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Numerical aspects of the advection-diffusion equation

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SILAM winter school,

February 2013, FMI

Outline

- **Intro**
- **Some common requirements for numerical transport schemes**
- **Lagrangian approach**
- **Eulerian schemes**
  - features and error sources
  - SILAM: Galperin's scheme
- **Vertical transport in Eulerian models**
  - vertical levels
  - solving diffusion

Introduction

- **The following aims to provide an only slightly technical view to numerical solution of the advection-diffusion equation**

$$\frac{\partial c}{\partial t} = \nabla \cdot (K \nabla c) - \nabla \cdot (\vec{v} c) \qquad (1)$$

- **Will focus separately in advection and diffusion**
  - > the approach of operator splitting: instead of solving (1) as whole, develop schemes for the individual terms
  - Advantages:
    - simpler implementation
    - numerical schemes can be tailored for each sub-problem
    - generalizable to include chemistry and other processes
  - Disadvantage:
    - additional numerical error not easily analysed
  - Operator splitting is used by nearly all chemistry-transport models

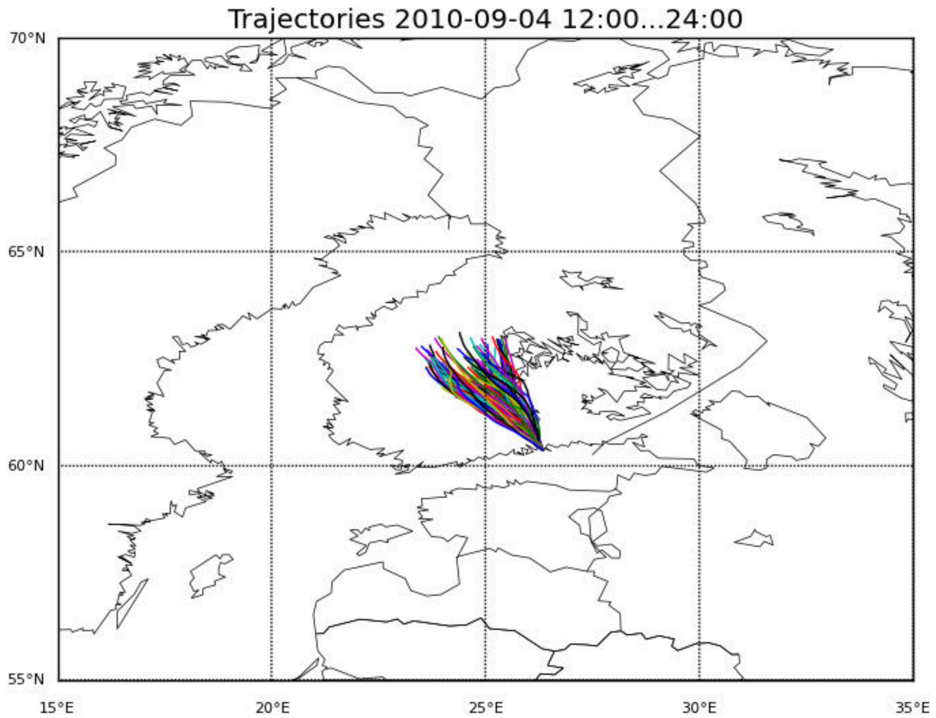
Some common requirements for numerical schemes in dispersion models

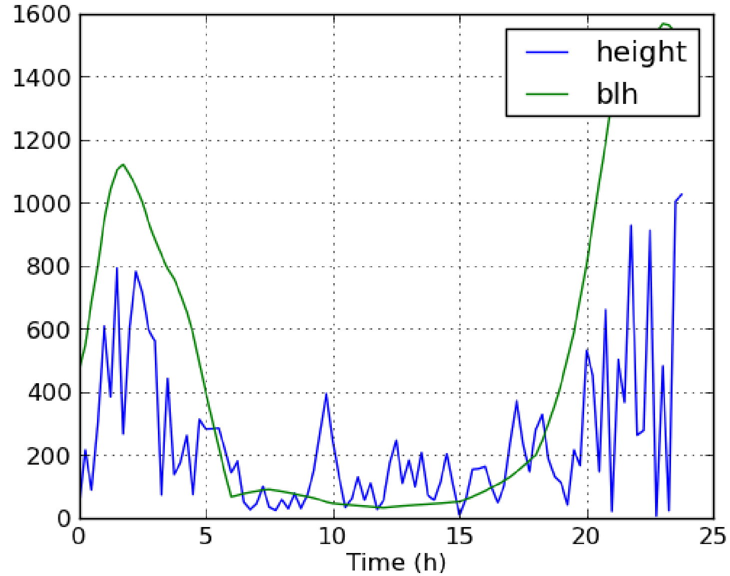
- **Mass conservation**
- **Positivity: no negative concentrations**
- **Stability: no infinite concentrations**
- **“sufficient accuracy”…**
- **“sufficiently low” computational cost**
- **Two approaches frequently satisfy the above:**
  - Lagrangian, particle based models
  - Eulerian, finite volume models
- **spectral, finite element, finite difference, collocation, etc.…**

Eulerian and Lagrangian schemes

- **Euler**
  - split the domain in grid cells
  - track the mass budget of each cell
  - turbulent mixing described as diffusion
  - SILAM v4, v5
- **Lagrange**
  - track the motion of the pollutant represented by finite number of model particles
  - count model particle density to obtain concentration (mass/volume)
  - turbulent mixing described as a random process
  - SILAM v4, v5.x
- **Lagrange attractive especially for point sources, but**
  - handling diffuse emission sources is expensive
  - handling nonlinear chemistry is very difficult

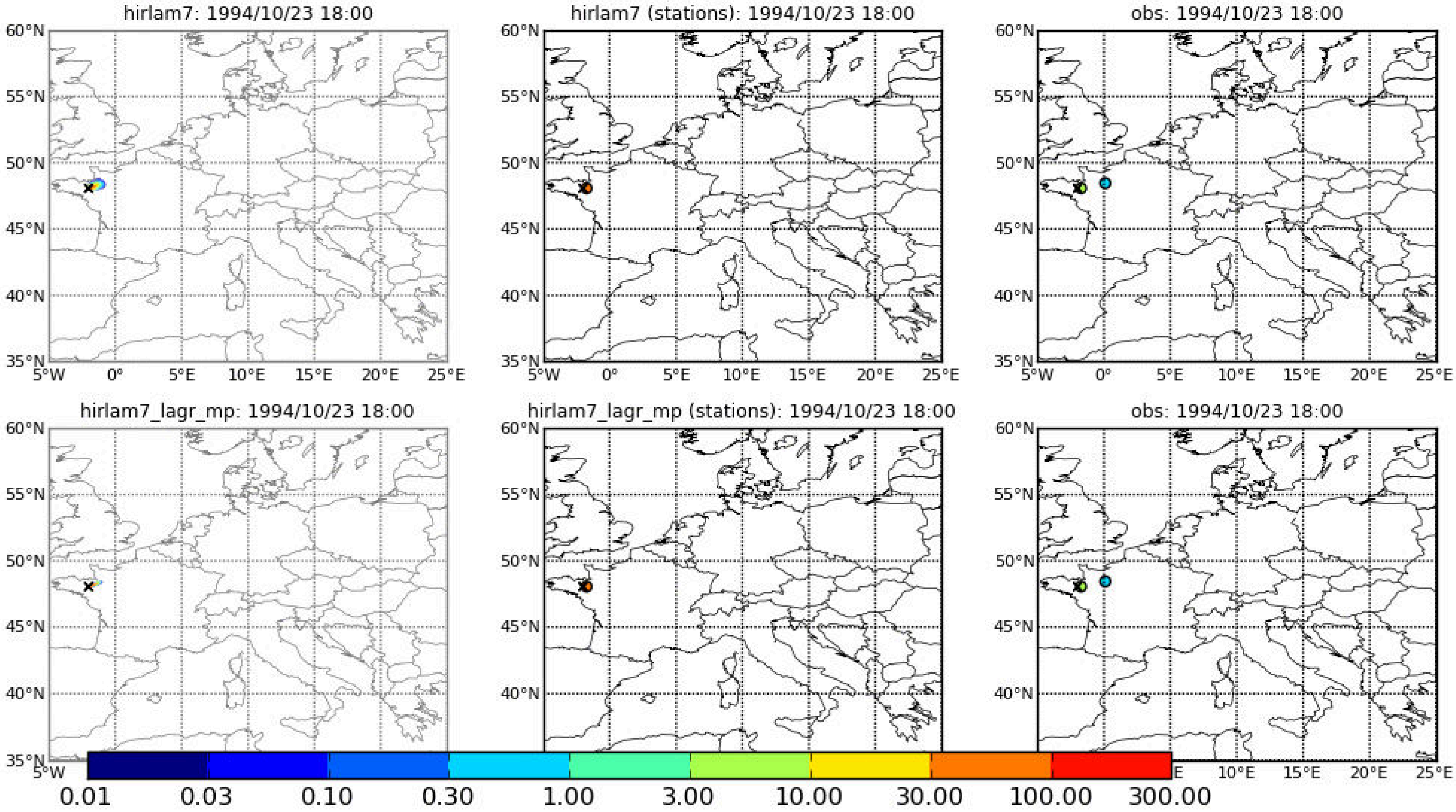
Lagrangian dynamics: particle trajectories





> A single particle trajectory is not meaningful – their statistics are!

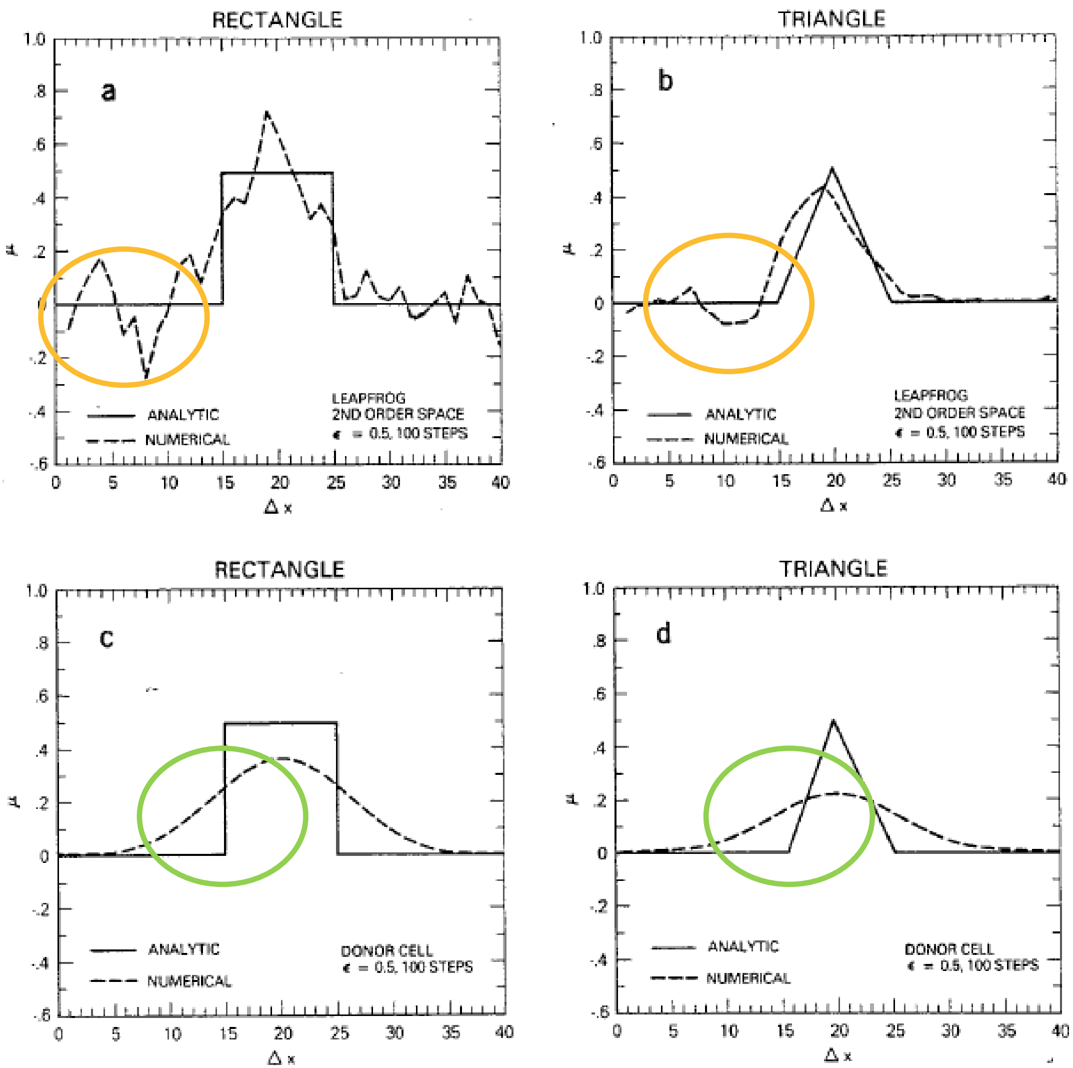
SILAM Euler / Lagrange



Eulerian advection schemes

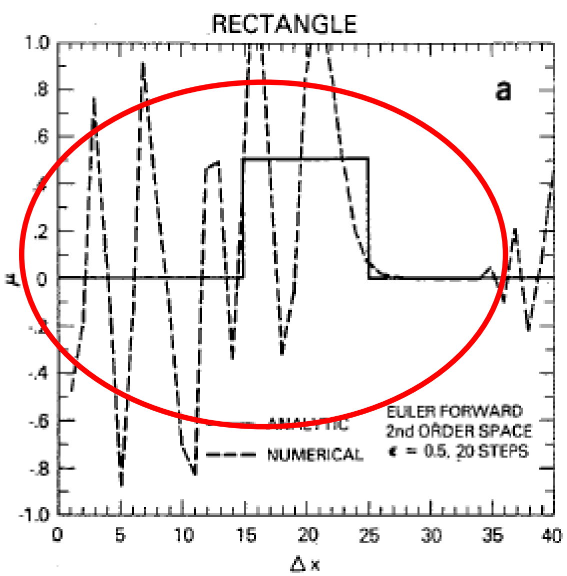
- **Finite volume schemes usually mass conservative by construction**
- **Everything else needs to be worked out…**
- **We'll look at some issues arising with Eulerian schemes**

Issues with Eulerian advection schemes



(From Rood, 1987)

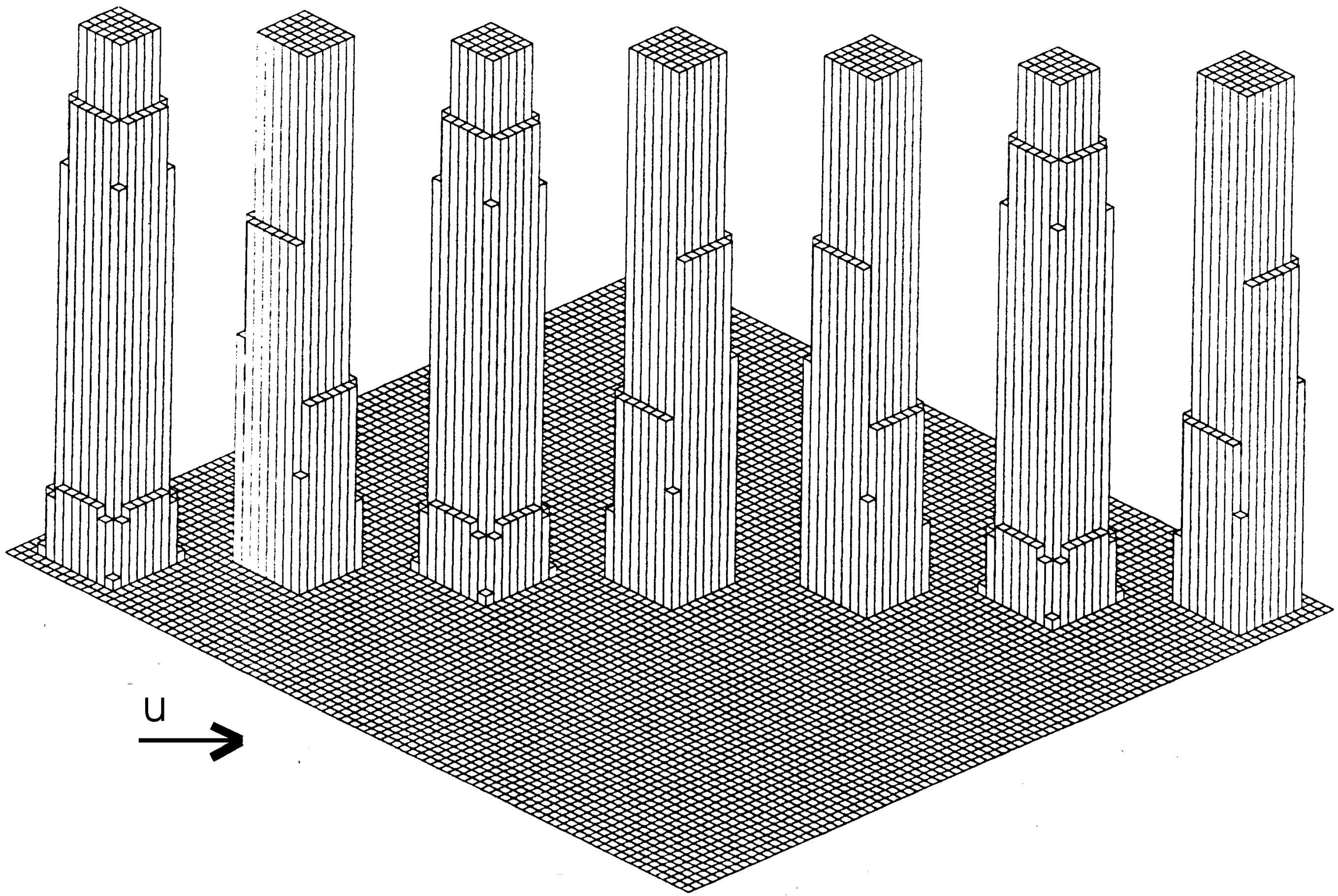
Monotonicity,
positivity (lack of),
Numerical diffusion,
Instability



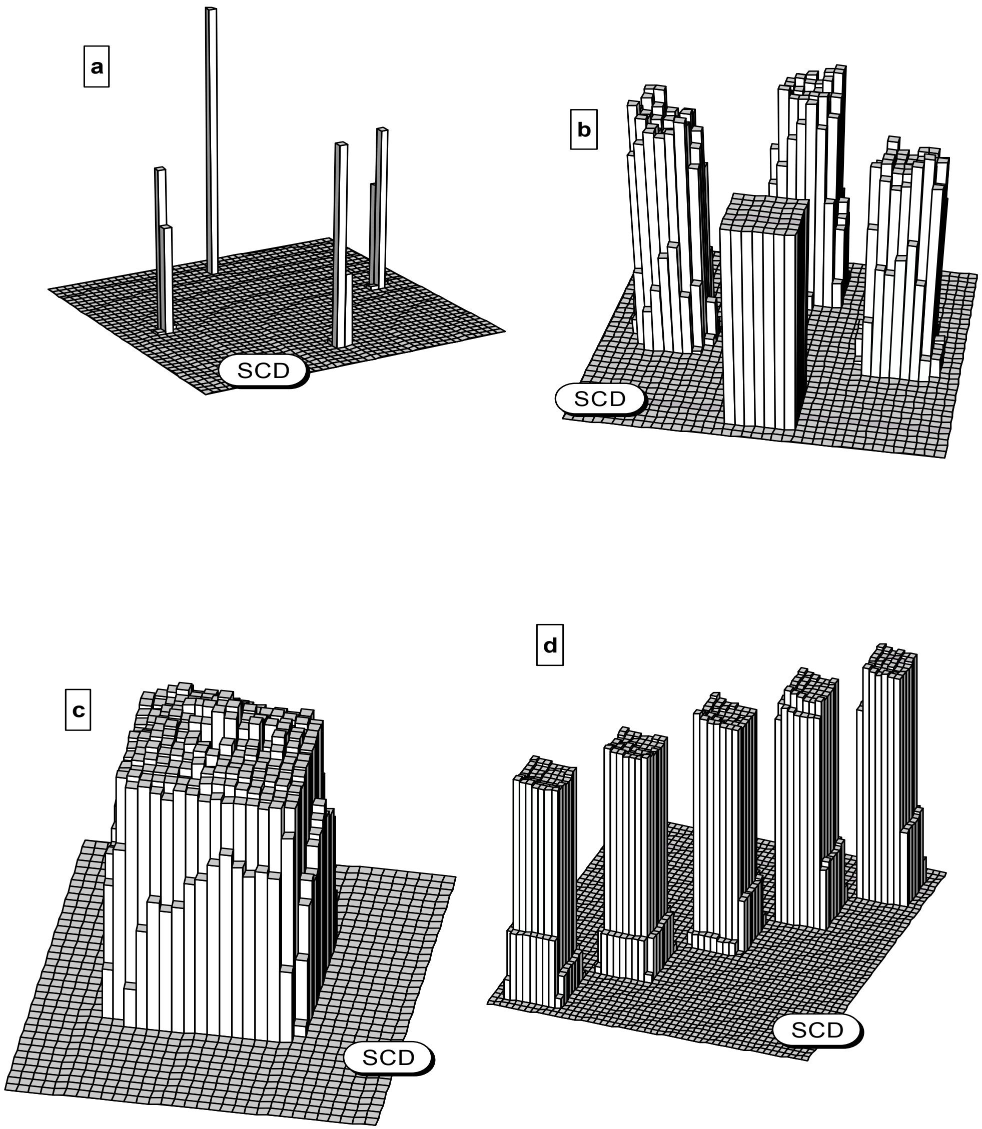
Eulerian advection schemes

- **Classical finite difference schemes rarely useful for advection**
  - Behave poorly with sharp gradients
  - Godunov's theorem: a linear, monotonous scheme is at most first order accurate
  - Stability requires a small Courant number $C = \frac{v\Delta t}{\Delta x}$
- **Practical advection schemes are nonlinear**
- **One approach: borrow elements from Lagrangian schemes**
  - no strict stability constraints
  - Example: the Galperin scheme, as used in SILAM

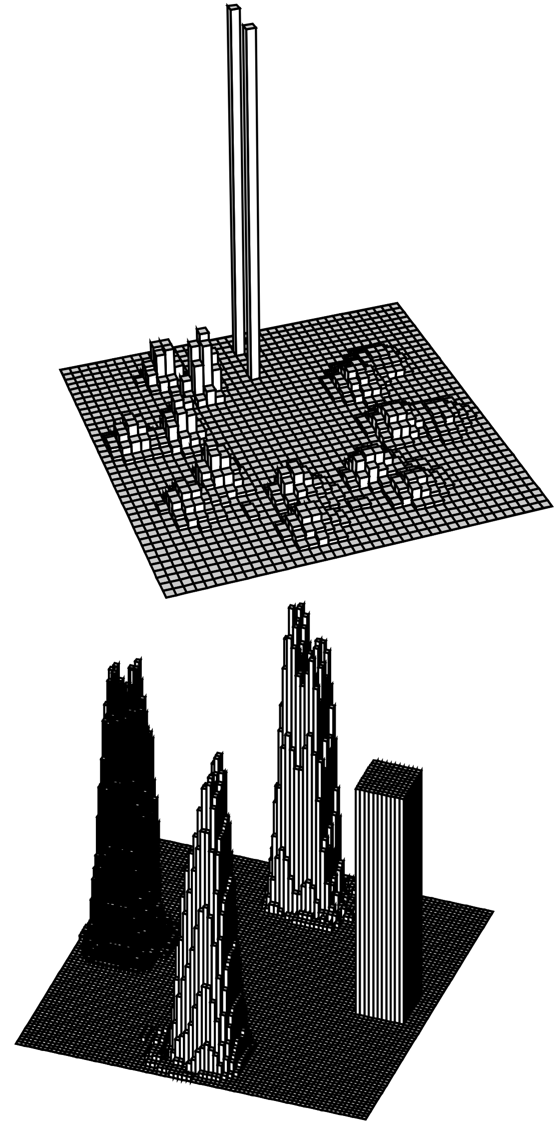
Galperin's scheme: examples



Galperin scheme:



Bott scheme:



Comments on the Galperin scheme

- **Very low numerical diffusion**
- **Mass conservative**
- **Positively definite, but not monotonous**
- **Stable at any Courant number**
  - but accuracy suffers at high *C*!
- **Good computational performance, but requires 3 additional tracers for each chemical species (first moment of mass in 3 dimensions)**
- **In SILAM:**
  - V2 advection: first order time integration
  - V3 advection: second order implicit time integration
  - V3 slower than V2, but better performance for long-lived species (especially in complex terrain)

Additional issues: mass consistency

- **Mass conservation is a global feature of advection scheme (ignore diffusion for a moment…)**
- **concentration: the conservative form**

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{v}) = 0 \qquad (2)$$

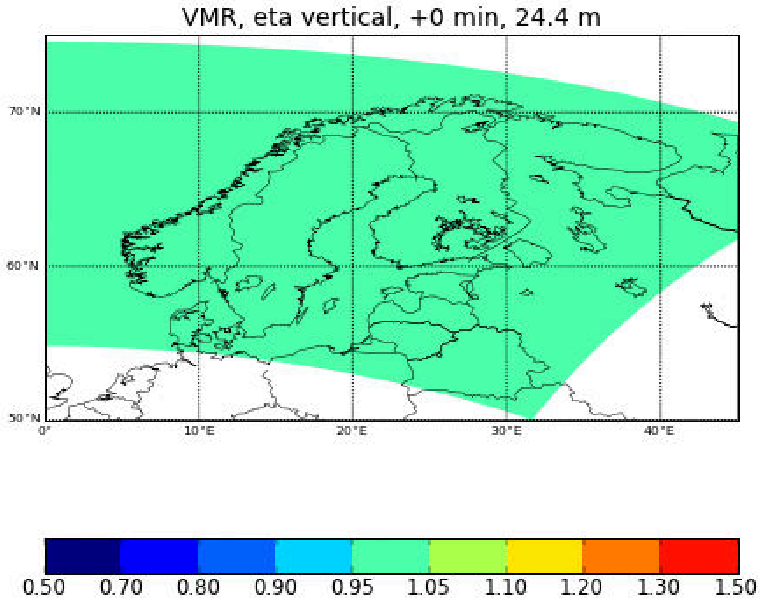
- **mixing ratio: the advective form**

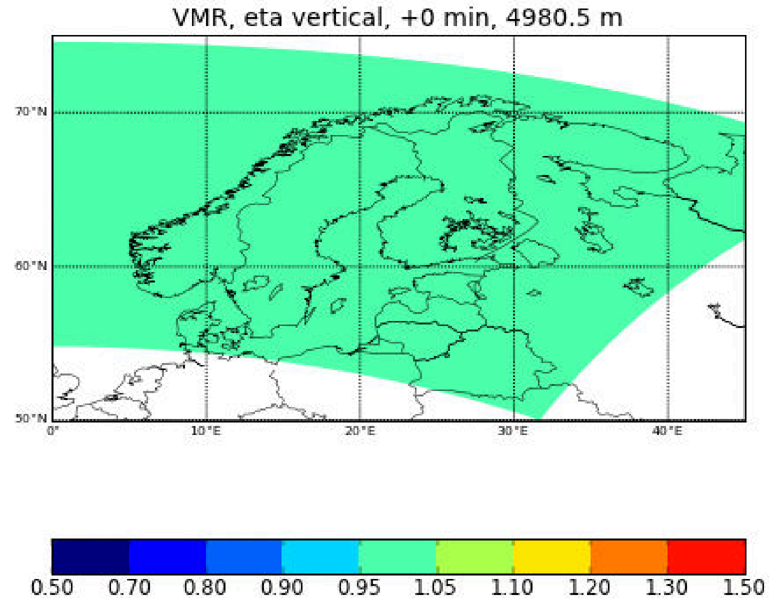
$$\frac{\partial \xi}{\partial t} + \vec{v} \cdot \nabla \xi = 0, \quad \xi = c/\rho \qquad (3)$$

- **Is the mixing ratio computed from solution of (2) guaranteed to satisfy (3)?**
- **Consider a consequence of (3): initially constant mixing ratio stays constant…**

Additional issues: mass consistency

- **…or not**





- **Problem is related to differences in schemes for computing the winds (weather model) and the advection (CTM)**
- **Surprisingly recent issue in the AQ modelling community**

Vertical discretization in Eulerian models

- **Model vertical layers may be defined in terms of pressure, height from ground, altitude, etc.**
  - constant height
  - hybrid terrain influenced
- **SILAM:**
  - “standard” setup – levels defined by height
  - “hybrid levels” as option since v5.1
- **Vertical advection:**
  - slower than horizontal, but not negligible!
  - Galperin’s scheme
- **Vertical diffusion…**

Vertical diffusion

- **This time classical schemes work (almost!)**
- **Textbook solution of the 1D diffusion**
- **Flux-preserving averaging of the diffusivities *K_z* *(Sofiev, 2002)***

$$< K_z >_{i,\, i+1} = \frac{\Delta z_i}{\int_i^{i+1} \frac{dz}{K_z(z)}}$$

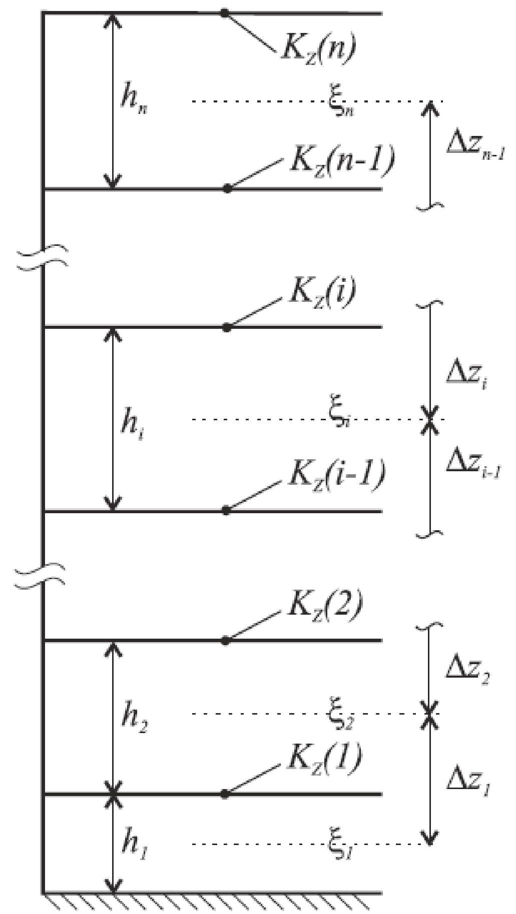


Figure 1. Multilayer structure of the vertical column.

Final comments

- **Different simulations and pollutants are sensitive to different features of numerical schemes**
  - pollutants with concentrated sources, short term simulations: numerical diffusion, resolving gradients
  - long-lived pollutants, long term simulations: mass consistency issues, overall accuracy
- **Excluding input/output, computing tranport takes ~20% of run time in chemistry simulations, closer to 100% in non-chemistry runs**

Literature

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