Mass conservation and continuity equations !!!

In the absence of sources/sinks it is possible to attain formal local mass conservation in models based on the volume density continuity equation.

This is generally NOT the case if the advection equation is used to forecast the mixing ratio. This is because one needs to evaluate the mass as a product of two separate numerical forecasts: one for the mixing ratio (q_t) and another for the dry air density (ρ_d) and then evaluate $\rho_t = q_t \rho_d$.

The problem is that two different numerical approximations have to be used since it is two different equations that are solved: the advection equation and the continuity equation.

Mass conservation

Strategies one can follow in order to obtain formal mass conservation:

- Flux based Eulerian schemes (e.g. Bott, Easter)
- Flux based semi-Lagrangian (e.g. Leonard, Lin and Rood, Xiao et al. (CIP))
- Cell integrated semi-Lagrangian schemes (e.g. Rancic, Machenhauer et al., Lauritzen (CSLAM))

} Finite volume methods

- Partition of unity based semi-Lagrangian schemes (Kaas (LMCSL))
- Full Lagrangian mass conservation is also possible (total mass of all Langrangian particles is conserved).

Finite volume methods

Integro- diffential forms of the continuity equation (here omitting dissipative and source/sink terms)

Eulerian form (fixed control volume ΔV):

$$\frac{\partial \Delta V \bar{\rho}}{\partial t} = \frac{\partial}{\partial t} \iiint_{\Delta V} \rho \, dV = -\iiint_{\Delta V} \nabla \cdot (\rho \boldsymbol{V}) dV = \; -\oiint_{\Delta A} \rho \boldsymbol{V} \cdot \boldsymbol{n} dA$$

Lagrangian form (Lagrangian control volume δV):

$$\frac{d}{dt}\left(\delta V \bar{\rho}\right) = \frac{d}{dt}\left(\iiint_{\delta V} \rho \, dV\right) = 0$$

Flux based finite volume methods

Example in one dimension. Eulerian form of the integro-differential form

$$\frac{\partial \Delta x \bar{\rho}}{\partial t} = -(F(x+\Delta x,t) - F(x,t)) \quad ,$$

where

$$F(x,t) = \rho(x,t)u(x,t)$$

Integration in time of the above equation. Example in one dimension (i.e. density is a function of location x and time t):

$$\bar{\rho}_i^{n+1} = \bar{\rho}_i^n - \frac{\Delta t}{\Delta x}\left(F_{e_i}^n - F_{w_i}^n\right)$$

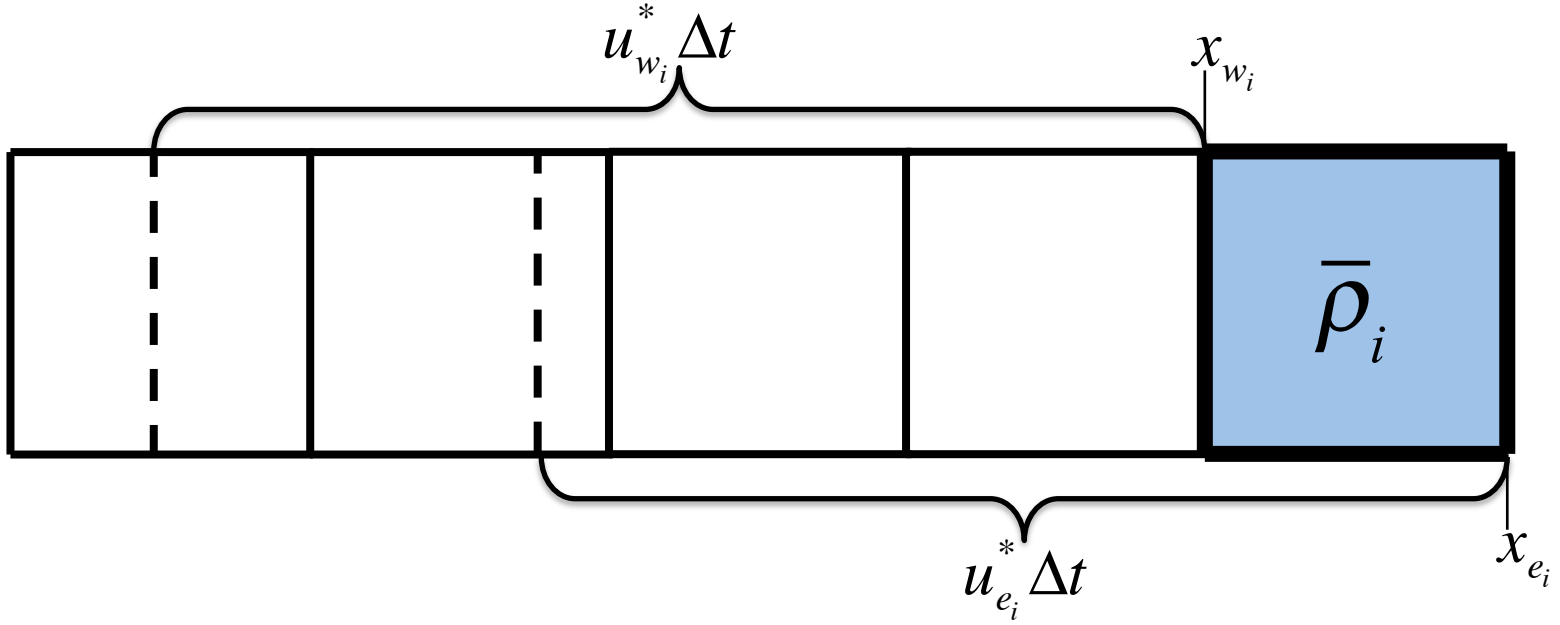
Note that $F_{w_i}^n = F_{e_{i-1}}^n$

where $F_{e_i}^n = \frac{1}{\Delta t}\int_{x_{e_i}-u_{e_i}^*\Delta t}^{x_{e_i}} \rho^n \, dx$ and $F_{w_i}^n = \frac{1}{\Delta t}\int_{x_{w_i}-u_{w_i}^*\Delta t}^{x_{w_i}} \rho^n \, dx$

Flux based finite volume methods

Example in one dimension (cont).

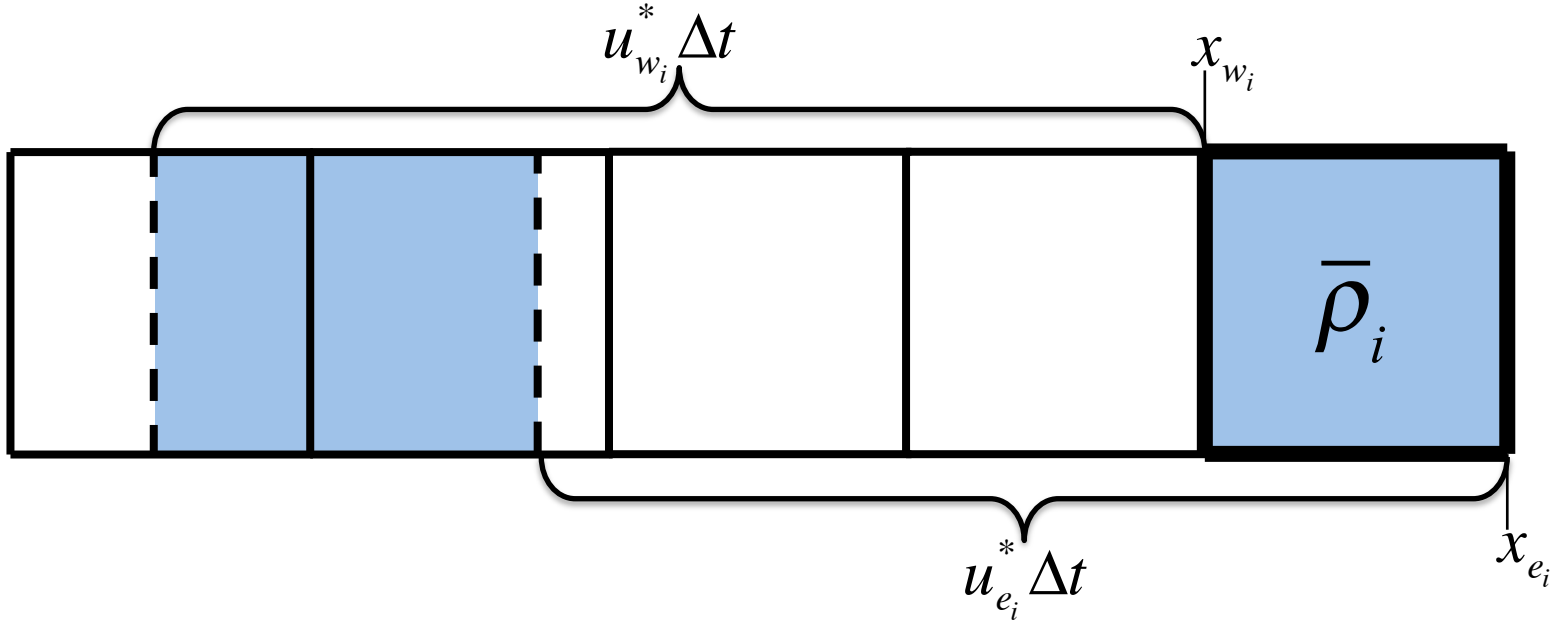
$$\bar{\rho}_i^{n+1} = \bar{\rho}_i^n + \frac{1}{\Delta x}\int_{x_{w_i} - u_{w_i}^* \Delta t}^{x_{w_i}} \rho^n \, dx - \frac{1}{\Delta x}\int_{x_{e_i} - u_{e_i}^* \Delta t}^{x_{e_i}} \rho^n \, dx$$



Cell integrated finite volume methods

Example in one dimension (cont).

$$\bar{\rho}_i^{n+1} = \frac{1}{\Delta x} \int_{x_{w_i} - u^*_{w_i} \Delta t}^{x_{e_i} - u^*_{e_i} \Delta t} \rho^n \, dx$$



Equivalence of cell integrated and flux based finite volume methods

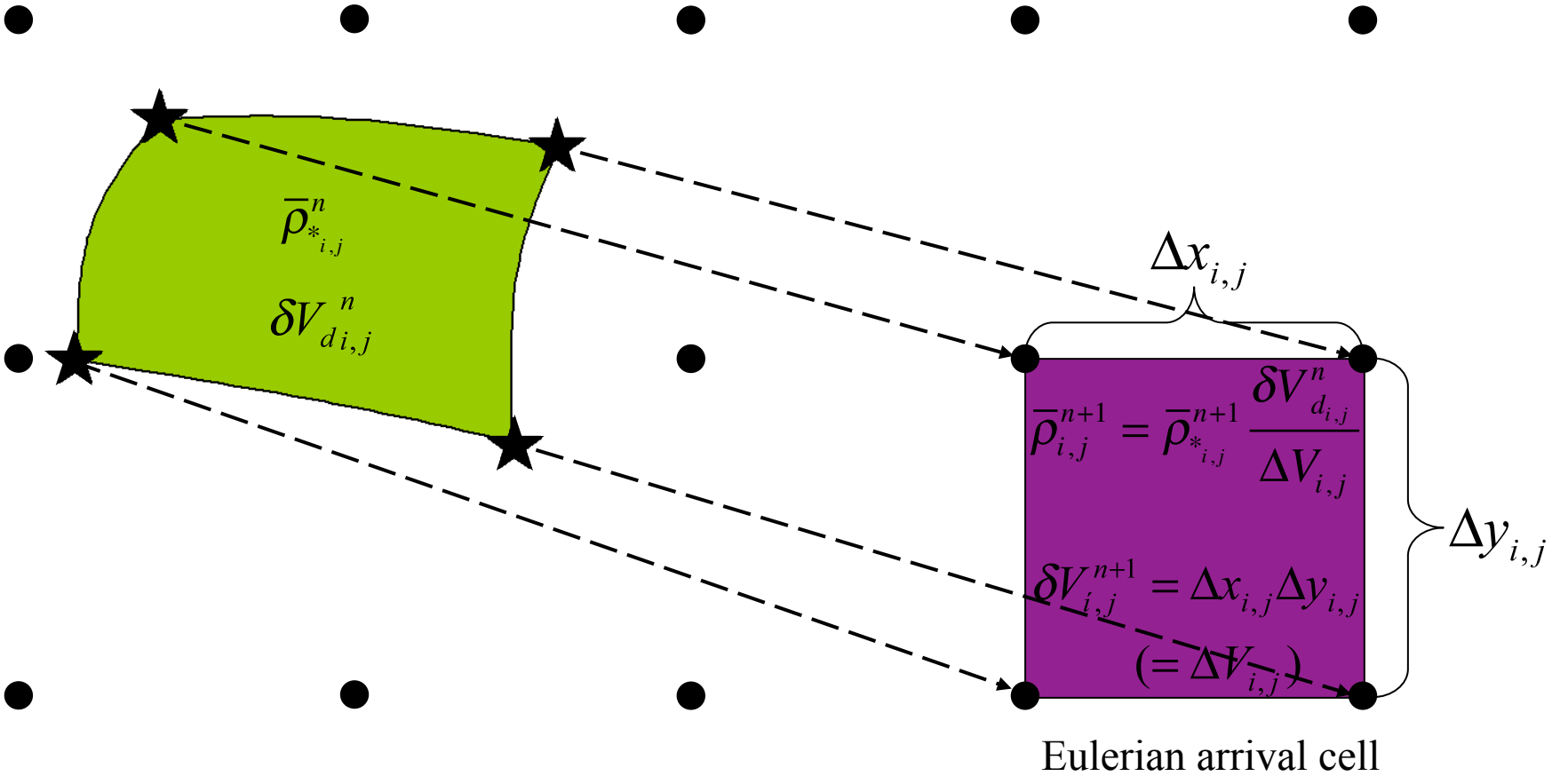
But the two are identical since:

$$\bar{\rho}_i^{n+1} = \bar{\rho}_i^n + \frac{1}{\Delta x}\int_{x_{w_i}-u^*_{w_i}\Delta t}^{x_{w_i}} \rho^n\, dx - \frac{1}{\Delta x}\int_{x_{e_i}-u^*_{e_i}\Delta t}^{x_{e_i}} \rho^n\, dx$$

$$= \frac{1}{\Delta x}\int_{x_{w_i}}^{x_{e_i}} \rho^n\, dx + \frac{1}{\Delta x}\int_{x_{w_i}-u^*_{w_i}\Delta t}^{x_{w_i}} \rho^n\, dx + \frac{1}{\Delta x}\int_{x_{e_i}\Delta t}^{x_{e_i}-u^*_{e_i}\Delta t} \rho^n\, dx$$

$$= \frac{1}{\Delta x}\int_{x_{w_i}-u^*_{w_i}\Delta t}^{x_{e_i}-u^*_{e_i}\Delta t} \rho^n\, dx$$

Cell integrated finite volume methods:

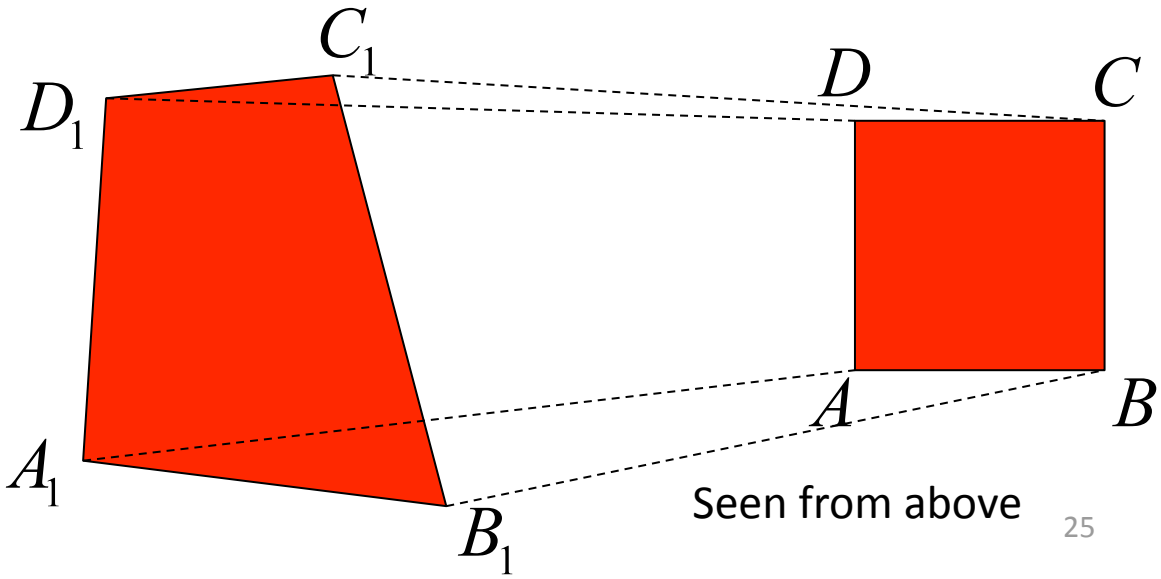


$$\overline{(\tilde{\rho}_k\,\delta_k h)}^{+}\,\Delta A = \iint_{ABCD} (\tilde{\rho}_k\,\delta_k h)\,dx\,dy + \iint_{A_1B_1BA} (\tilde{\rho}_k\,\delta_k h)\,dx\,dy$$

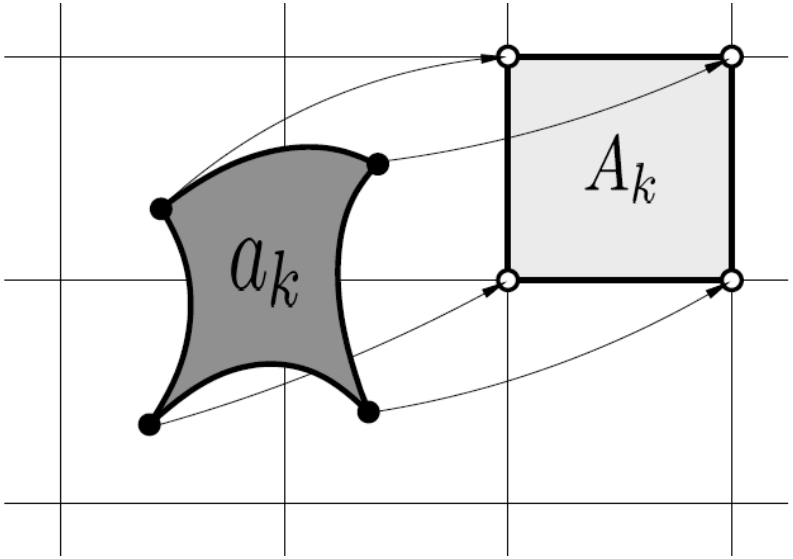
$$+ \iint_{A_1ADD_1} (\tilde{\rho}\,\delta_k h)\,dx\,dy + \iint_{D_1DCC_1} (\tilde{\rho}_k\,\delta_k h)\,dx\,dy$$

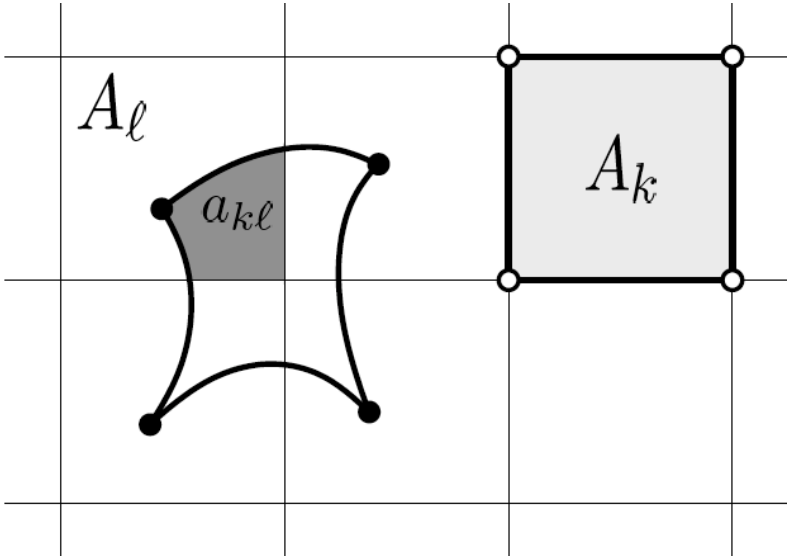
$$- \iint_{B_1BCC_1} (\tilde{\rho}_k\,\delta_k h)\,dx\,dy$$

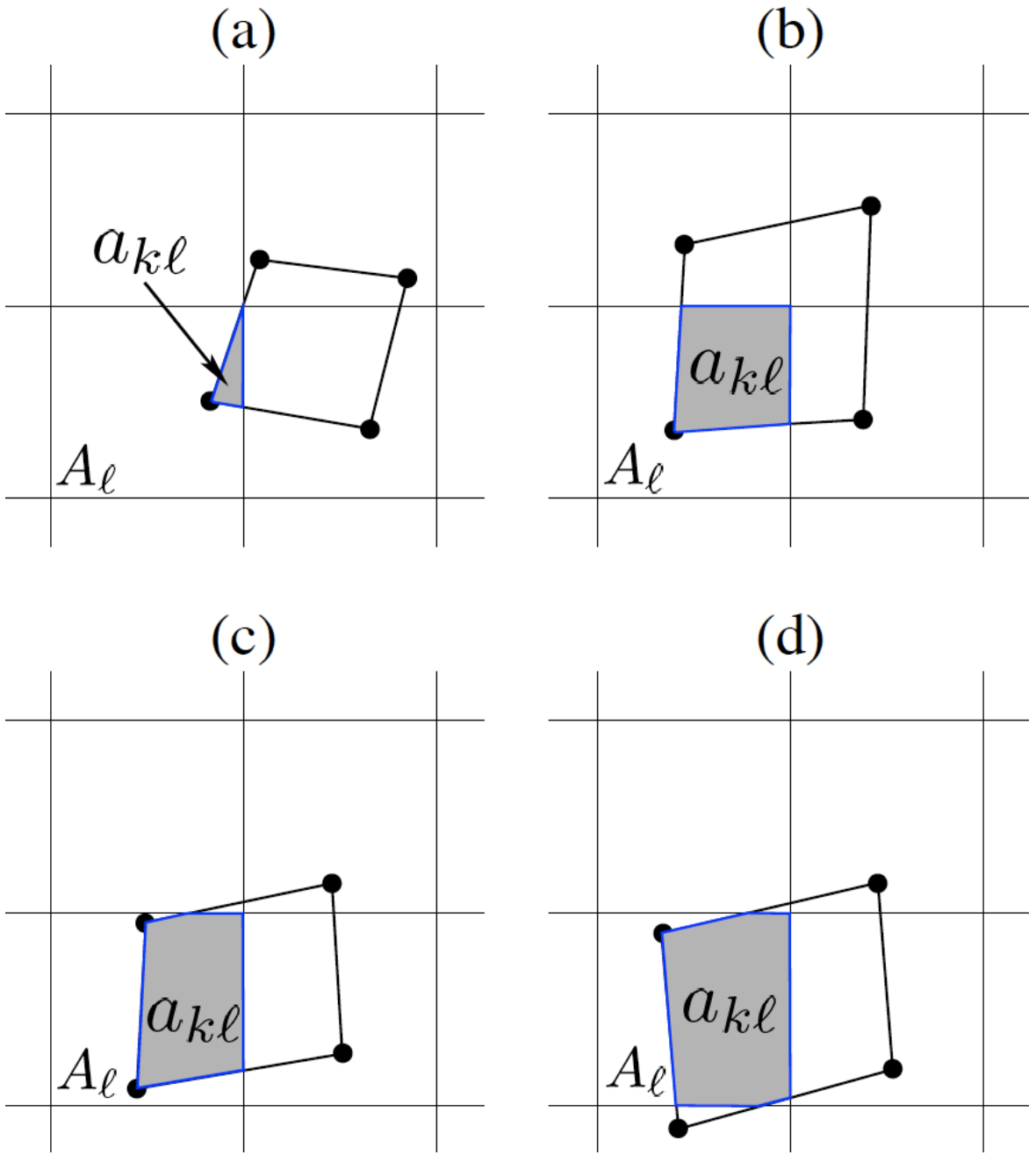
$$= \iint_{A_1B_1C_1D_1} (\tilde{\rho}_k\,\delta_k h)\,dx\,dy$$



Cell integrated semi-Lagrangian scheme



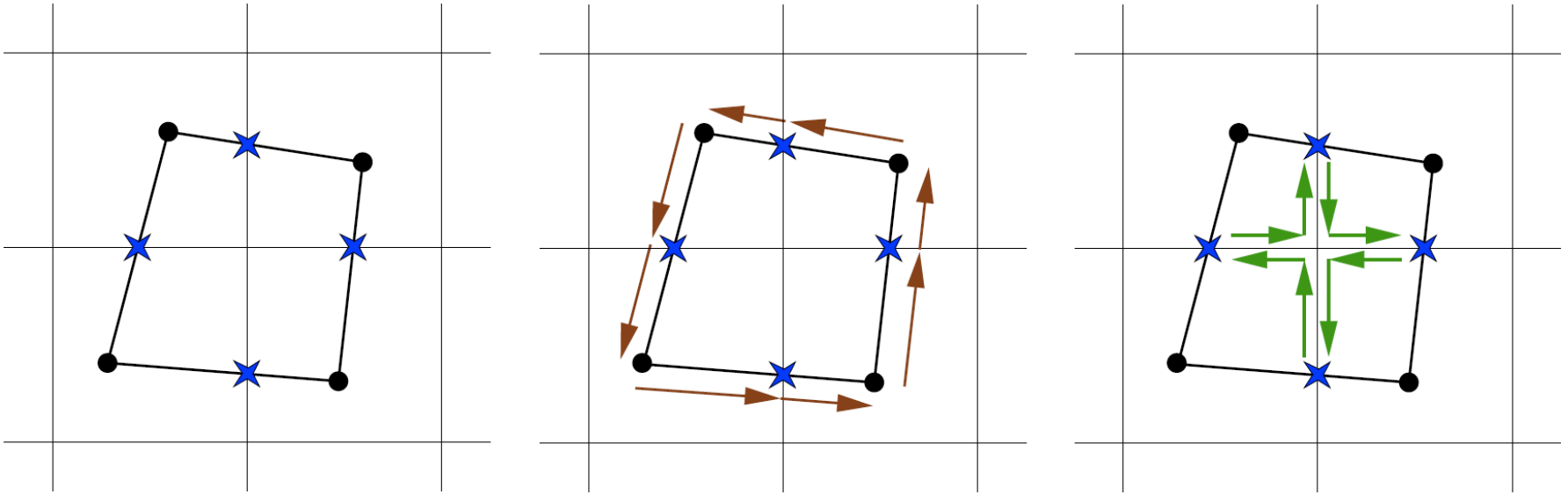



(a)
$a_{k\ell}$
A_ℓ
(b)
$a_{k\ell}$
A_ℓ
(c)
$a_{k\ell}$
A_ℓ
(d)
$a_{k\ell}$
A_ℓ

Cell integrated semi-Lagrangian scheme

Applying the Gauss-Green theorem one can convert surface integrals into line-integrals (Lauritzen)

$$\iint_{a_{k\ell}} f_\ell(x,y)\,dx\,dy = \oint_{\partial a_{k\ell}} [P\,dx + Q\,dy]$$



The LMCSL approach: A simple modification of the advection equation by applying a partition of unity principle!

Locally mass conserving semi-Lagrangian (LMCSL) scheme:

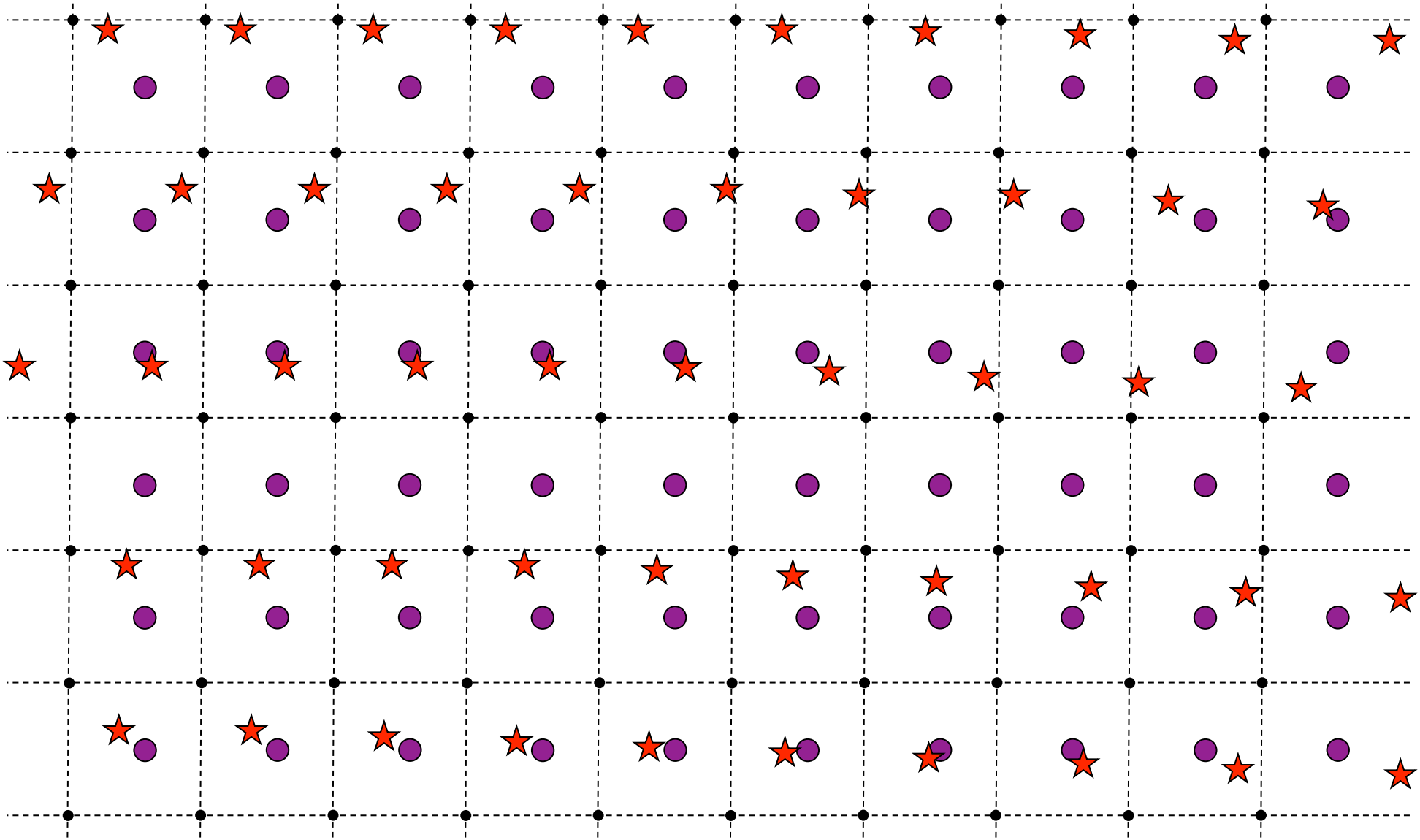
Explicit forecast in grid point k :

$$\rho_{k\ \mathrm{LM}}^{n+1} = \left\{\bar{\rho}\right\}_{**_k}^{n} \equiv \sum_{l=1}^{K} \hat{w}_{k,l} \bar{\rho}_l^n$$

where $$\hat{w}_{k,l} = \frac{A_l}{A_k} \frac{w_{k,l}}{\sum_{m}^{K} w_{m,l}}$$

and A_k is the volume represented by the k'th Eulerian grid point.

Semi Lagrangian scheme



LMCSL (continued):

Formally mass conserving :

$$\sum_{k=1}^{K} A_k \rho_{k\ \mathrm{LM}}^{n+1} = \sum_{k=1}^{K}\sum_{l=1}^{K} A_k \hat{w}_{k,l} \rho_l^n = \sum_{k=1}^{K}\sum_{l=1}^{K} \frac{A_l w_{k,l}}{\sum_{m=1}^{K} w_{m,l}} \rho_l^n = \sum_{l=1}^{K} A_l \frac{\sum_{k=1}^{K} w_{k,l}}{\sum_{m=1}^{K} w_{m,l}} \rho_l^n$$

$$= \sum_{l=1}^{K} A_l \rho_l^n$$

Divergence is defined implicitly from the weighted weights, i.e. by the trajectories:

$$\mathcal{D}_{LM_k} = \frac{1}{\Delta t}\left(1 - \sum_{l}^{K} \hat{w}_{k,l}\right)$$

Reference:
Kaas, E, 2008: A simple and efficient locally mass conserving semi-Lagrangian transport scheme, Tellus, 60A, 305-320

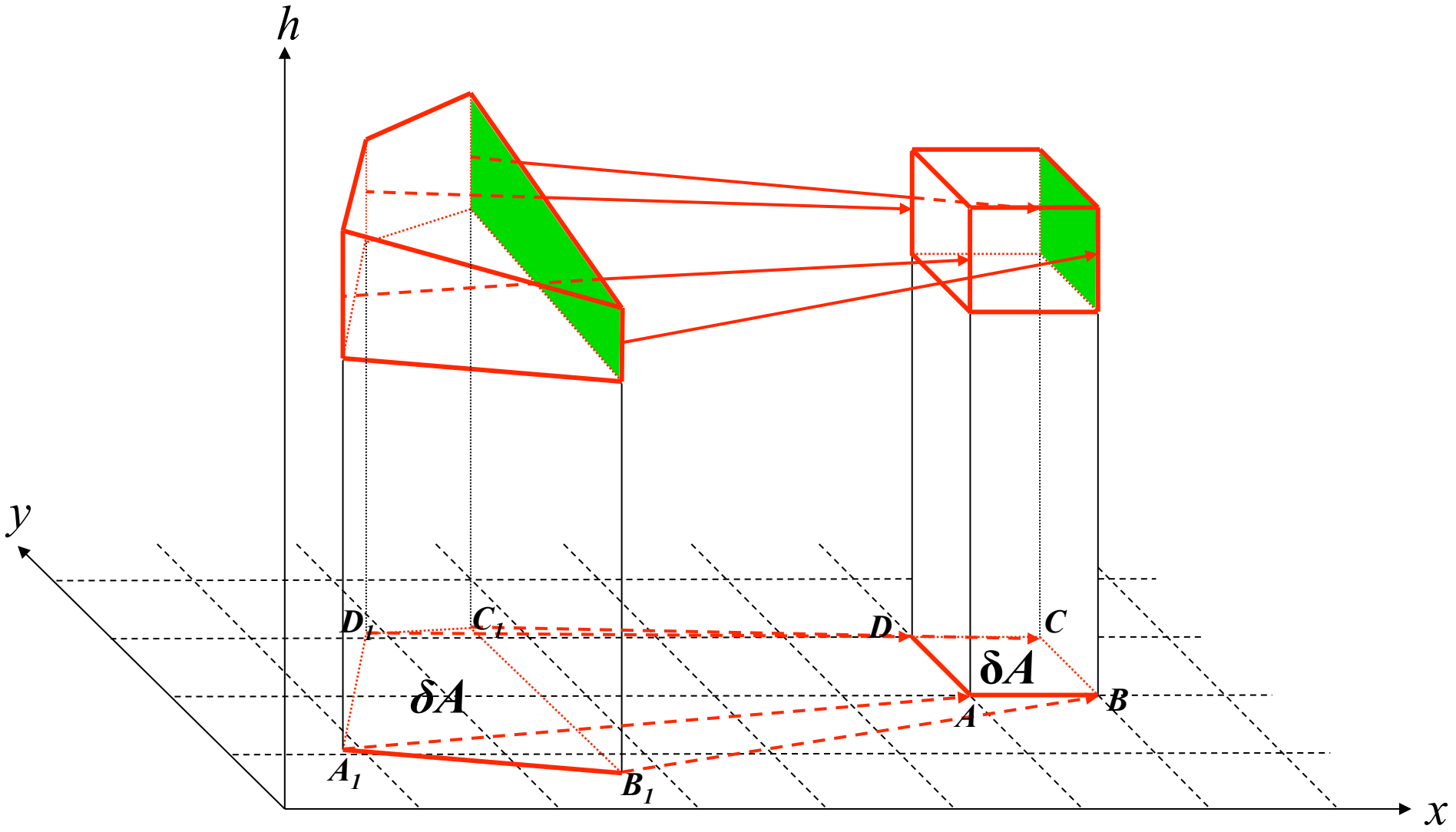
Generalisation to three dimensions. Possible strategies:

Introducing a Lagrangian or a quasi-Lagrangian vertical coordinate

Use a purely flux based transport in the vertical (i.e. an extra term on the right hand side representing mass flux convergence in the vertical)

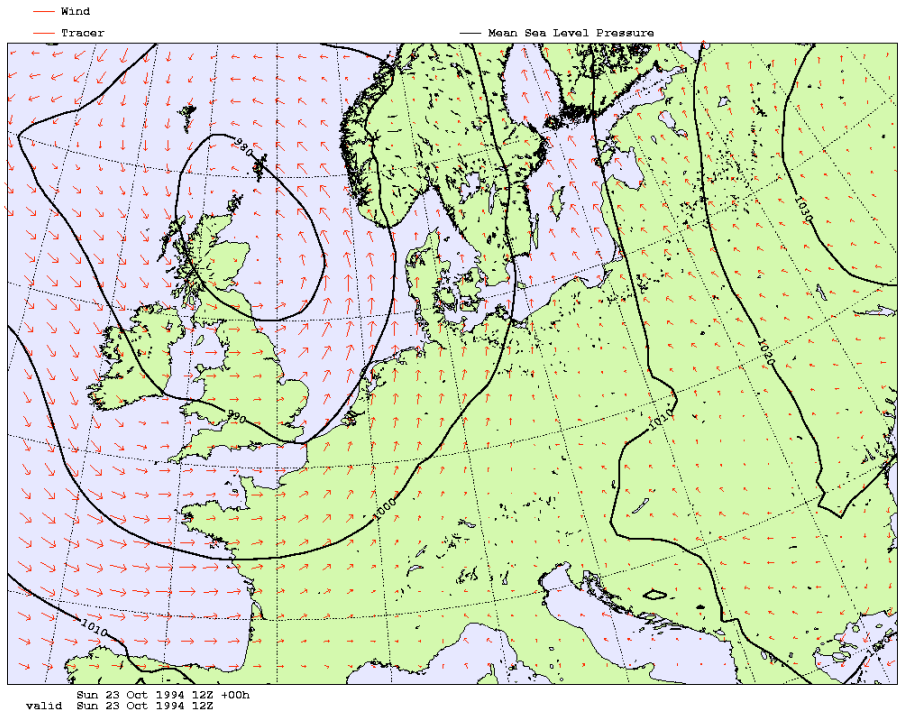
Use cascade interpolation in the vertical, i.e. perform a complete transport of density in the vertical, including divergence effects. Then perform the horizontal transport (or visa versa)

Generalisation to three dimensions.

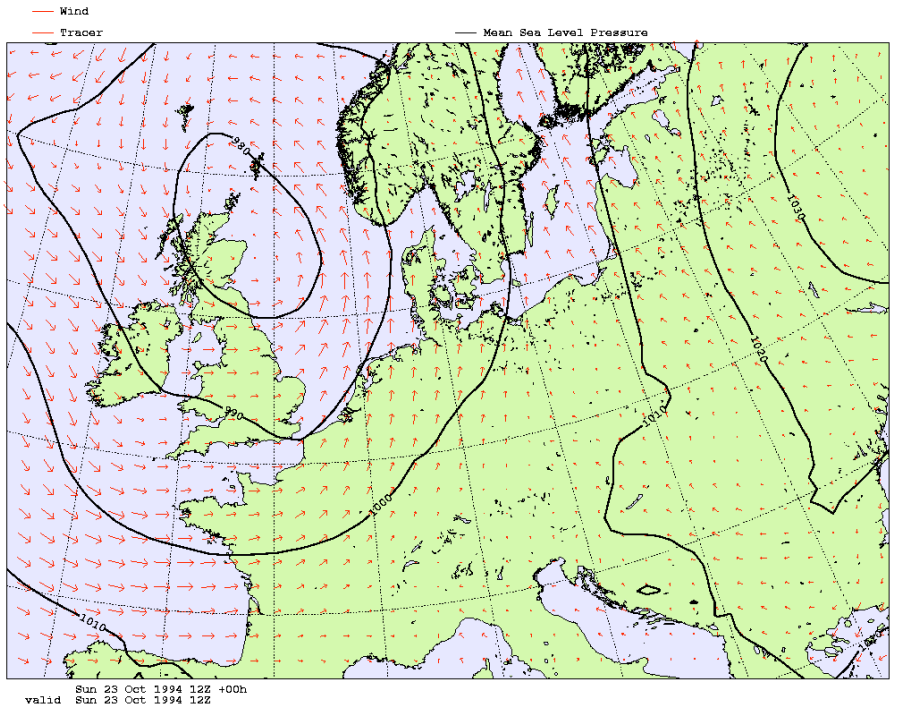


ETEX experiment

D-CISL

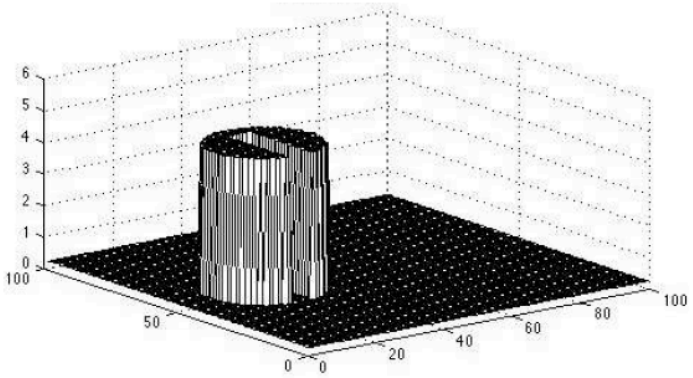


LMCSL

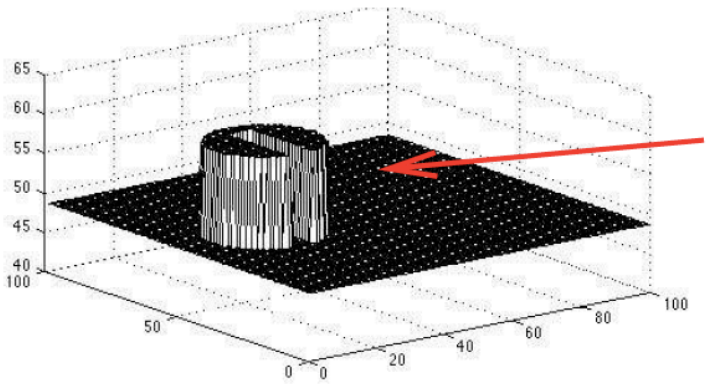


Numerical mixing.

Exact solution one revolution, no chemistry

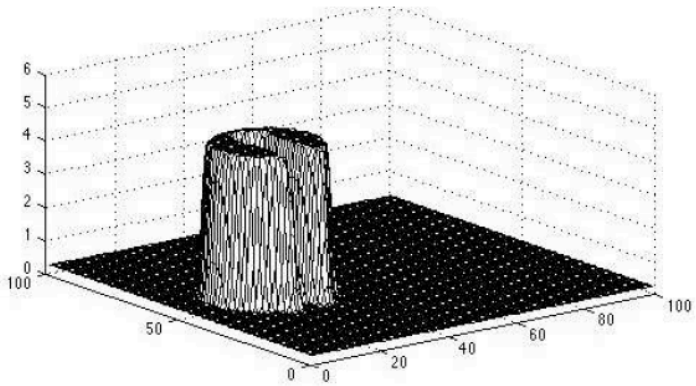


"Exact" solution, v=0, urban chemistry

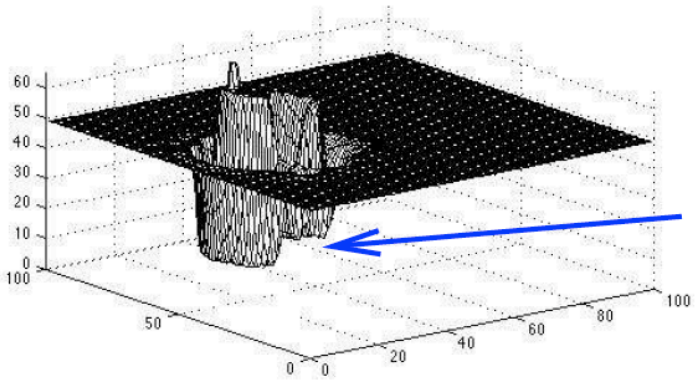


correponds to doing chemistry in Lagrangian space

LMCSL solution one revolution, no chemistry

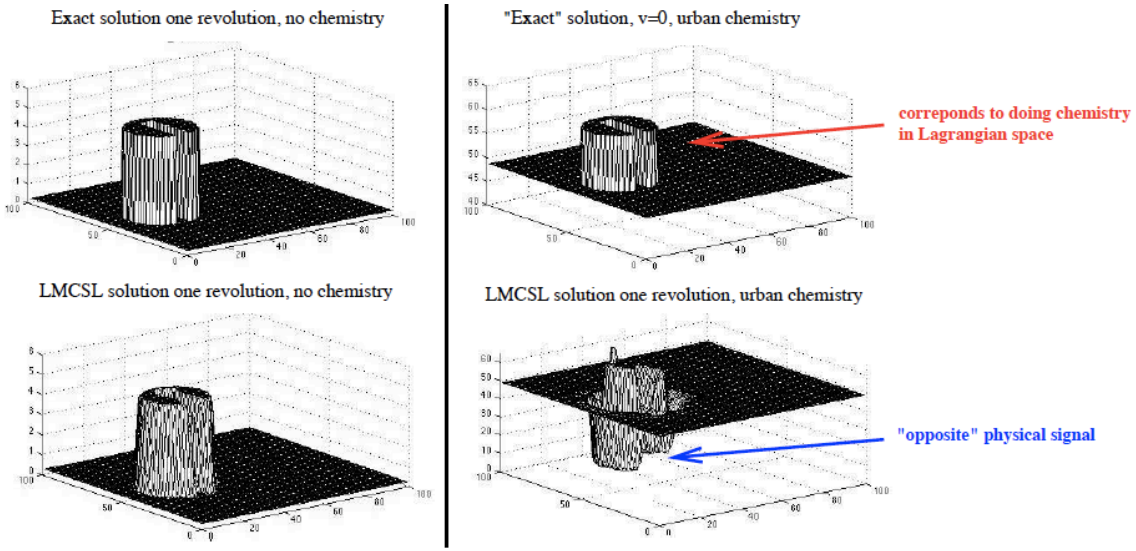


LMCSL solution one revolution, urban chemistry



"opposite" physical signal

Numerical mixing.



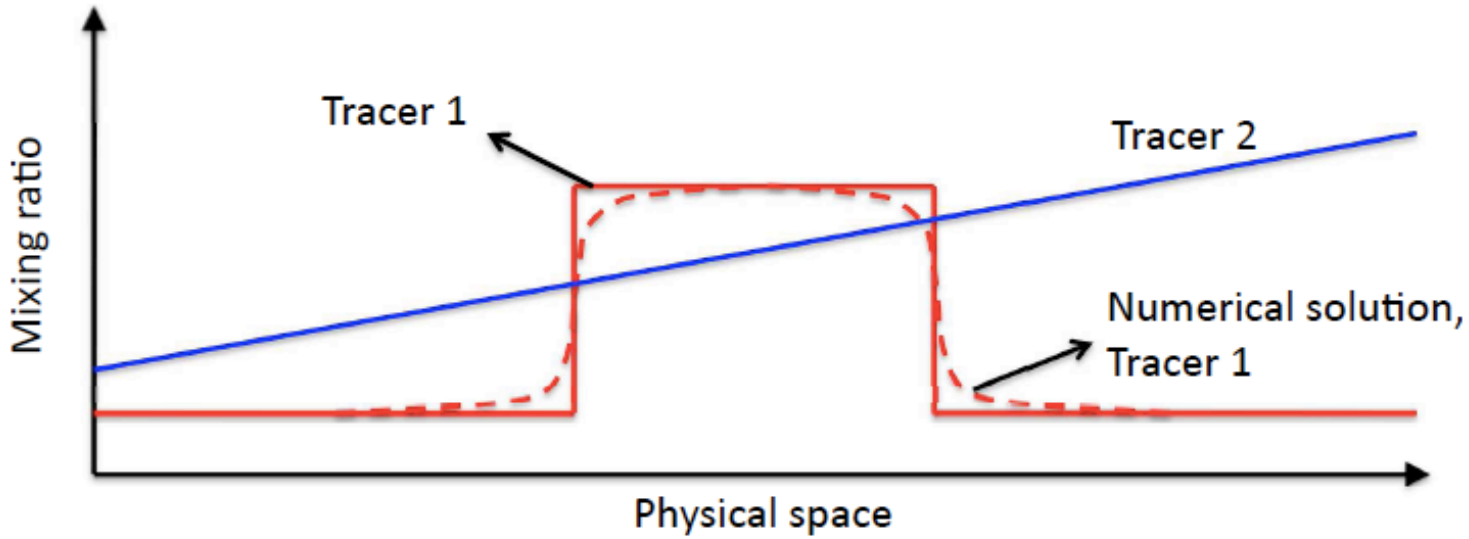
But in the real world there is mixing!

- Depends on meteorological conditions (flow). If strong shear, yes. If linear flow, no!
- Two modeling philosophies: 1. Implicit numerical diffusion in scheme represents physical diffusion. 2. Diffusion is added explicitly. In any case: The resulting diffusion should match the physical diffusion.

E.g., a fully Lagrangian method needs explicit diffusion operators; traditional finite-volume methods may need it.

What matters for chemistry

- Relative concentration is the important factor for chemistry (reactions between tracers are controlled by relative concentrations!).
- This is more general than preservation of linear correlations: $q_1 = A + Bq_2$
- Some chemical processes are highly non-linear (e.g., NOx, O_3, example on previous slide)



Wind-mass inconsistency

Assume one require strict mass conservation. Then using a mass conservative numerical technique to solve the volume density continuity for a tracer in spatial cell *k* and at time step *n* gives

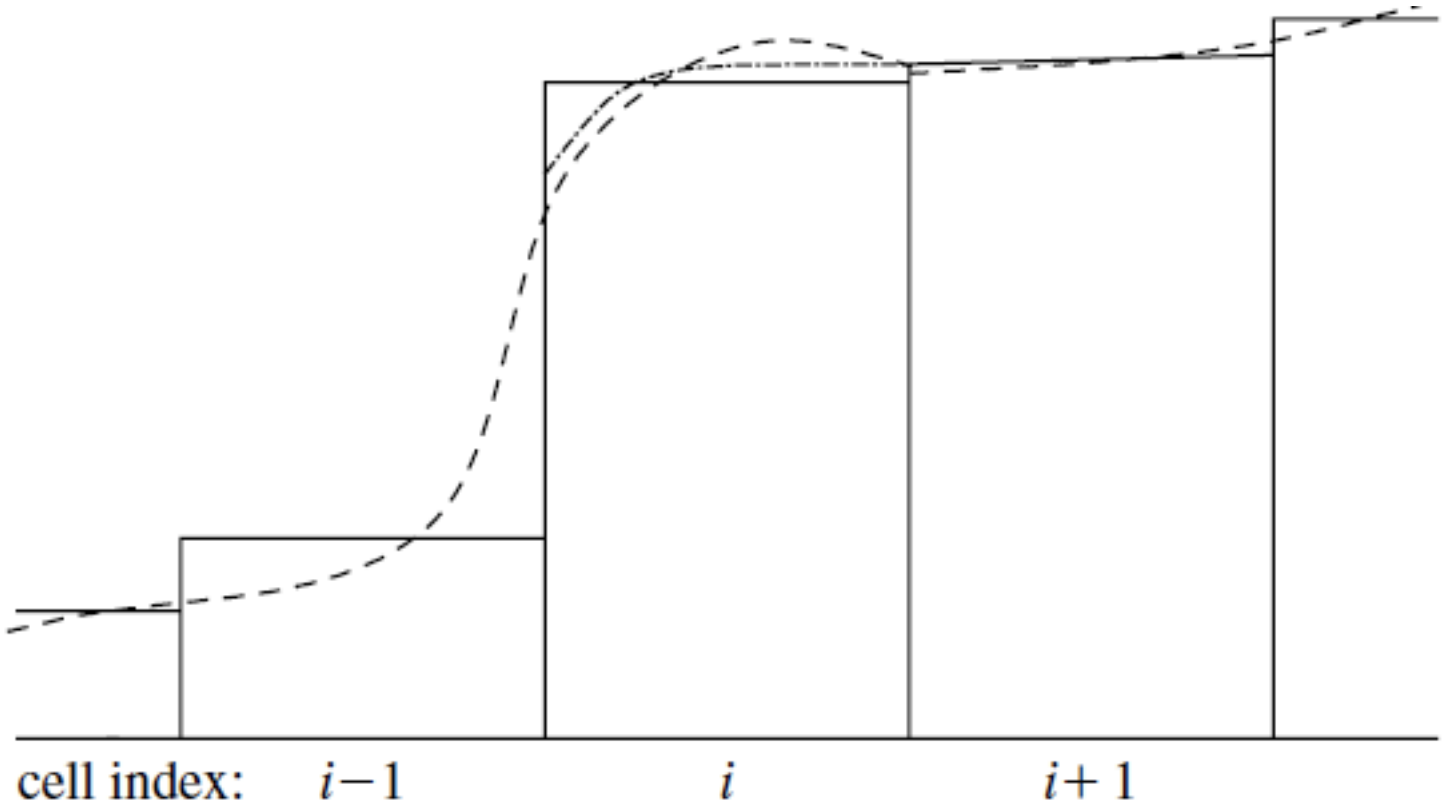
$$\left(\rho_t\right)_k^n$$

Now the mixing ratio required for chemical calculations should be evaluated as:

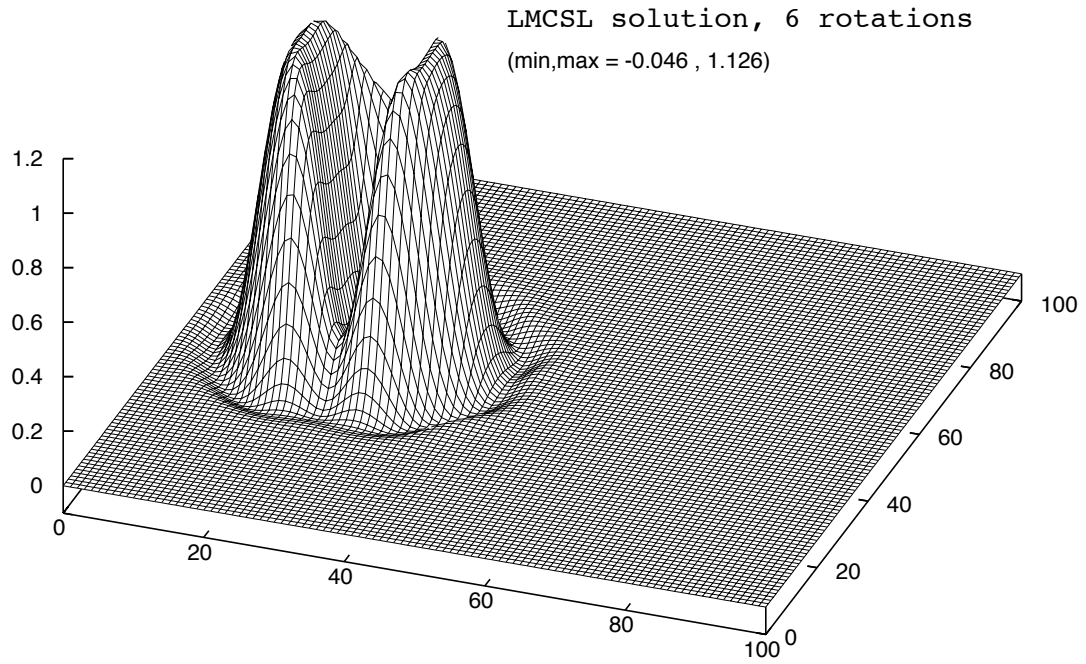
$$\left(q_t\right)_k^n = \left(\rho_t\right)_k^n \Big/ \left(\rho_d\right)_k^n$$

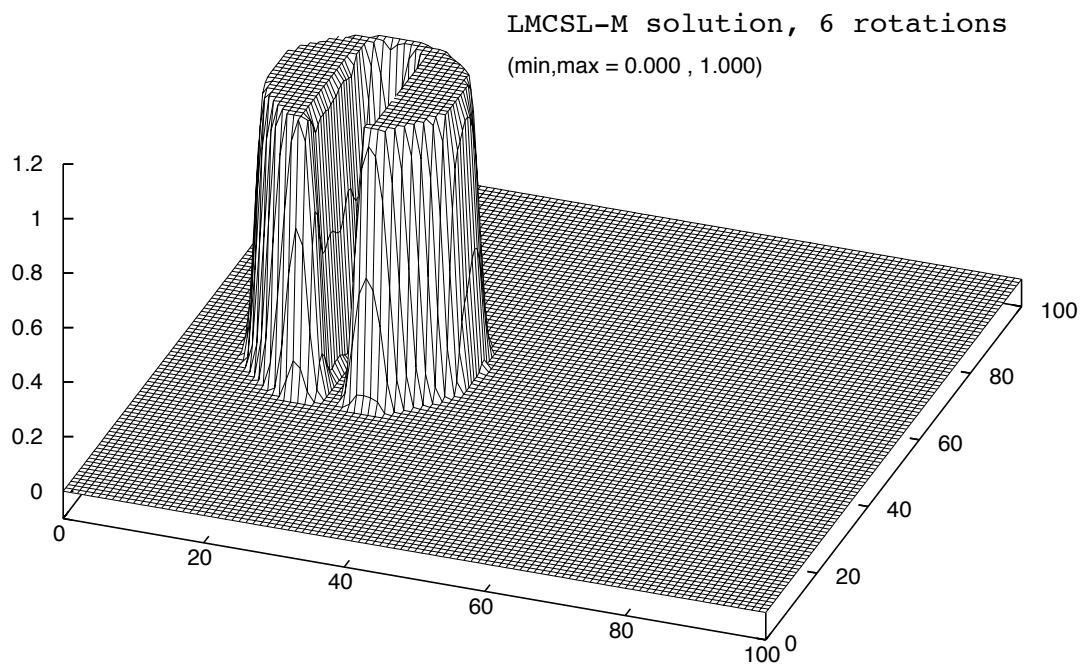
Problem: if we did not use exactly the same numerical scheme to forecast the the tracer density and the dry air density we commit an error, which may evolve seriously (e.g. Jöckel et al. 2001). Special fixers are required.

Monotonic filters and flux limiters



General idea in finite volume method approaches: Modify the subgrid cell representation to avoid the problem. (here Colella and Woodward (1984))


LMCSL solution, 6 rotations
(min,max = -0.046 , 1.126)
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
0
20
40
60
80
100


LMCSL-M solution, 6 rotations
(min,max = 0.000 , 1.000)
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
0
20
40
60
80
100

Additional reading

Durran, D.R. 2010: Numerical Methods for Fluid Dynamics. Springer, ISBN 978-1-4419-6411-3

”COMPUTATIONAL METHODS FOR THE ATMOSPHERE AND THE OCEANS” published by Elsevier. Editors: Roger Temam, Joe Tribbia and Philippe Ciarlet. 784 pages. ISBN 978-0-444-51893-4.

T H A N K Y O U