Mass-Conservative Transport of Atmospheric Constituents

First Lecture (# 6)

by

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References on new developments:

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Mass Transport-not only Advection

The Continuity Equation:

Rate of change of mass density = mass advection + mass convergence = mass flux convergence

$$\boxed{\frac{\partial \rho}{\partial t} = -\vec{V}_3 \bullet \nabla \rho - \rho \nabla \bullet \vec{V}_3 = -\nabla \bullet \rho \vec{V}_3}$$

$$\rho = dencity\ of\ (moist)\ air\ [kg/m^3]$$

For atmospheric constituent:

$$\boxed{\frac{\partial q\rho}{\partial t} = -\vec{V}_3 \bullet \nabla q\rho - q\rho \nabla \bullet \vec{V}_3 = -\nabla \bullet q\rho \vec{V}_3}$$

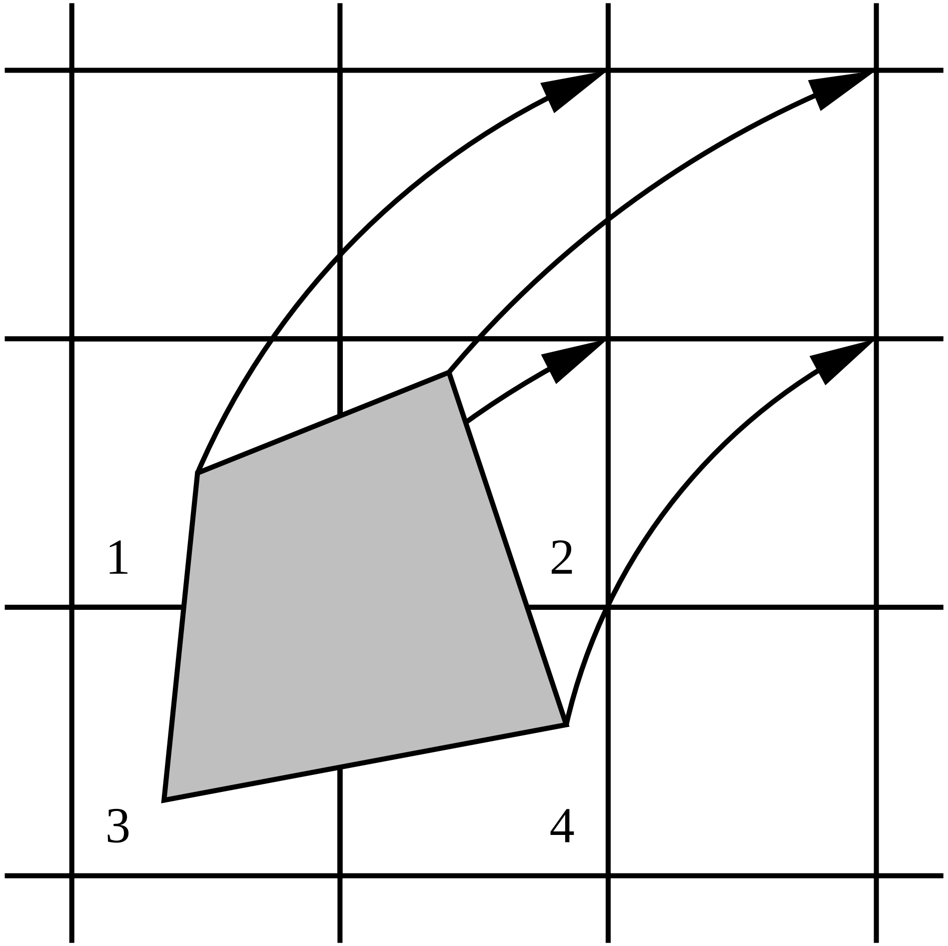
$$q\rho = dencity\ of\ constituent\ [kg/m^3]$$

$$q = specific\ consentration = \frac{mass\ of\ constituent}{mass\ of\ moist\ air}\left[\frac{kg}{kg}\right]$$

$$\boxed{\frac{dq}{dt} = \frac{\partial q}{\partial t} + \vec{V}_3 \bullet \nabla q = 0}$$

Jockel et al. (2001): The mass-wind inconsistency can only be avoided in on-line ***consistent*** models.
(Conservation of specific concentrations may be used as a consistency

check.)



$$\min(\overline{q}_1^{\,n}, \overline{q}_2^{\,n}, \overline{q}_3^{\,n}, \overline{q}_4^{\,n}) \leq \overline{q}^{\,n+1} \leq \max(\overline{q}_1^{\,n}, \overline{q}_2^{\,n}, \overline{q}_3^{\,n}, \overline{q}_4^{\,n})$$

3a

Finite Volume or Cell Integrated method

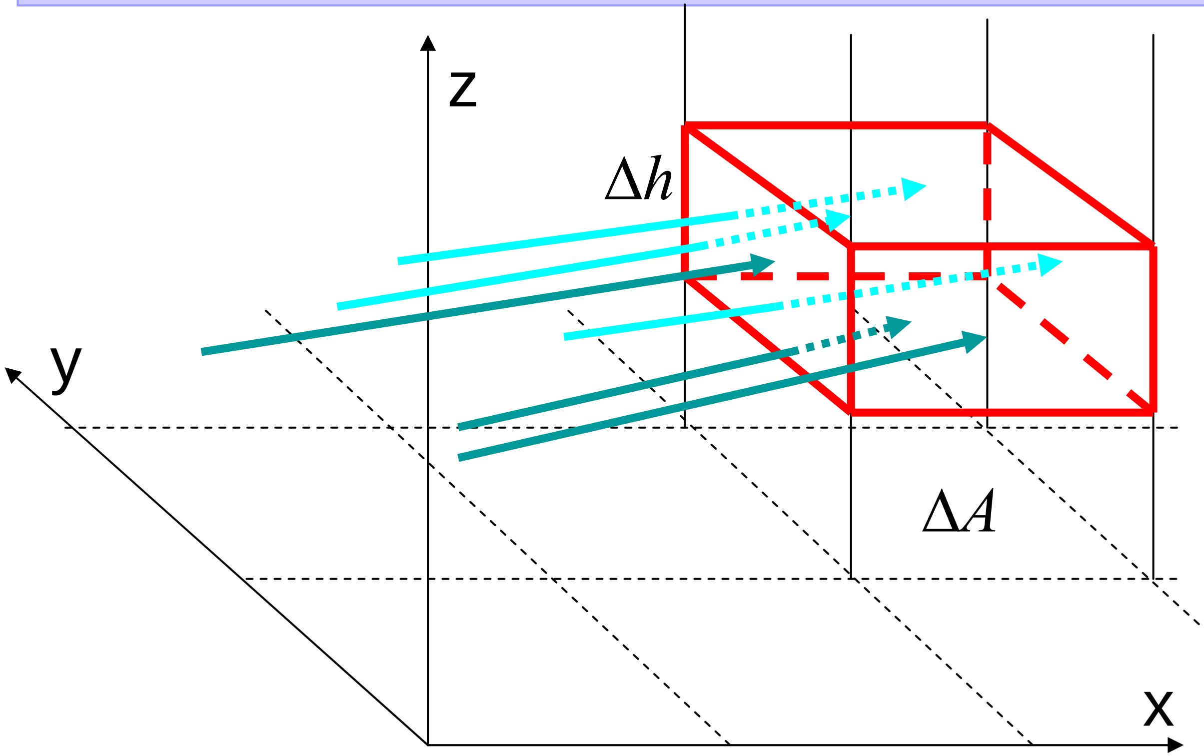
- The prognostic variable is a cell integrated mean value:

$$\bar{\tilde{\rho}} = \frac{1}{\Delta h \Delta A} \iiint_{\delta h\, \delta A} \rho \; dxdydz$$

where $h = z - z_s$

A cell integrated prognostic equation is obtained by integrating the Continuity Equation over an Eulerian grid cell

Traditional approach:
To estimate 3-D mass fluxes during a time interval Δt through all 6 faces of an Eulerian grid cell



$$\frac{\partial \rho}{\partial t} = -\nabla \bullet \rho \vec{V}_3$$

$$\overline{\widetilde{X}} = \frac{1}{\Delta h \Delta A} \iiint_{\Delta h \, \Delta A} X \, dxdydz$$

$$\overline{\overline{X}} = \frac{1}{\Delta t} \int_t^{t+\Delta t} X \, dt$$

$$h = z - z_s$$

Inward mass fluxes through west, south and bottom faces

Outward mass fluxes through east, north and top faces

$$\overline{\widetilde{\rho}}^{+} - \overline{\widetilde{\rho}} = \frac{\Delta t}{\Delta h \Delta A} \sum_{i=1}^{6} \left(\overline{\overline{< \rho \vec{V} >}} \bullet \vec{n} \, \delta a \right)_i$$

New approach*:
Vertically discretized quasi-horizontal transport along *3-D trajectories or Lagrangian particle tracks*

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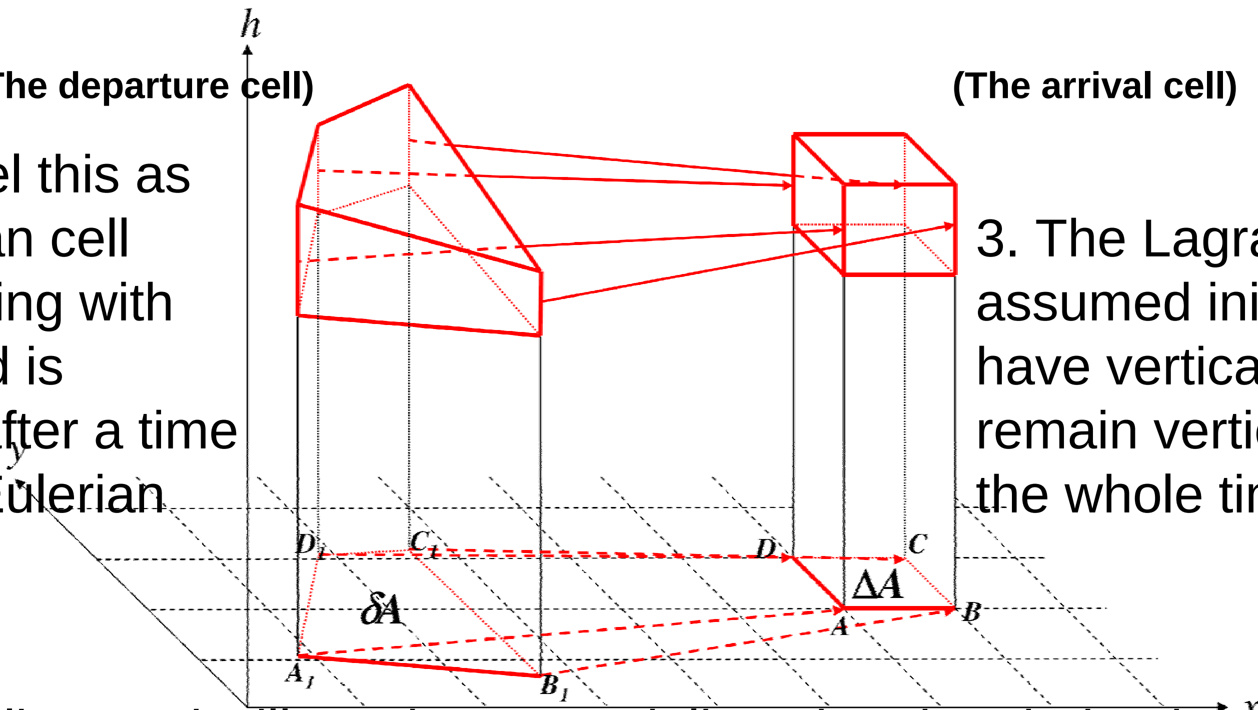
(The departure cell) (The arrival cell)



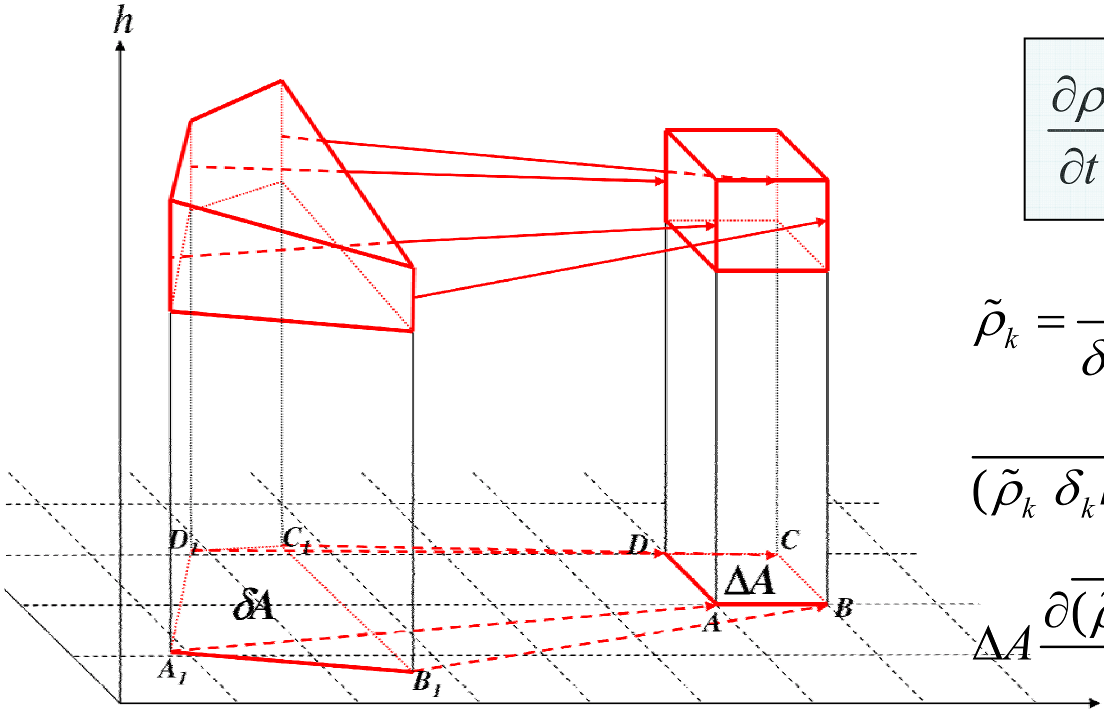
2. We model this as a Lagrangian cell that is mowing with the flow and is ending up after a time step in an Eulerian Cell.

3. The Lagrangian cell is assumed initially to have vertical walls, which remain vertical during the whole time step.

1. We realize, and will use in our modeling, that the air that is ending up in an Eulerian cell (the arrival cell) after a time step has been moving with the flow along 3-D trajectories that originates in a so-called departure cell, also called a Lagrangian cell.

* **Machenhauer and Olk (1998)**

Transport along a ”vertical Lagrangian coordinate” *



$$\frac{\partial \rho}{\partial t} = -\nabla_{\xi} \cdot \rho \vec{V} - \frac{\partial \rho \dot{\xi}}{\partial \xi} \qquad \dot{\xi} = \frac{d\xi}{dt} = 0$$

$$\tilde{\rho}_k = \frac{1}{\delta_k h} \int_{\delta_k h} \rho \, dz \qquad \frac{\partial \tilde{\rho}_k \delta_k h}{\partial t} = -\nabla_{\xi} \cdot \tilde{\rho}_k \delta_k h \, \vec{V}_k$$

$$\overline{(\tilde{\rho}_k \ \delta_k h)} = \frac{1}{\Delta A} \iint_{\Delta x \Delta y} (\tilde{\rho}_k \ \delta_k h) \ \ dxdy$$

$$\Delta A \frac{\partial \overline{(\tilde{\rho}_k \ \delta_k h)}}{\partial t} = -\sum_{i=1}^{4} (< (\tilde{\rho}_k \ \delta_k h) \, \vec{V}_k > \cdot \, \vec{n} \ \Delta l \ )_i$$

The *Flux Form* of the continuity equation:

$$\Delta A \, (\overline{(\tilde{\rho}_k \ \delta_k h)}^{+} - \overline{(\tilde{\rho}_k \ \delta_k h)}) = -\Delta t \sum_{i=1}^{4} (\overline{\overline{< (\tilde{\rho}_k \ \delta_k h) \vec{V}_k > \cdot \, \vec{n} \ \Delta l}})_i \qquad \textbf{(1)}$$

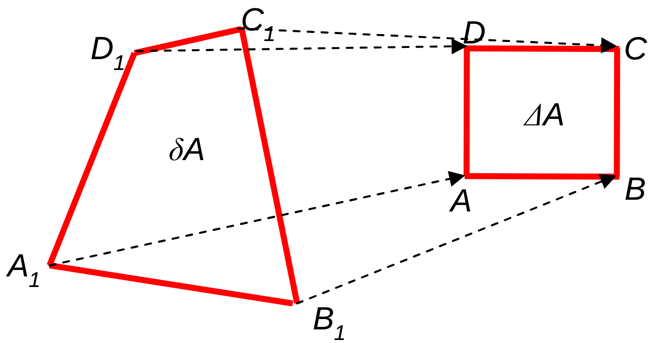
* **Starr (1945)**

The *Flux Form* is equivalent with a *Lagrangian Form* of the Continuity Equation

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

$$+\iint_{A_1ADD_1}(\tilde{\rho}_k\ \delta_k h)\,dx\,dy + \iint_{D_1DCC_1}(\tilde{\rho}_k\ \delta_k h)\,dx\,dy - \iint_{B_1BCC_1}(\tilde{\rho}_k\ \delta_k h)\,dx\,dy$$

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



$$\boxed{\overline{(\tilde{\rho}_k\ \Delta_k h)}^{+}\Delta A = \overline{(\tilde{\rho}_k\ \delta_k h)}\,\delta A}$$

$$\boxed{\overline{(\tilde{\rho}_k\ )}^{+} = \frac{1}{\Delta_k h\ \Delta A}\iint_{A_1B_1C_1D_1}(\tilde{\rho}_k\ \delta_k h)\,dx\,dy = \frac{1}{\Delta_k V}\iiint_{\delta_k V}\rho_k\ dx\ dy\ dz} \quad \textbf{(2)}$$

Direct derivation of the *Lagrangian Form* of the Continuity Equation

The mass in a cell with the volume δV :

$$M_{\delta_k V} = \iiint\limits_{\delta_k V} \rho_k \; dx\, dy dz$$

This mass must be conserved. So

$$\frac{d\ M_{\delta_k V}}{dt} = 0$$

When integrated over Δt we get

$$\overline{(\tilde{\rho}_k\ )}^{+} \Delta_k V = \iiint\limits_{\delta_k V} \rho_k \; dx\, dy\, dz$$

Two categories of Finite Volume schemes

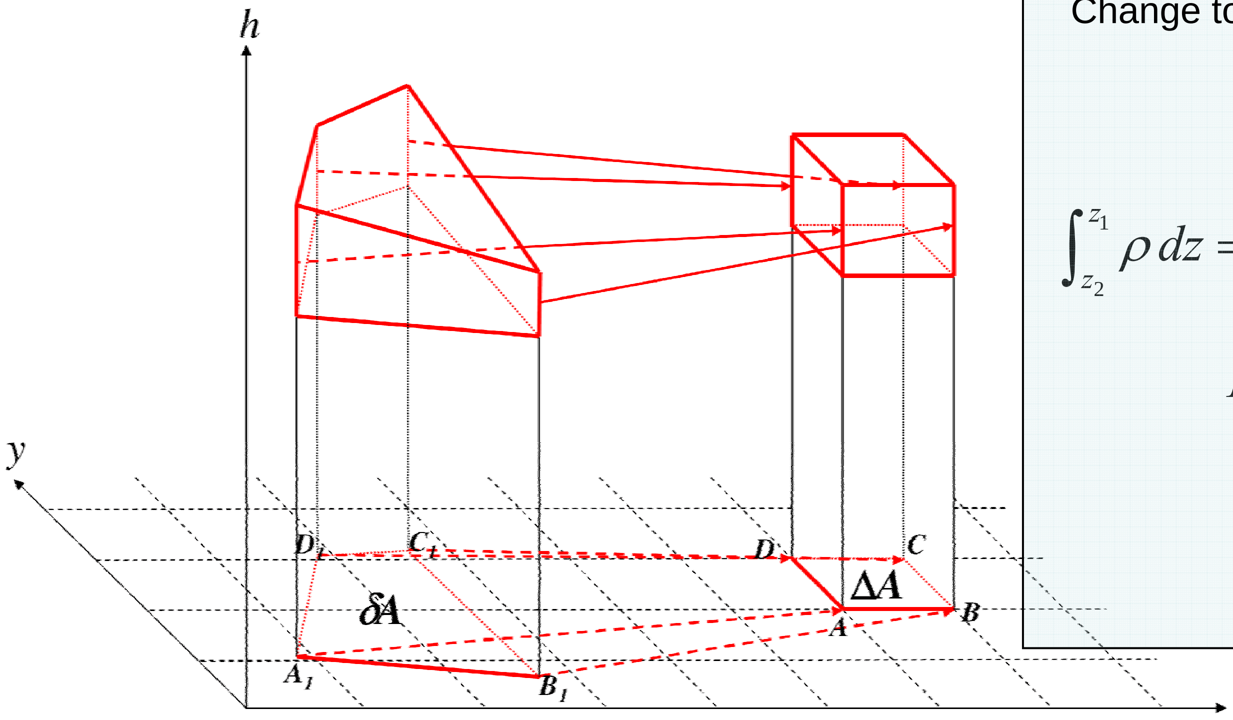
1. Semi-Lagrangian schemes based on approximations of a direct integration over an up-stream departure area:

$$\overline{(\tilde{\rho}_k \;)}^{+} = \frac{1}{\Delta_k h \; \Delta A} \iint\limits_{A_1 B_1 C_1 D_1} (\tilde{\rho}_k \; \delta_k h) \, dx \, dy = \frac{1}{\Delta_k V} \iiint\limits_{\delta_k V} \rho_k \; dx \; dy \; dz$$

So called *DCISL schemes*. Pioneering example: HIRLAM-DCISL

2. Flux Form schemes based on approximations of the fluxes through the walls of an Eulerian arrival cell. Pioneering example: the FFSL

Traditional upstream DCISL scheme



Change to HIRLAM vertical coordinate:

$$M_{\delta V} = \iint_{\delta A} \left(\int_{z_2}^{z_1} \rho \, dz \right) dx dy$$

$$\int_{z_2}^{z_1} \rho \, dz = \frac{1}{g} \int_{p_1}^{p_2} dp = \frac{1}{g}(p_2 - p_1) = \frac{1}{g} \delta p$$

$$M_{\delta V} = \frac{1}{g} \iint_{\delta A} \delta p dx dy = \frac{1}{g} \overline{\delta p} \delta A$$

$$\frac{dM_{\delta V}}{dt} = \frac{1}{g} \frac{d}{dt} \left(\overline{\delta p} \delta A \right) = 0$$

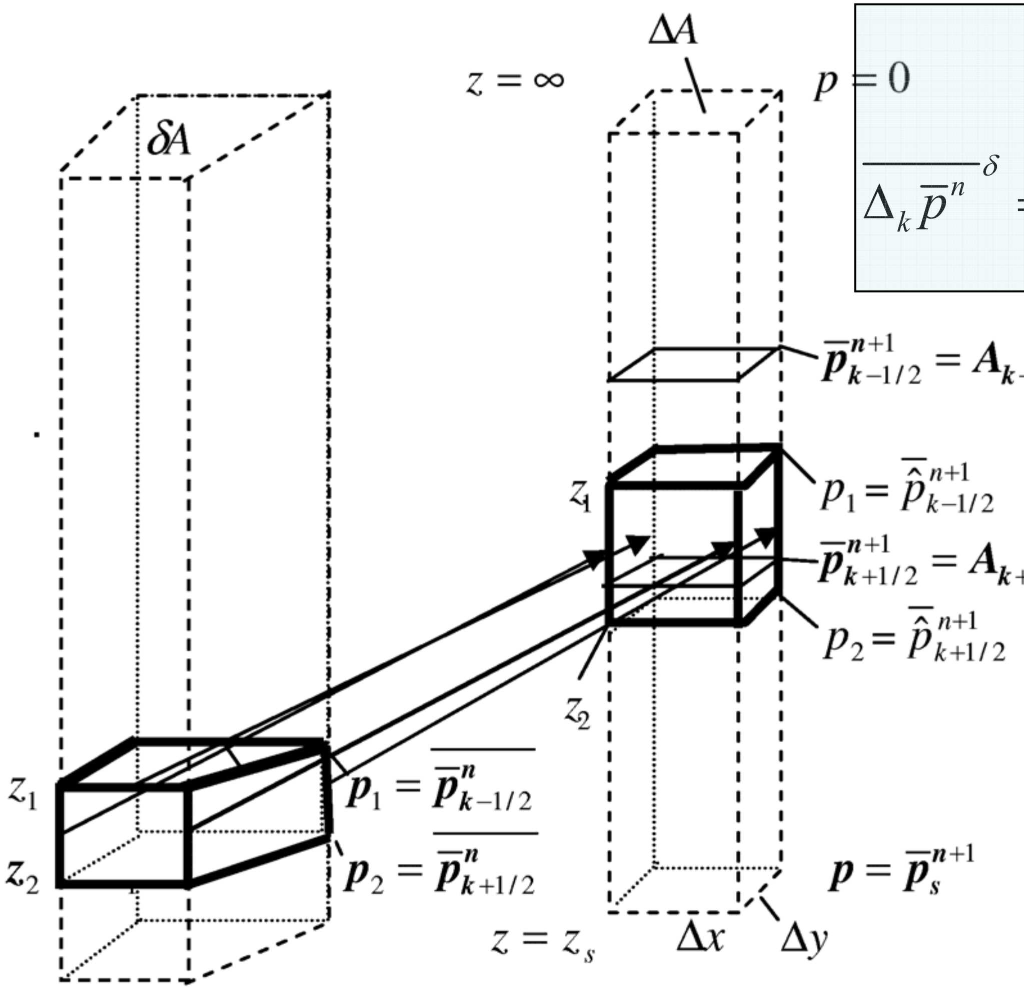
$$\overline{(\tilde{\rho}_k \, \Delta_k h)}^{+} \Delta A = \overline{(\tilde{\rho}_k \, \delta_k h)} \, \delta A$$

$$\overline{(\tilde{\rho}_k \,)}^{+} = \frac{1}{\Delta_k h \, \Delta A} \iint_{A_1 B_1 C_1 D_1} (\tilde{\rho}_k \, \delta_k h) \, dx \, dy = \frac{1}{\Delta_k V} \iiint_{\delta_k V} \rho_k \, dx \, dy \, dz$$

(2)

The ***HIRLAM-DCISL (Lauritzen et al., 2008)***

*- a new direct cell integrated semi-Lagrangian (DCISL) approach: based on quasi-horizontally backward and vertically forward trajectories (*Machenhauer and Olk, 1998)



$$\delta_k \bar{\hat{p}}^{n+1}\Delta A = \overline{\Delta_k \bar{p}^n}^{\delta}\,\delta_k A^n$$

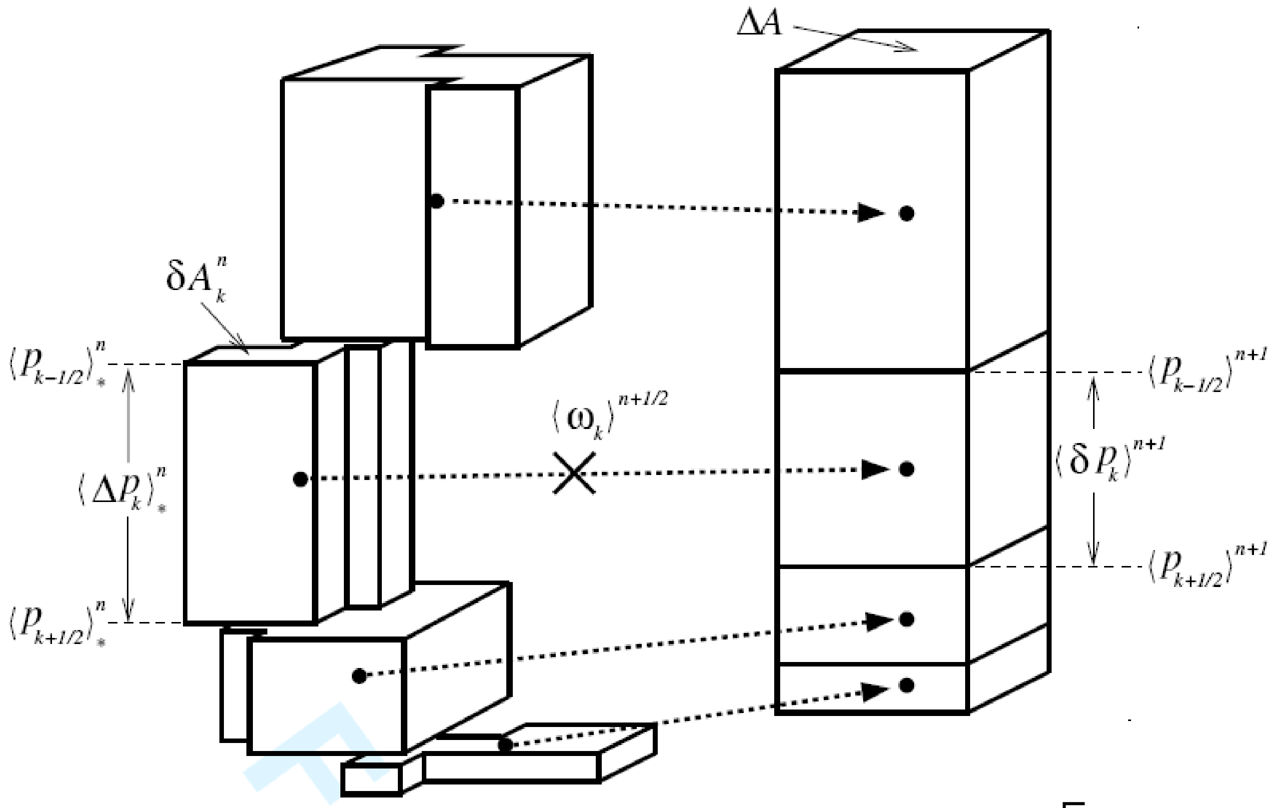
$$\overline{\Delta_k \bar{p}^n}^{\delta} = \overline{\bar{p}^n_{k+1/2} - \bar{p}^n_{k-1/2}}^{\delta} = \frac{1}{\delta A}\iint_{\delta A} \Delta_k \bar{p}^n \, dxdy$$

$$\bar{\hat{p}}^{n+1}_{k-1/2} = \sum_{l=1}^{k-1} \delta_l \bar{\hat{p}}^{n+1}$$

$$\bar{p}^{n+1}_s = \sum_{l=1}^{NLEV} \delta_l \bar{\hat{p}}^{n+1}$$

$$\bar{p}^{n+1}_{k-1/2} = A_{k-1/2} + B_{k-1/2}\,\bar{p}^{n+1}_s$$

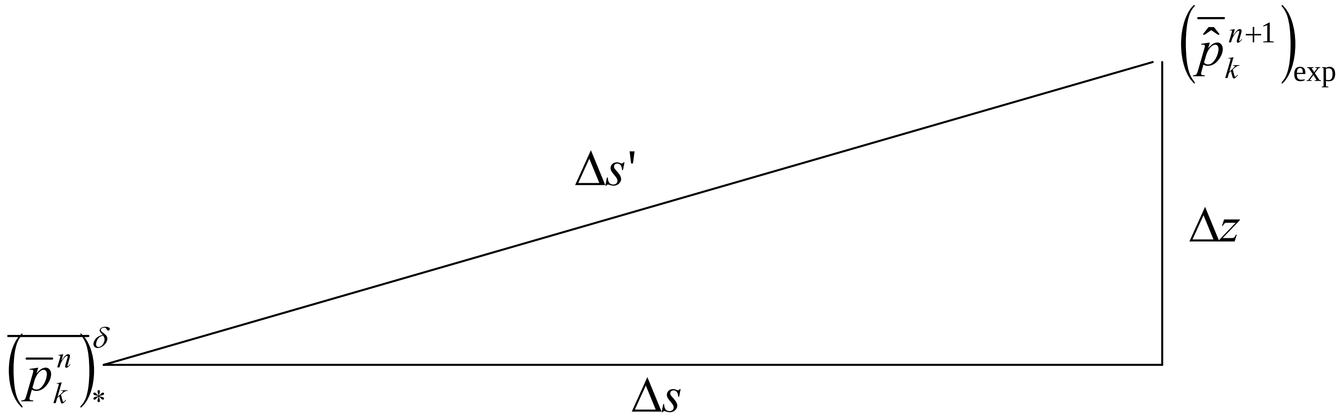
Consistent ω applied in the energy conversion term in the thermodynamic equation



$$\omega = \frac{dp}{dt}$$

$$\Delta t\left[\left(\frac{R_d T_v}{c_p}\frac{\omega}{p}\right)_k\right]^{n+1} = \frac{R_d}{c_p}\left[T_v^{\,n} + \tilde{T}_v^{\,n+1}\right]_k \left[\frac{\bar{\hat{p}}_k^{\,n+1} - \overline{\left(\bar{p}_k^{\,n}\right)_*}^{\delta}}{\bar{\hat{p}}_k^{\,n+1} + \overline{\left(\bar{p}_k^{\,n}\right)_*}^{\delta}}\right]$$

Consistent mean pressure gradient force along the trajectory



$$PGF_{\Delta s'} = \left[\left(-\frac{1}{\rho}\frac{\partial p}{\partial s'}\right)_k\right]_{\exp}^{n+1/2} = -\frac{1}{\bar{\bar{\rho}}}\frac{\left(\hat{\bar{p}}_k^{n+1}\right)_{\exp} - \overline{\left(\bar{p}_k^{n}\right)_*}^{\delta}}{\Delta s'} = -\frac{1}{\bar{\bar{\rho}}}\frac{\left(\hat{\bar{p}}_k^{n+1}\right)_{\exp} - \overline{\left(\bar{p}_k^{n}\right)_*}^{\delta}}{\Delta s}\cos(\vartheta)$$

$$\cos(\vartheta) = \frac{\Delta s}{\Delta s'}$$

$\bar{\bar{\rho}}$ is an approximation of the mean density along the trajectory

$$PGF_h = \sqrt{\left(PGF_{\Delta s'}\right)^2 - g^2}$$

Trajectory algorithm (I)

Hybrid trajectory scheme developed by LAURITZEN et al. [2007]:

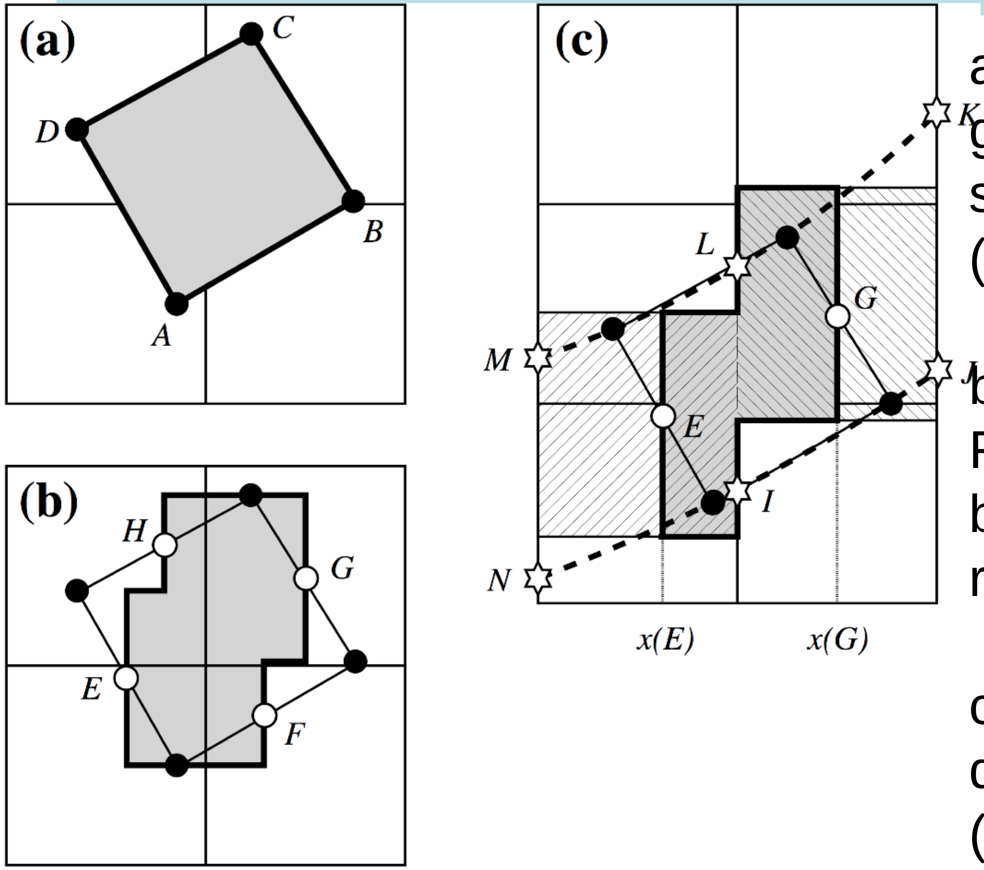
$$\vec{r}_* = \vec{r} + \vec{\breve{V}}\Delta t$$

$$\vec{\breve{V}} = \frac{\vec{V}_*^{\,n}}{2} + \frac{\Delta t}{4}\frac{d\vec{V}_*^{\,n}}{dt} + \frac{\vec{\tilde{V}}^{\,n+1}}{2} + \frac{\Delta t}{4}\frac{d\vec{\tilde{V}}^{\,n+1}}{dt}$$

$$\vec{\tilde{V}}^{\,n+1} = 2\vec{V}^{\,n} - \vec{V}^{\,n-1}$$

$$\frac{d\vec{V}}{dt} \approx \vec{V} \bullet \nabla \vec{V}$$

Integration over departure area (II)



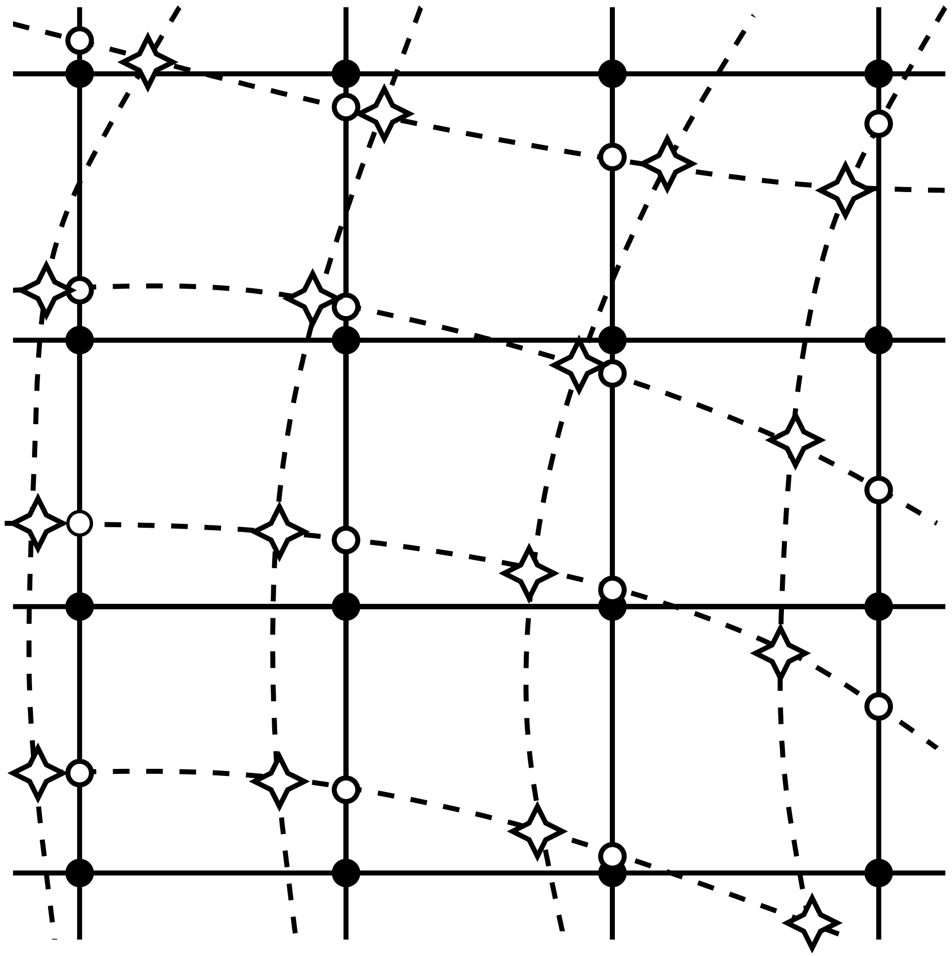
a) RANCIC [1992]: Fully 2D integration of piecewise bi-parabolic sub-grid-scale representation. (250% overhead)

b) MACHENHAUER AND OLK [1998] Fully 2D integration of pseudo bi-parabolic sub-grid-scale representation. (10% overhead)

c) NAIR et al. [2002): Two one-dimensional cascade integrations. (more than twice as efficient as b))

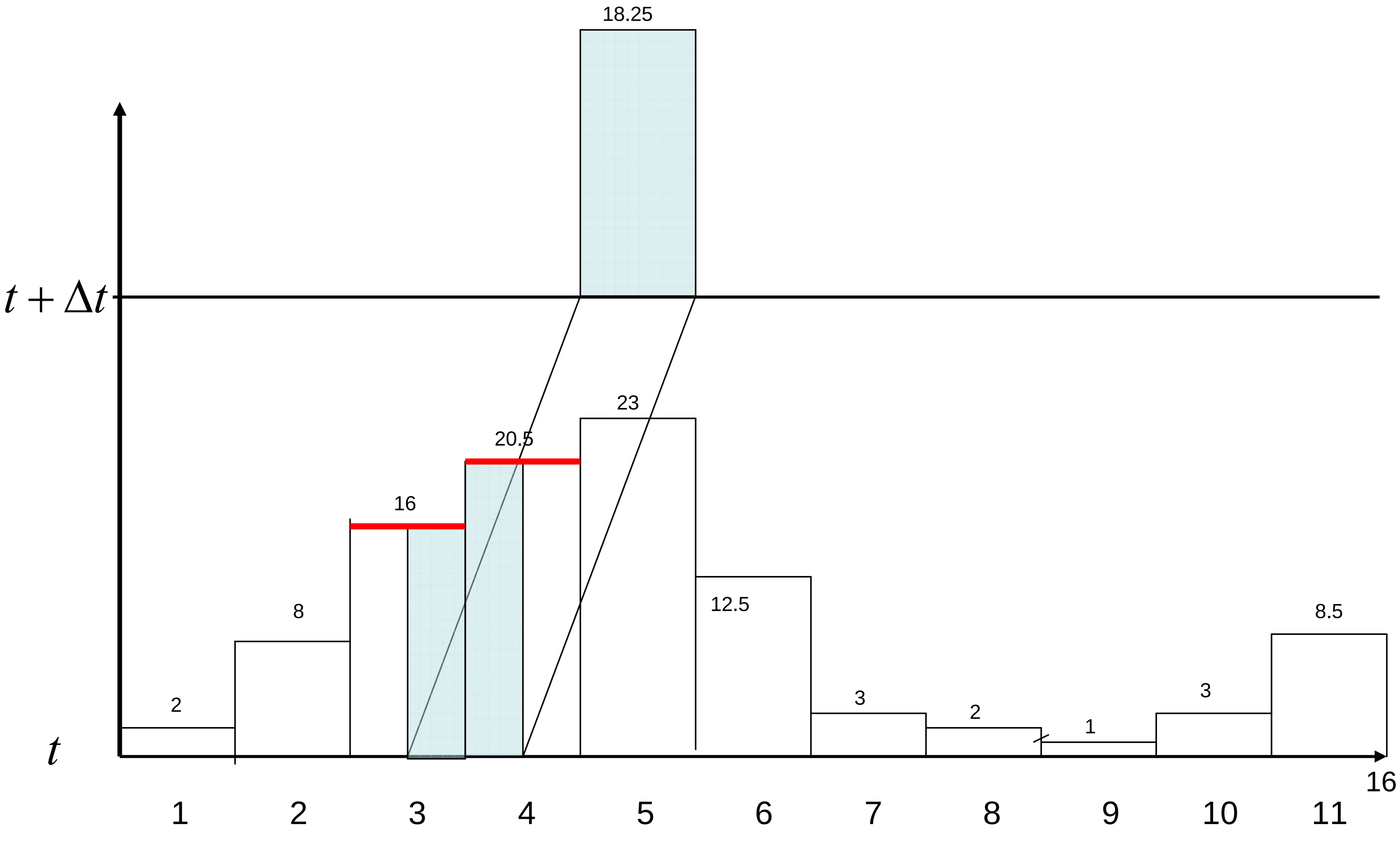
$$\overline{\Delta_k \overline{p}^n}^{\delta} = \overline{\overline{p}^n_{k+1/2} - \overline{p}^n_{k-1/2}}^{\delta} = \frac{1}{\delta A} \iint_{\delta A} \Delta_k \overline{p}^n \, dxdy$$

Cascade Interpolation

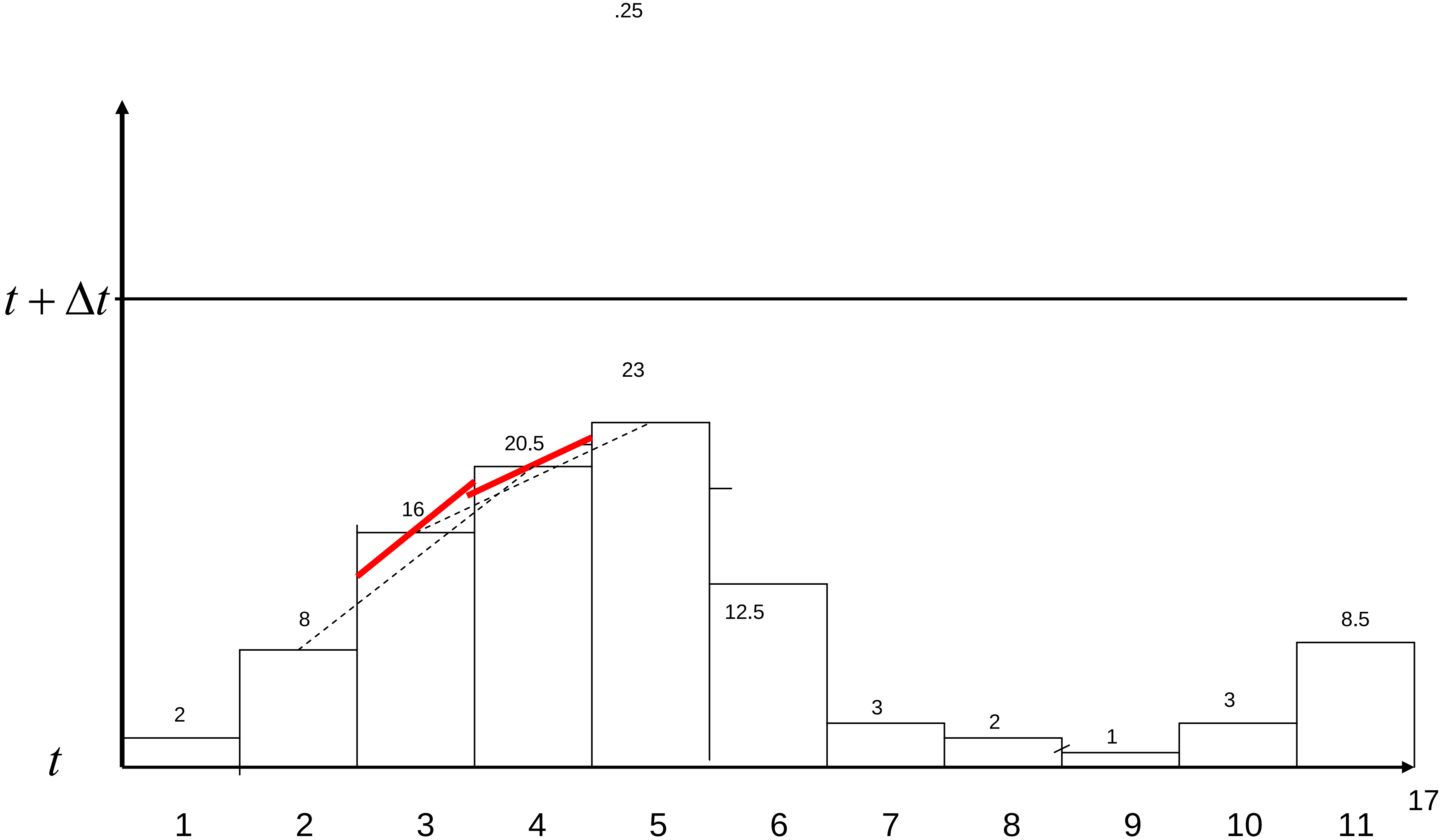


PURSER, R.J., LESLIE, L.M. (1991). An Efficient Interpolation Procedure for High-Order Three-Dimensional Semi-Lagrangian Models. *Mon. Wea. Rev* , **119** (10), 2492–2498

Piese-weise constant sub-grid representation

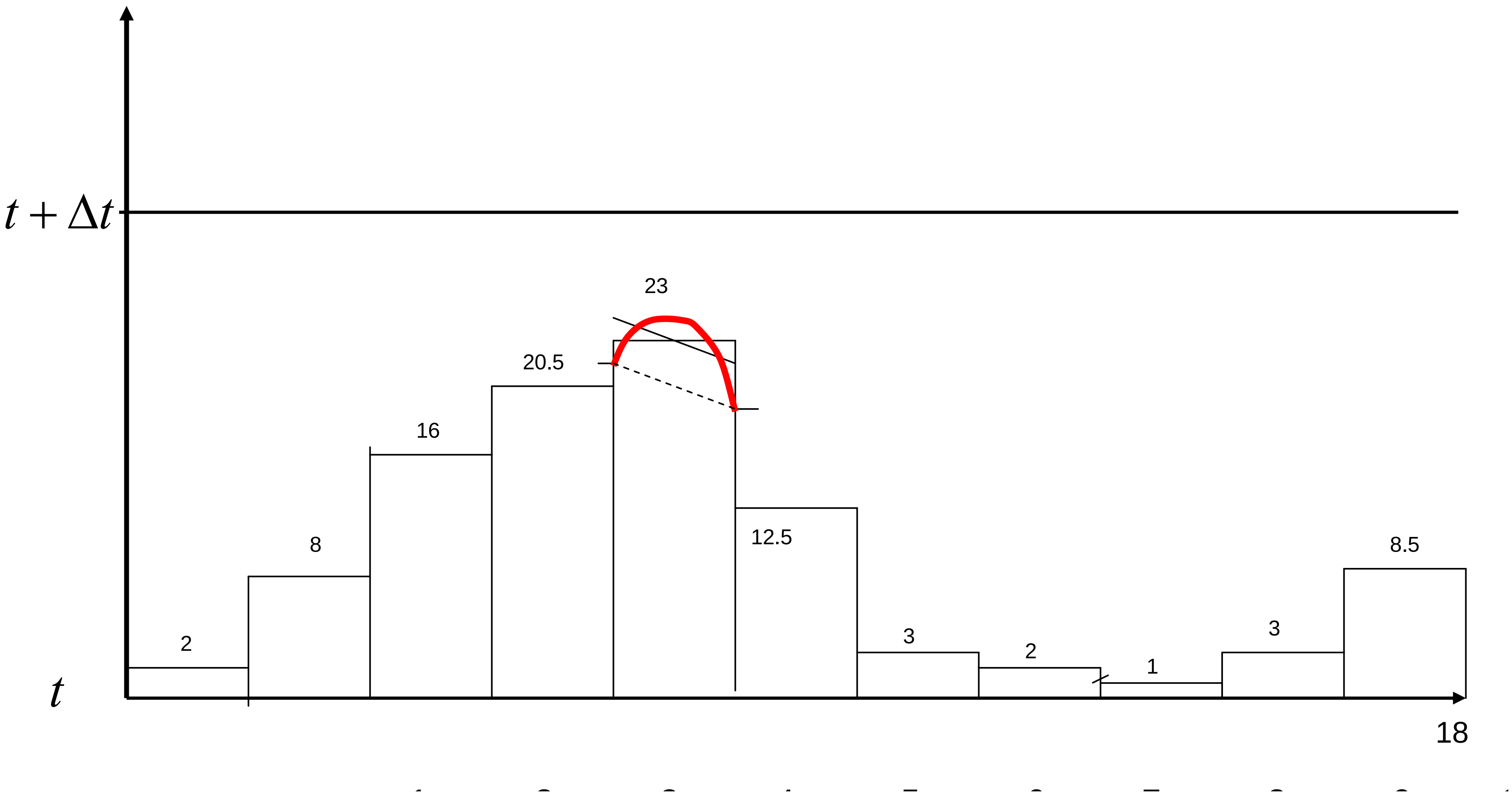


Piece-wise linear representation

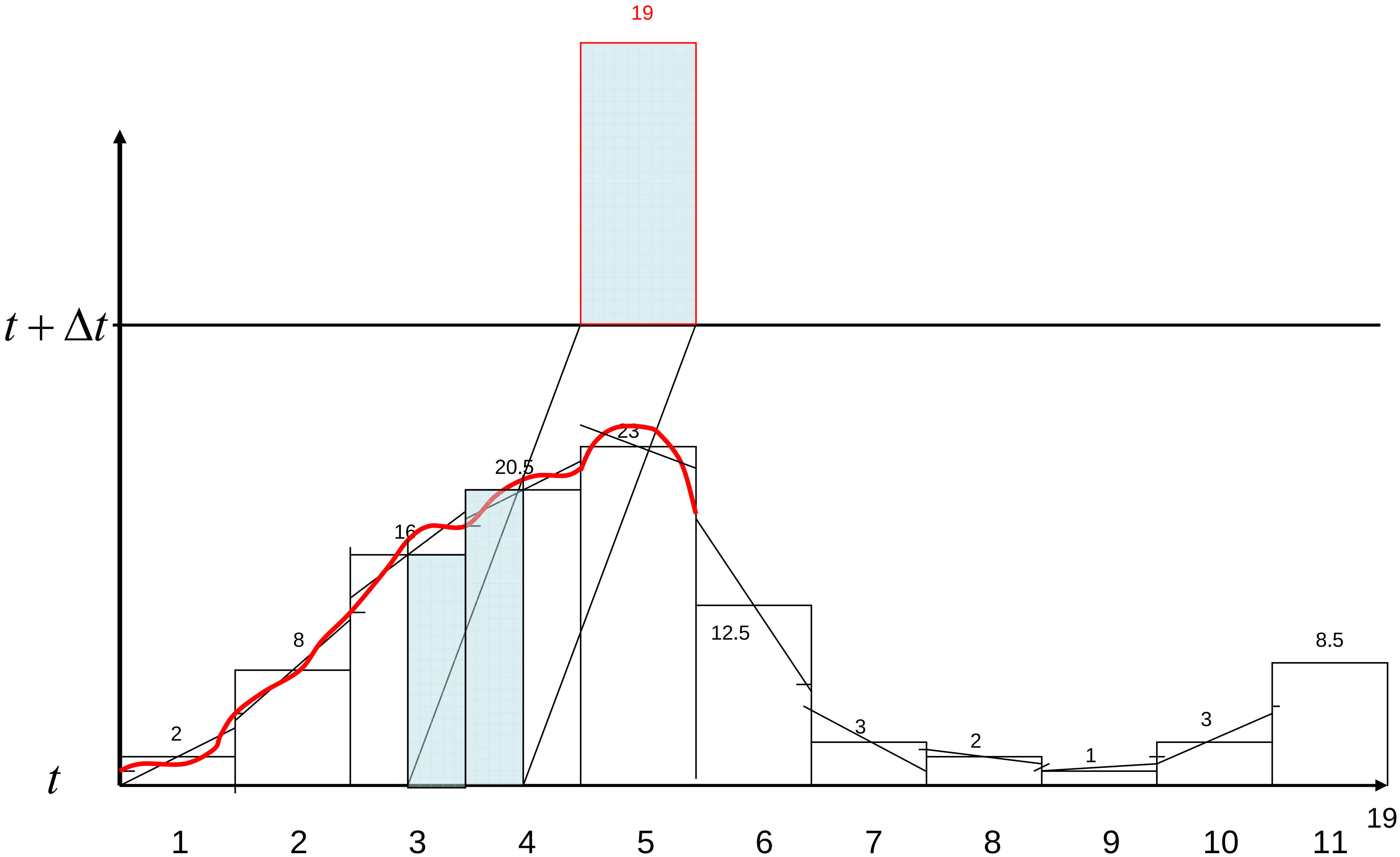


Piece-wise parabolic representation

.25



Piece-wise parabolic representation



Application of the semi-implicit technique.

So, large time steps are possible.

In HIRLAM-DCISL (Lauritzen et al., 2008) the above described transport scheme has been combined with the semi-implicit time stepping technique resulting in a dynamical model with a consistent on-line coupling for passive tracers that is numerically absolute stable for advection as well as gravity wave motion. *Hence large time steps is possible as in the traditional semi-implicit semi-Lagrangian HIRLAM*. This is the very first finite volume model with semi-implicit time stepping implemented.