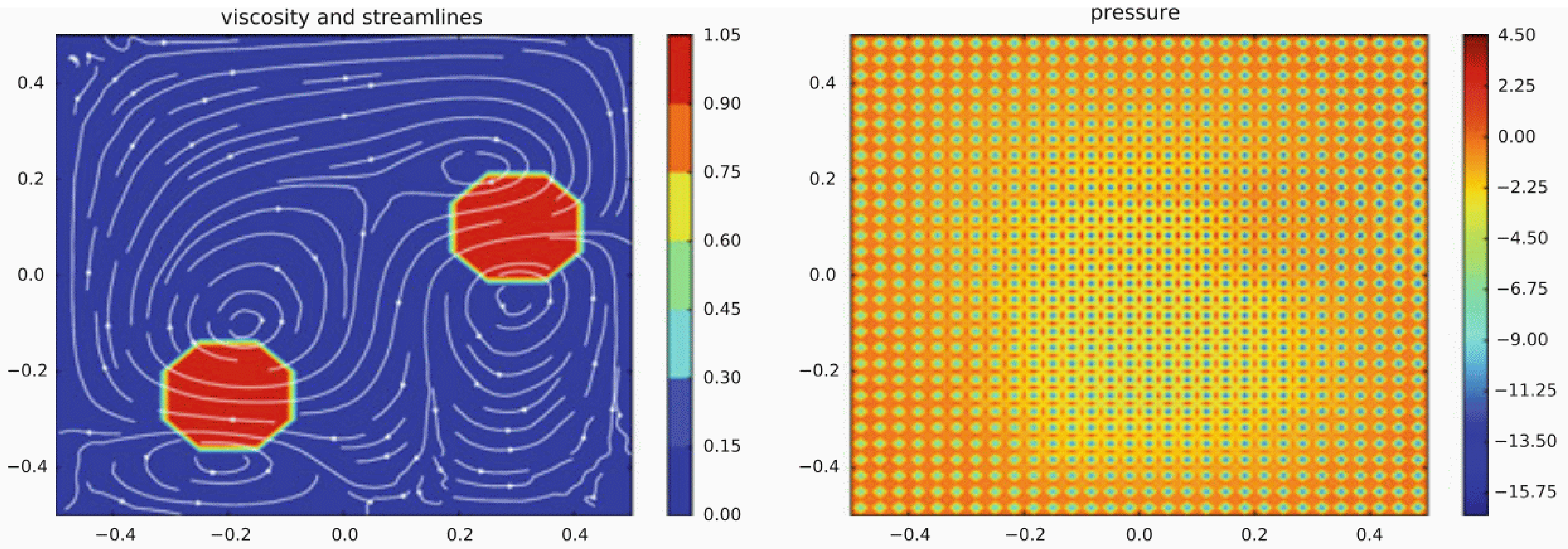


Fig. 10.1 *Left* velocity field determined with a full momentum+pressure solver for the same two particles in a box, using the full Stokes operator. Here, the solution is the same as the one in Fig. 9.5 except near the walls, due to the different Boundary conditions (free slip in the other case, no-slip in this case). *Right* pressure field for the same case. One observes that an instability arises. It arises because velocity and pressure are both solved on the same nodes

Simple 1D advection problem

$$\frac{\partial u}{\partial t} + \frac{\partial v(u)}{\partial x} = 0$$

Solution u_i at node i represents average value over cell

$$\overline{u}_i(t) = \frac{1}{x_{i+1/2} - x_{i-1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t)\mathrm{d}x$$

$$\int_{t_1}^{t_2} \frac{\partial u}{\partial t} = u(x,t_2) - u(x,t_1) = -\int_{t_1}^{t_2} \frac{\partial v(u)}{\partial x}$$

Finite Volume schemes

Simple 1D advection problem

$$u(x, t_2) = u(x, t_1) - \int_{t_1}^{t_2} \frac{\partial v(u)}{\partial x}$$

$$\overline{u}(t_2) = \frac{1}{x_{i+1/2} - x_{i-1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \left(u(x, t_1) - \int_{t_1}^{t_2} \frac{\partial v(u)}{\partial x} \right)$$

$$\overline{u}(t_2) = \overline{u}(t_1) - \frac{1}{x_{i+1/2} - x_{i-1/2}} \left(\int_{t_1}^{t_2} v_{i+1/2} \mathrm{d}t - \int_{t_1}^{t_2} v_{i-1/2} \mathrm{d}t \right)$$

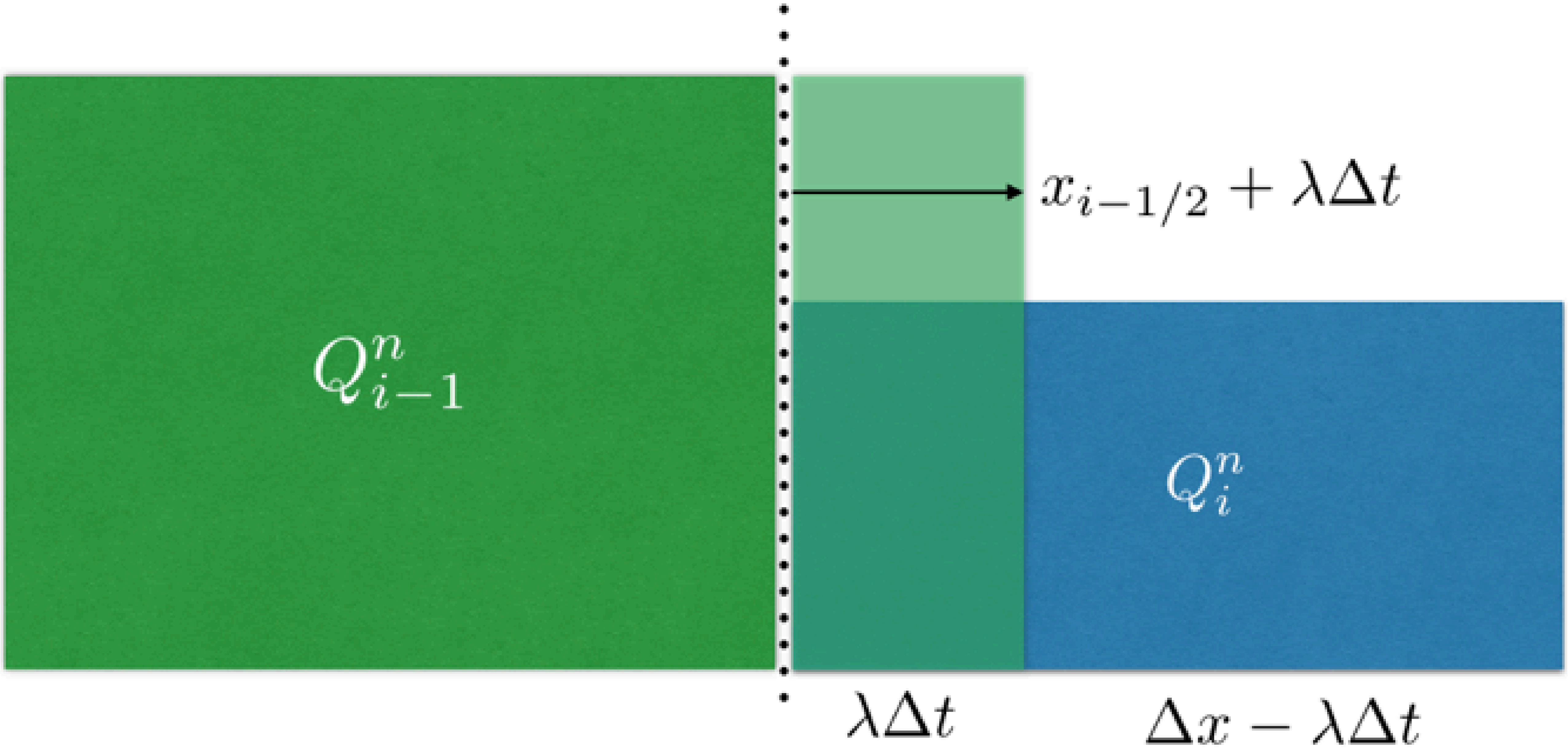
Result

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{1}{\Delta x_i}\left(v_{i+1/2} - v_{i-1/2}\right) = 0$$

Note

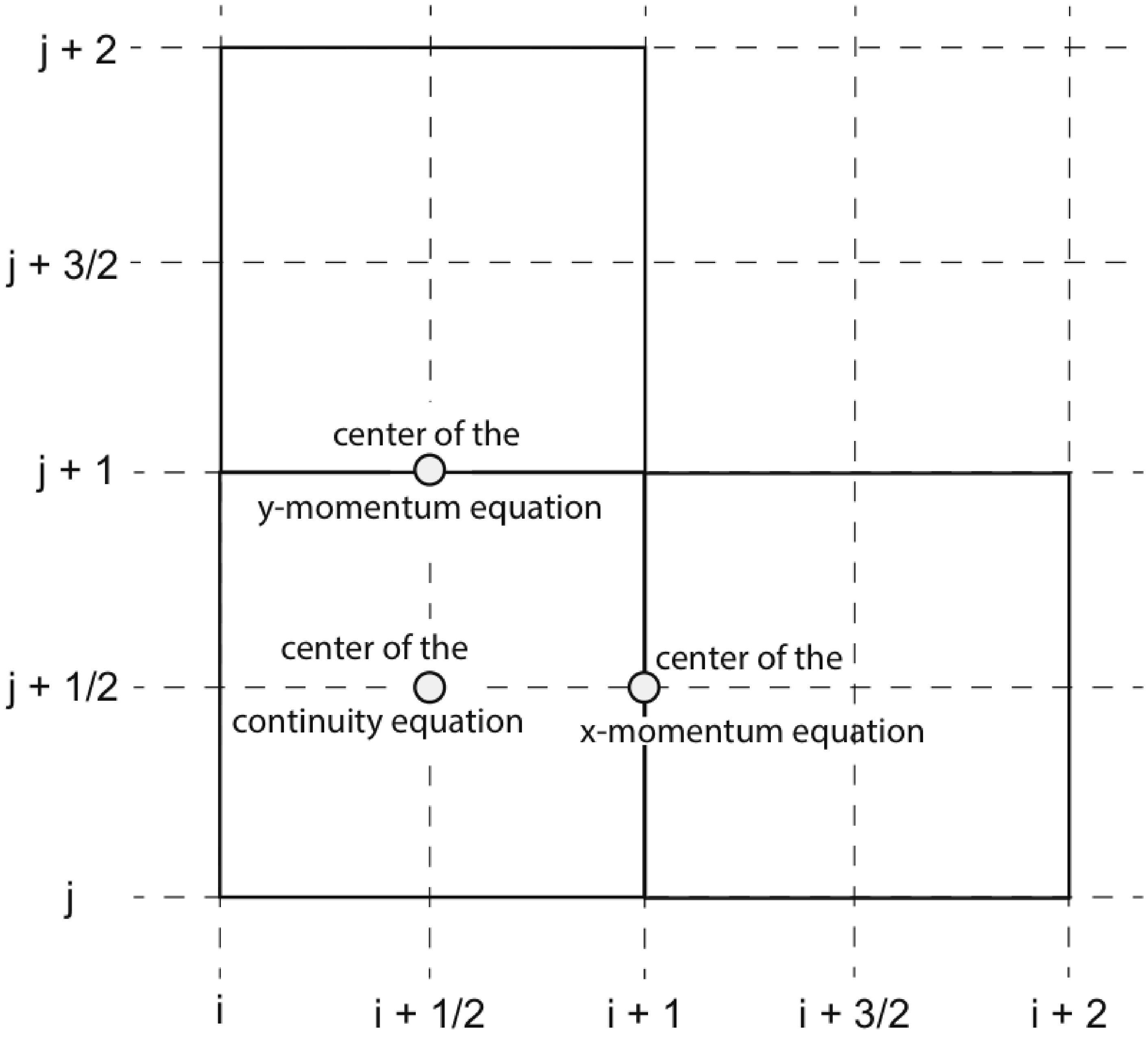
Finite volume schemes are conservative as cell averages change through the edge fluxes. In other words, one cell's loss is always another cell's gain!

Visualization



Similarity to staggered (E, B) grid methods

Fig. 10.2 Sketch of the of the indices and of the positions where the continuity, the x-momentum and the y-momentum equations are calculated. The mid indexes ($\frac{1}{2}$ and $\frac{3}{2}$) indicate the center between two edges of the volume. By calculating the finite volume at the center of each side one is also implicitamente integrating the momentum equations on each side. It is possible to show that this choice makes this algorithm second-order accurate.



Conservation law (3D) problem

$$\frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{v}(u) = 0$$

volume integral over cell, using Gauss' law

$$\int_{\Omega_i} \frac{\partial \mathbf{u}}{\partial t} \mathrm{d}\Omega + \int_{\Omega_i} \boldsymbol{\nabla} \cdot \mathbf{v}(u) \mathrm{d}\Omega = 0 = \int_{\Omega_i} \frac{\partial \mathbf{u}}{\partial t} \mathrm{d}\Omega + \int_{\Gamma_i} \mathbf{v}(u) \cdot \mathbf{n} \, \mathrm{d}\Gamma$$

$$\Rightarrow \frac{\partial \overline{u}}{\partial t} + \frac{1}{V_i} \int_{\Gamma_i} \mathbf{v}(u) \cdot \mathbf{n} \, \mathrm{d}\Gamma = 0$$

Godunov's scheme

1. Define piece-wise constant approximation u^{n+1}
2. Obtain solution for local Riemann problem at cell interfaces
3. Average state variables from 2. over

The methods

The Finite Difference method

approximates the partial derivatives by difference quotients (beware Δx and Δa)

The Finite Element method

approximates the solution through base functions in integrative sense

The Finite Volume method

approximates the solution by piecewise constant values and ensures conservation law by fluxes

Discontinuous Galerkin scheme

- use Galerkin method (multiply test function and take as basis)
- discretize fields by piece-wise constant functions
  - fields are becoming discontinuous
- communicate flux between elements by Riemann problem scheme
- every element independent (also mesh size)
- fully parallelized (element-wise)