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Different numerical approaches and numerical schemes for solving the governing equations.

Special subject: numerical methods for solving continuity equations

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On-line and off-line atmospheric chemistry transport (ACT) models

On-line chemistry permits explicit simulation of feedbacks between atmospheric dynamic and chemical processes.

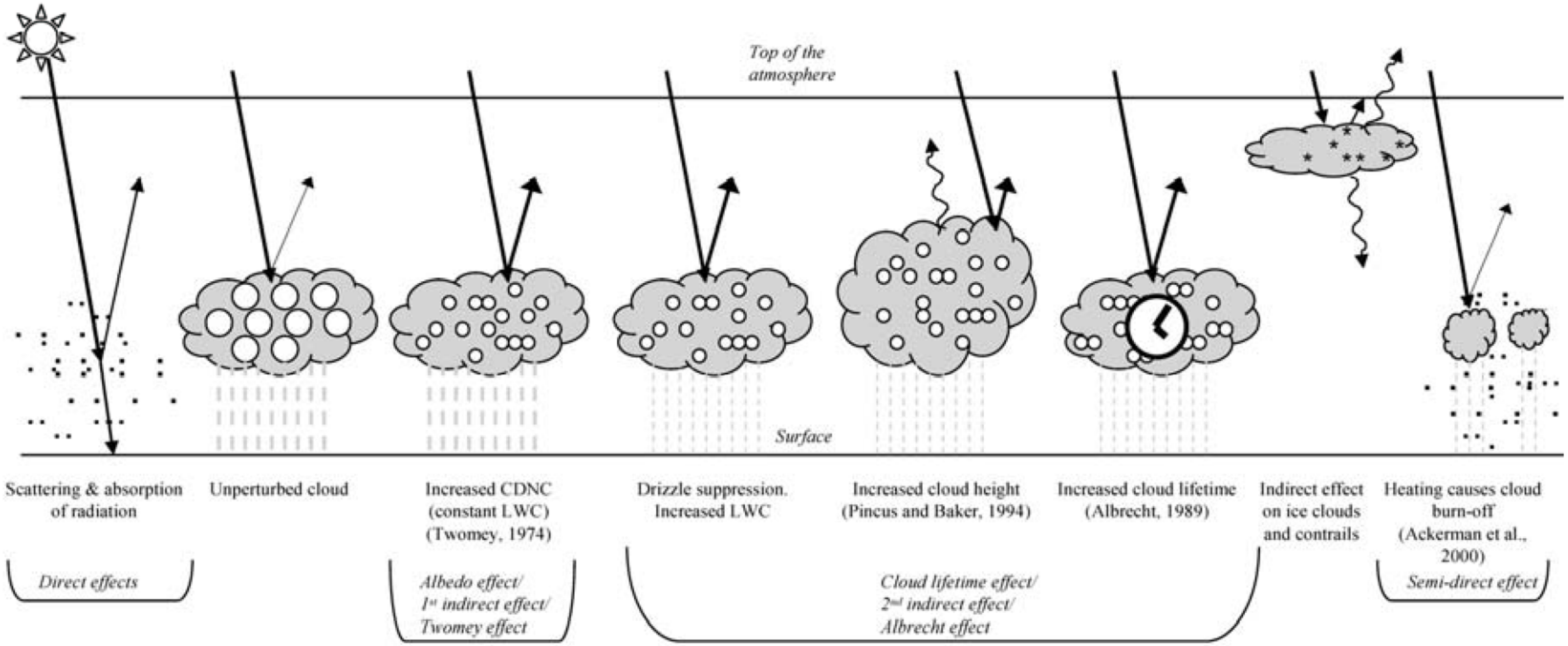
On different time-scales the following issues are particularly relevant:

- CO_2 and CH_4 cycles (well mixed greenhouse gases)
- O_3 (effects in both the short and longwave domain)
- Direct effect of aerosols (mainly shortwave)
- Indirect/semi-direct aerosol forcing (coupling to clouds and related radiation)

Applications

Air quality predictions (e.g. Enviro HIRLAM)

Earth system (climate) simulations (global and regional models, e.g. HadCM3, ECHAM6, RegClim).



Governing equations

Repetition from Sergyi’s presentation

Exact governing dynamical equations

Navier-Stokes equation (Unit mass version of "Newton's second law) expressed in the accelerated coordinate system of the Earth

$$\frac{d\boldsymbol{U}}{dt} = -2\boldsymbol{\Omega} \times \boldsymbol{U} - \frac{1}{\rho}\nabla p + \boldsymbol{g} + \boldsymbol{F}$$

The first equation of thermodynamics

$$c_v \frac{dT}{dt} + p\frac{d\alpha}{dt} = c_p \frac{dT}{dt} - \alpha \frac{dp}{dt} = Q$$

Continuity equation for dry air

$$\frac{d\rho_d}{dt} = -\rho_d \nabla \cdot \boldsymbol{U}$$

Continuity equation for various tracers (e.g. water vapour, liquid and solid water, SO_2, ^{137}Cs, particles …)

$$\frac{d\rho_t}{dt} = -\rho_t \nabla \cdot \boldsymbol{U} + S_{\rho_t}$$

$$\frac{dq_t}{dt} = S_{q_t}$$

Equation of state for ideal gases (no particle density included in ρ).

$$p = \rho RT$$

$$\rho = \rho_d + \sum_t \rho_t$$

Continuity equations

Conservation of mass or conservation of mixing ration?

Conservation of dry air mass. The volume density continuity equation:

$$\frac{\partial \rho_d}{\partial t} = -\nabla \cdot (\rho_d \boldsymbol{V})$$ Eulerian formulation

$$\frac{d\rho_d}{dt} = -\rho_d \nabla \cdot \boldsymbol{V}$$ Lagrangian formulation

ρ_d density of dry air

Conservation of mass of a chemical species, *t*:

$$\frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\rho_t \boldsymbol{V}) + D_{\rho_t} + S_{\rho_t}$$

$$\frac{d\rho_t}{dt} = -\rho_t \nabla \cdot \boldsymbol{V} + D_{\rho_t} + S_{\rho_t}$$

ρ_t density of tracer *t*

S_{ρ_t} sources/sinks

Continuity equations

Chemistry works on mixing ratio - NOT on density!

$$q_t = \frac{\rho_t}{\rho_d} \qquad \text{mixing ratio of chemical tracer } t$$

From the volume density continuity equation for tracer *t* we have:

$$\frac{dq_t\rho_d}{dt} = -q_t\rho_d\nabla\cdot\boldsymbol{V} + D_{\rho_t} + S_{\rho_t}$$

$$q_t\frac{d\rho_d}{dt} + \rho_d\frac{dq_t}{dt} = -q_t\rho_d\nabla\cdot\boldsymbol{V} + D_{\rho_t} + S_{\rho_t}$$

Continuity equations

Using the continuity equation for dry air, and re-ordering terms we get the advection equation for mixing ratio:

$$q_t\left(\frac{d\rho_d}{dt}+\rho_d\nabla\cdot\boldsymbol{V}\right)+\rho_d\frac{dq_t}{dt}=D_{\rho_t}+S_{\rho_t}$$

$$\Rightarrow$$

$$\frac{dq_t}{dt}=D_{q_t}+S_{q_t}$$ Lagrangian form

or $$\frac{\partial q_t}{\partial t}=-\boldsymbol{V}\nabla q_t+D_{q_t}+S_{q_t}$$ Eulerian form

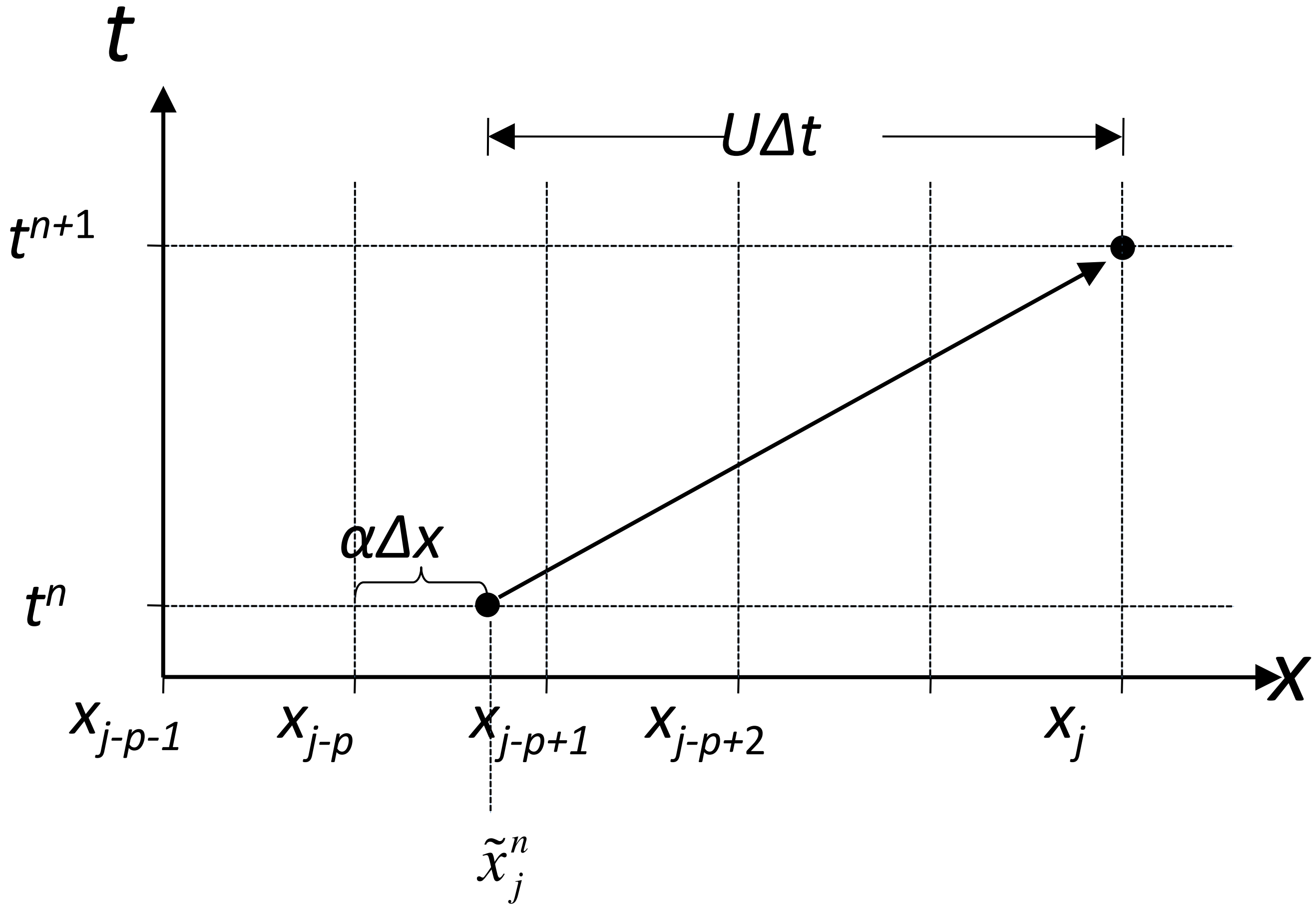
with $S_{q_t}=\dfrac{S_{\rho_t}}{\rho_d}$ and $D_{q_t}=\dfrac{D_{\rho_t}}{\rho_d}$

Desired properties for numerical solutions to the continuity equation

- Locally mass conserving
- Shape conserving (positive definite, monotonic and non-oscillatory)
- Avoid numerical mixing of tracers
- Transportive and local (solution must follow characteristics)
- Consistent (avoid mass-wind inconsistency problem)
- Conserving a constant field in a non-divergent flow
- Computationally efficient (i.e. high accuracy for a given computational resource). E.g numerically stable for long time steps

Semi-Lagrangian integration

$$\frac{d\rho_t}{dt} = -\rho_t \frac{\partial u}{\partial x}$$



Semi-Lagrangian approximation to the continuity equation

One-dimensional

$$\frac{d\rho}{dt} = -\rho\frac{\partial u}{\partial x}$$

$$\rho_k^{n+1}{}_{\mathrm{SL}} = \left\{\rho - 0.5\Delta t\left(\rho\frac{\partial u}{\partial x}\right)\right\}_{*_k}^{n} - 0.5\Delta t\left(\rho\widetilde{\frac{\partial u}{\partial x}}\right)_k^{n+1}$$

Any-dimensional

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\vec{v}$$

$$\rho_k^{n+1}{}_{\mathrm{SL}} = \left\{\rho - 0.5\Delta t\left(\rho\nabla\cdot\vec{v}\right)\right\}_{*_k}^{n} \underbrace{- 0.5\Delta t\left(\widetilde{\rho\nabla\cdot\vec{v}}\right)_k^{n+1}}_{\text{Second order Adams-Bashforth type}}$$

Traditional semi-Lagrangian (SL) scheme. Here solving the volume density continuity equation as an example:

Explicit forecast in grid point k :

$$\rho_{k\ \mathrm{SL}}^{n+1} = \rho_{*_k}^{n} - 0.5\Delta t\left(\rho\nabla\cdot\boldsymbol{v}\right)_{*_k}^{n} - 0.5\Delta t\left(\widetilde{\rho\nabla\cdot\boldsymbol{v}}\right)_{k}^{n+1}$$

$$= \sum_{l}^{K} w_{k,l}\left(\rho_l^n - 0.5\Delta t\left(\rho\nabla\cdot\boldsymbol{v}\right)_l^n\right) - 0.5\Delta t\left(\widetilde{\rho\nabla\cdot\boldsymbol{v}}\right)_k^{n+1}$$

k Grid point/cell index. $k = 1, \ldots, K$, $K = nlon*nlat$

l Grid point/cell index. $l = 1, \ldots, K$.

$w_{k,l}$ Weights on upstream departure grid points representing the polynomial upstream interpolations. These weights are only different from zero in Eulerian points l close to the semi-Lagrangian departure point.

Per definition we have $\sum_{l}^{K} w_{k,l} = 1$

$(\tilde{\bullet})^{n+1}$ Extrapolated value $(\tilde{\bullet})^{n+1} = 2(\tilde{\bullet})^{n} - (\tilde{\bullet})^{n-1}$

Semi-Lagrangian approximation to the continuity equation

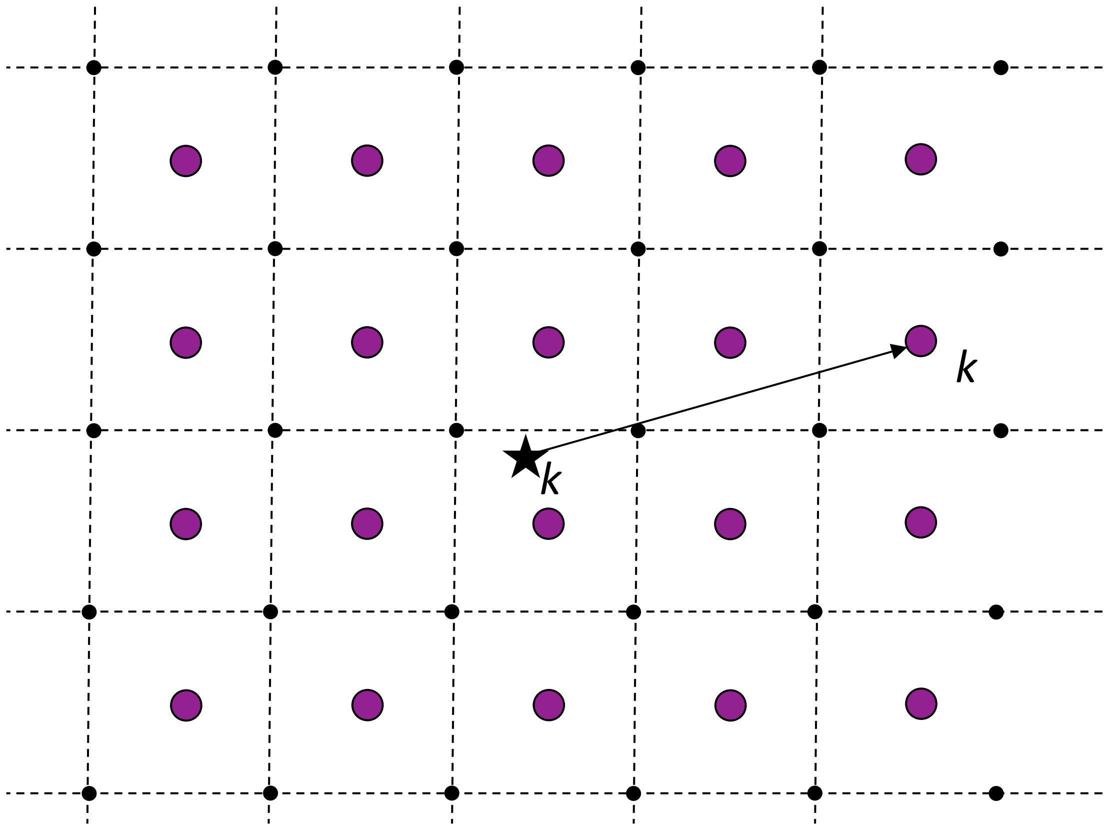
$$
\begin{aligned}
{\rho_k^{n+1}}_{\mathrm{SL}} &= \left\{\rho - 0.5\Delta t\left(\rho\nabla\cdot\vec{v}\right)\right\}_{*_k}^{n} - 0.5\Delta t\left(\widetilde{\rho\nabla\cdot\vec{v}}\right)_k^{n+1} \\
&= \sum_{l=1}^{K} w_{k,l}\left(\rho_l^n - 0.5\Delta t\left(\rho\nabla\cdot\vec{v}\right)_l^n\right) - 0.5\Delta t\left(\widetilde{\rho\nabla\cdot\vec{v}}\right)_k^{n+1}
\end{aligned}
$$

E.g. cubic (third order) interpolating scheme for the case of pure 1-D advection of a tracer:

$$
\begin{aligned}
{\phi_k^{n+1}}_{\mathrm{SL}} &= \phi_{k_*}^n \\
&= \overbrace{\boxed{-\frac{\alpha(1-\alpha)(2-\alpha)}{6}}}^{=w_{k,k-p-1}}\phi_{k-p-1}^n \overbrace{\boxed{+\frac{(1-\alpha^2)(2-\alpha)}{2}}}^{=w_{k,k-p}}\phi_{k-p}^n \\
&\quad \underbrace{\boxed{+\frac{\alpha(1+\alpha)(2-\alpha)}{2}}}_{=w_{k,k-p+1}}\phi_{k-p+1}^n \underbrace{\boxed{-\frac{\alpha(1-\alpha^2)}{6}}}_{=w_{k,k-p+2}}\phi_{k-p+2}^n
\end{aligned}
$$

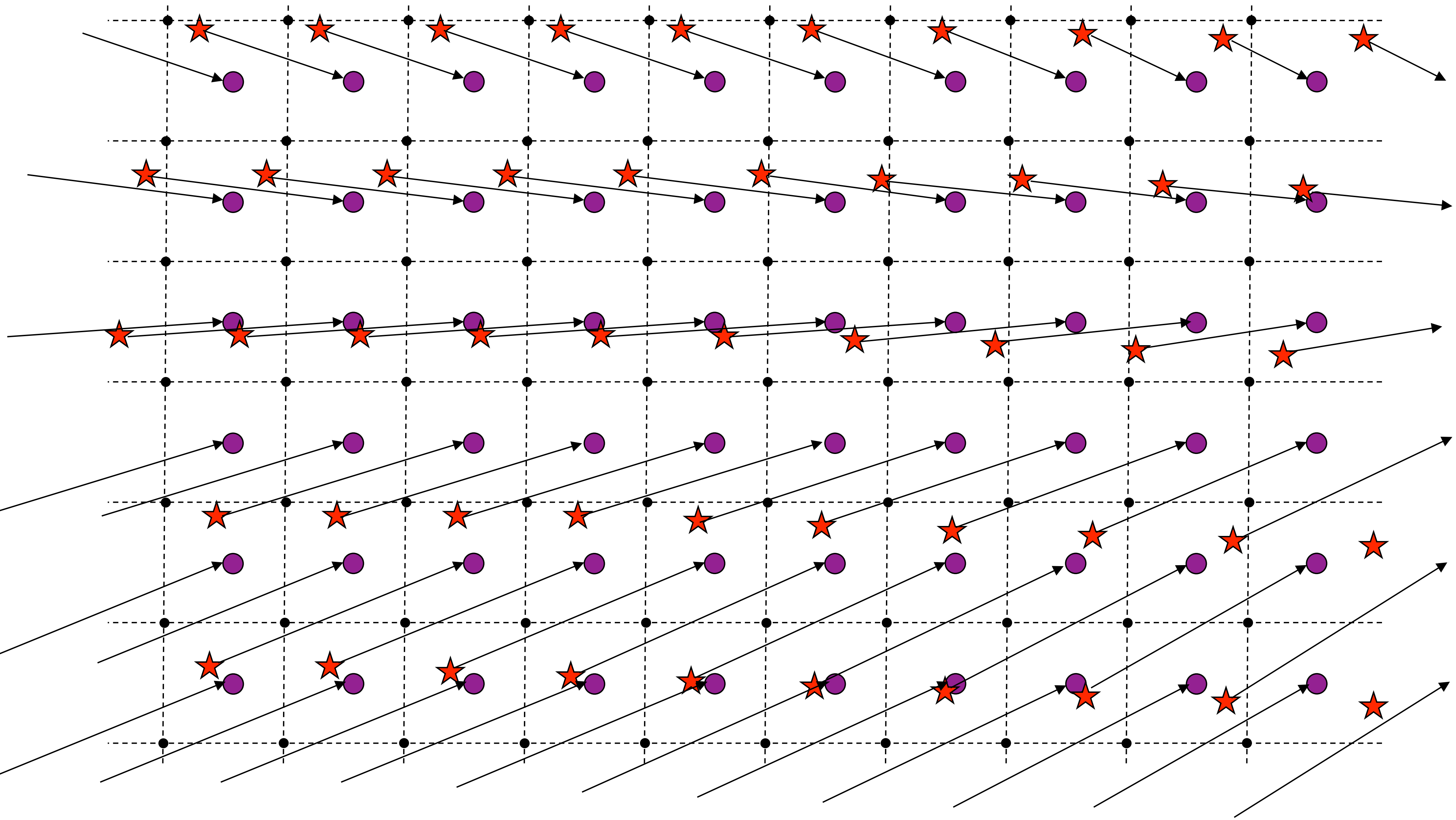
Semi Lagrangian scheme for solving the volume density continuity equation (two dimensions)

$$\rho_{k\ \mathrm{SL}}^{n+1} = \rho_{*_k}^{n} - 0.5\Delta t\left(\rho\nabla\cdot\boldsymbol{v}\right)_{*_k}^{n} - 0.5\Delta t\left(\widetilde{\rho\nabla\cdot\boldsymbol{v}}\right)_{k}^{n+1}$$



Bicubic interpolation requires 4×4 = 16 points.

Semi Lagrangian scheme



Semi Lagrangian scheme