Tracer Advection I
Atmospheric tracer transport & design philosophies

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Picture: Eruption of Iceland’s Eyjafjallajökull volcano (NASA-MODIS)
Continuity equation's in climate models

Desirable properties for transport schemes intended for climate applications
- Mass-conservation, shape-preservation, multi-tracer efficiency, ...
- Preservation of pre-existing functional relations (correlations) between species

A semi-Lagrangian view on finite-volume schemes
Continuity equations in climate models: dry air

Continuity equation for dry air mass

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0,
\]

where \( \vec{v} \) is the velocity field and \( \rho \) density.

- Mass of dry air \( \approx N_2 \) (ca. 78.08%), \( O_2 \) (ca. 20.95%), \( Ar \) (ca. 0.93%), \( CO_2 \) (at present ca. 0.038%); these well-mixed gases make up 99.998% of the volume of dry air.

- Trenberth and Smith (2005) estimated that the mass of dry air corresponds to a surface pressure of 983.05 hPa and it varies less than 0.01 hPa based on changes in atmospheric composition.

- \( \Rightarrow \) to a very good approximation there are no source/sink terms on the right-hand side of continuity equation for dry air.
Continuity equations for water species

\[
\frac{\partial (\rho q_i)}{\partial t} + \nabla \cdot (\rho q_i \vec{v}) = P \rho q_i,
\]

where \(q_i\) are dry mixing ratios\(^a\) \([m_i^{(d)}/m^{(d)}]\) and \(P\) represent source and sink terms.

- \(q_i\): water vapor, cloud liquid and cloud ice.
  - 99% of the total weight of the atmosphere is the mass of dry air. The remaining 1% is approximately the mass of water (large local variations though!)

- \(q_i\): Meso-scale models also have prognostic rain, snow, graupel, ...
  - If rain, snow, graupel, etc. are diagnostic it is assumed that they fall to the ground in one physics time-step!

\(^a\)the subtleties between using ‘dry’ and ‘wet’ mixing ratios is not discussed here - see, e.g., Lauritzen et al. (2011b)
Continuity equations in climate models: water

Very ‘oscillatory’ fields:
- Production/loss terms are large, however, clouds (e.g., ‘ice clouds’ such as Cirrus) can have lifetimes on the order of days.
- Transport operator must not produce negative values.
- Overshooting in water vapor, for example, can trigger irreversible physical processes.

In other words: the transport scheme should be shape-preserving with respect to $q$. 

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Continuity equations in climate models: aerosols

- Microphysics: continuity equations for aerosol number and mass concentrations
  - CAM5 physics: 22 aerosol continuity equations (particulate organic matter, dust, sea salt, secondary organic aerosols, ...)

Example mass fields in CAM

Example from CAM5 at 'standard' $1.9 \times 2.5^\circ$ resolution

Variation of number concentration with height

Near the surface 'drastic' variations in horizontal and vertical!

Large sources and sinks, however, without scavenging (e.g. with precipitation) aerosols can have long lifetimes (e.g. Saharan dust can be transported 1000s of miles)

$\Rightarrow$ advective tendencies can locally be the largest signal!

Check you scheme for such fields (especially if limiters use 'magic numbers'!)

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Transport in global climate models
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Tracer Advection I
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Chemistry: continuity equations for chemical species

- CAM-chem: approximately 127 continuity equations (ozone, chlorine compounds, bromine, ...)
  - some highly reactive and some long-lived

Example mass fields in CAM

- Example from chemistry version of CAM
  - HNO$_3$:
    - Produced in the stratosphere and wet removed in the troposphere, i.e.
      - strong vertical gradients
    - Variation with height
  - Br:
    - Strong diurnal cycle (produced by photolysis)

Figure: Bromine has a strong diurnal cycle (produced by photolysis)
Continuity equations in climate models: desirable properties

Important properties of transport schemes intended for atmospheric models:

- The number of prognostic continuity equations in climate and chemistry-climate models is increasing fast to accommodate more advanced physical parameterizations (e.g., microphysics), online chemistry, ....

  \( \Rightarrow \) multi-tracer efficiency is becoming increasingly important (closely tied to compute platform)!

- Atmospheric tracer fields can have very large gradients:
  - Shape-preservation is paramount!
  - Preservation of gradients is important

- Inherent conservation of mass is desirable, in particular, to consistently enforce shape-preservation and tracer-air mass consistency.

- Optimal preservation of pre-existing functional relationships (correlations)
Correlations between long-lived species in the stratosphere

Relationships between long-lived stratospheric tracers, manifested in similar spatial structures on scales ranging from a few to several thousand kilometers, are displayed most strikingly if the mixing ratio of one is plotted against another, when the data collapse onto remarkably compact curves. - Plumb (2007)

E.g., nitrous oxide ($N_2O$) against 'total odd nitrogen' ($NO_y$) or chlorofluorocarbon (CFC's)

Figures from Plumb (2007).
Relationships between long-lived stratospheric tracers, manifested in similar spatial structures on scales ranging from a few to several thousand kilometers, are displayed most strikingly if the mixing ratio of one is plotted against another, when the data collapse onto remarkably compact curves. - Plumb (2007)

E.g., nitrous oxide ($N_2O$) against ‘total odd nitrogen’ ($NO_y$) or chlorofluorocarbon (CFC’s)

Similarly:
- The total of chemical species within some chemical family may be preserved following an air parcel although the individual species have a complicated relation to each other and may be transformed into each other through chemical reactions (e.g., total chlorine)
- Aerosol-cloud interactions (Ovtchinnikov and Easter, 2009)

The transport operator should ideally not perturb pre-existing functional relationships
Analyzing scatter plots

Analytical pre-existing functional relationship curve $\psi$ (linear)

$$\xi = \psi(\chi) = a \cdot \chi + b, \quad \chi \in [\chi^{(\text{min})}, \chi^{(\text{max})}],$$

where $a$ and $b$ are constants, and $\chi$ and $\xi$ are the mixing ratios of the two tracers
Analyzing scatter plots

Analytical pre-existing functional relationship curve $\psi$ (linear)

$\chi$ and $\xi$ are transported separately by the transport scheme

\[
\begin{align*}
\chi_k^{n+1} &= \mathcal{T}(\chi_j^n), \quad j \in \mathcal{H}, \\
\xi_k^{n+1} &= \mathcal{T}(\xi_j^n), \quad j \in \mathcal{H},
\end{align*}
\]

where $\mathcal{T}$ is the transport operator and $\mathcal{H}$ the set of indices defining the ‘halo’ for $\mathcal{T}$. 
Analyzing scatter plots

Analytical pre-existing functional relationship curve $\psi$ (linear)

If $\mathcal{T}$ is ‘semi-linear’ then linear pre-existing functional relations are preserved:

$$\xi^{n+1}_k = \mathcal{T}(\xi^n_j) = \mathcal{T}(a \chi^n_j + b) = a\mathcal{T}(\chi^n_j) + b\mathcal{T}(1) = a\mathcal{T}(\chi^n_j) + b = a\chi^{n+1}_k + b.$$

→ If transport operator is non-linear the relationship might be violated.
Analyzing scatter plots

Analytical pre-existing functional relationship curve $\psi$ (linear)

→ carefully designed finite-volume schemes are ‘semi-linear’ even with limiters/filters! (Thuburn and McIntyre, 1997; Lin and Rood, 1996)
Analyzing scatter plots

Analytical pre-existing functional relationship curve $\psi$

$$\xi = \psi(\chi) = a \cdot \chi^2 + b,$$

where $a$ and $b$ are constants so that $\psi$ is concave or convex in $[\chi^{(\min)}, \chi^{(\max)}]$
Discrete pre-existing functional relation (initial condition)

\[ \xi_k = \psi(\chi_k) = a \cdot (\chi_k)^2 + b, \quad k = 1, \ldots, K, \]

where \( a \) and \( b \) are constants so that \( \psi \) is concave or convex in \([\chi^{(\text{min})}, \chi^{(\text{max})}]\)
A fully Lagrangian model will maintain pre-existing functional relation

\[ \chi_{k}^{n+1} = \chi_{k}^{n}, \quad \xi_{k}^{n+1} = \xi_{k}^{n} \]

following parcel trajectories (without ‘contour-surgery’ or other mixing mechanisms)
Any Eulerian/semi-Lagrangian scheme will disrupt pre-existing functional relation

\[ \xi_{k+1} = \mathcal{T}(\xi_j^n) \neq a \cdot \mathcal{T} \left( \chi_j^n \right)^2 + b, \quad j \in \mathcal{H} \]

where \( \mathcal{T} \) is the transport operator and \( \mathcal{H} \) the set of indices defining the ‘halo’ for \( \mathcal{T} \).
‘Real’ mixing, e.g., observed during polar vortex breakup (Waugh et al., 1997)

‘Real mixing’ (when occurring) will tend to replace the functional relation by a scatter by linearly interpolating along mixing lines between pairs of points.
‘Real’ mixing, e.g., observed during polar vortex breakup (Waugh et al., 1997)

‘Real mixing’ (when occurring) will tend to replace the functional relation by a scatter by linearly interpolating along mixing lines between pairs of points → Ideally numerical mixing should = ‘real mixing’!

However, it may be shown mathematically that schemes that exclusively introduce ‘real mixing’ are 1st-order schemes (Thuburn and McIntyre, 1997).
Classification of numerical mixing on scatter plots

Figure from (Lauritzen and Thuburn, 2012)

Show animation from idealized test case (Lauritzen and Thuburn, 2012; Lauritzen et al., 2012)
'Most fundamental equations in fluid dynamics can derived from first principles in either an *Eulerian* form or an *Lagrangian* form' - (see, e.g., text book of Durran, 1999)

Figure courtesy of J. Thuburn.
Consider the continuity equation for some inert (no sources/sinks) and passive (does not feed back on the flow) tracer.

semi-Lagrangian form

Eulerian (flux) form

For simplicity assume a quadrilateral mesh and leave out the ‘details’ of spherical geometry.

- Only consider two-time-level finite-volume schemes
Finite-volume approach: Integrate in space

semi-Lagrangian form

Eulerian (flux-form) form

\[ \frac{D}{Dt} \int_{A(t)} \psi \, dA = 0. \]

where \( A(t) \) is a Lagrangian\(^\dagger \) control volume and

\[ \frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla, \]

is the material/total derivative.

Integrate

\[ \frac{\partial \psi}{\partial t} + \nabla \cdot (\psi \, \vec{v}) = 0 \]

over an Eulerian control volume \( A_k \):

\[ \frac{\partial}{\partial t} \int_{A_k} \psi \, dA + \int_{A_k} \nabla \cdot (\psi \, \vec{v}) \, dA = 0. \]

\(^\dagger \) volume whose bounding surface moves with the local fluid velocity ⇔ volume which always contains the same material particles
Finite-volume approach: Integrate in space

**semi-Lagrangian form**

\[
\frac{D}{Dt} \int_{A(t)} \psi \, dA = 0.
\]

where \( A(t) \) is a Lagrangian\(^\dagger \) control volume and

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla,
\]

is the material/total derivative.

**Eulerian (flux-form) form**

Apply divergence theorem on second term:

\[
\frac{\partial}{\partial t} \int_{A_k} \psi \, dA + \oint_{\partial A_k} (\psi \, \vec{v}) \cdot \vec{n} \, dS = 0,
\]

where \( \partial A_k \) is the boundary of \( A_k \) and \( \vec{n} \) the outward normal vector to \( \partial A_k \).

\( \rightarrow \) instantaneous flux of tracer mass through boundaries of \( A_k \)

\(^\dagger\) volume whose bounding surface moves with the local fluid velocity \( \Leftrightarrow \) volume which always contains the same material particles
Finite-volume approach: Integrate in time

semi-Lagrangian form

\[
\int_{A(t+\Delta t)} \psi \, dA = \int_{A(t)} \psi \, dA,
\]

where \( \Delta t \) is time-step and \( t = n \Delta t \).

Upstream semi-Lagrangian approach:

\[
\overline{\psi^{n+1}} \Delta A_k = \overline{\psi^n} \Delta a_k,
\]

where \( \overline{()} \) is average value over cell.

Eulerian (flux-form) form

Apply divergence theorem on second term:

\[
\frac{\partial}{\partial t} \int_{A_k} \psi \, dA + \oint_{\partial A_k} (\psi \vec{v}) \cdot \vec{n} \, dS = 0,
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where \( \partial A_k \) is the boundary of \( A_k \) and \( \vec{n} \) the outward normal vector to \( \partial A_k \).

\( \rightarrow \) instantaneous flux of tracer mass through boundaries of \( A_k \).
Finite-volume approach: Integrate in time

**semi-Lagrangian form**

\[ \int_{A(t+\Delta t)} \psi \, dA = \int_{A(t)} \psi \, dA, \]

where \( \Delta t \) is time-step and \( t = n \Delta t \).

Upstream semi-Lagrangian approach:

\[ \bar{\psi}^{n+1}_{k} \Delta A_{k} = \bar{\psi}^{n}_{k} \Delta a_{k}, \]

where \( \bar{()} \) is average value over cell.

**Eulerian (flux-form) form**

\[ \frac{\partial}{\partial t} \int_{A_{k}} \psi \, dA + \oint_{\partial A_{k}} (\psi \, \vec{v}) \cdot \vec{n} \, dS = 0, \]

\[ \bar{\psi}^{n+1}_{k} \Delta A_{k} = \bar{\psi}^{n}_{k} \Delta A_{k} + \]

\[ \int_{n\Delta t}^{(n+1)\Delta t} \left[ \oint_{\partial A_{k}} (\psi \, \vec{v}) \cdot \vec{n} \, dS \right] dt = 0, \]

→ flux of tracer mass through boundaries of \( A_{k} \) during \( t \in [n\Delta t, (n+1)\Delta t] \).
Finite-volume approach:

semi-Lagrangian form

\[ \int_{A(t+\Delta t)} \psi \, dA = \int_{A(t)} \psi \, dA, \]
where \( \Delta t \) is time-step and \( t = n \Delta t \).

Upstream semi-Lagrangian approach:

\[ \overline{\psi}_{k}^{n+1} \Delta A_k = \overline{\psi}_{k}^{n} \Delta a_k, \]
where \( \overline{()}_k \) is average value over cell.

Eulerian (flux-form) form

\[ \overline{\psi}_{k}^{n+1} \Delta A_k = \overline{\psi}_{k}^{n} \Delta A_k - \sum_{\tau=1}^{4} F_{k}^{(\tau)}, \]
where

\[ F_{k}^{(\tau)} = s_{k}^{(\tau)} \int_{a_{k}^{\tau}} \psi^n(x, y) \, dA. \]

is flux of mass through face \( \tau \) during \( \Delta t \), and \( s_{k}^{(\tau)} = \pm 1 \)

for simplicity assume \( s_{k}^{\tau} \) is NOT multi-valued; for multi-valued case see, e.g., Harris et al. (2010).
Finite-volume approach:

semi-Lagrangian form

Eulerian (flux-form) form

\[ \psi_{k}^{n+1} \Delta A_{k} = \psi_{k}^{n} \Delta a_{k}, \]

Note equivalence between Lagrangian cell-integrated and Eulerian flux-form continuity equations:

\[ \Delta A_{k} - \sum_{\tau=1}^{4} \left( s_{k}^{(\tau)} \Delta a^{(\tau)}_{k} \right) = \Delta a_{k}. \]

i.e. the areas involved in Eulerian forecast equals upstream Lagrangian area \( a_{k} \).
Finite-volume approach:

semi-Lagrangian form

\[
\psi^{n+1}_k \Delta A_k = \psi^n_k \Delta a_k,
\]

Define a global piecewise continuous reconstruction function

\[
\psi(x, y) = \sum_{k=1}^{N} I_{A_k} \psi_k (x, y),
\]

where \(I_{A_k}\) is the indicator function

\[
I_{A_k} = \begin{cases} 
1, & (x, y) \in A_k, \\
0, & (x, y) \notin A_k.
\end{cases}
\]

Eulerian (flux-form) form

\[
\psi^{n+1}_k \Delta A_k = \psi^n_k \Delta A_k - \sum_{\tau=1}^{4} F^{(\tau)}_k,
\]
Finite-volume approach:

**semi-Lagrangian form**

\[
\overline{\psi}_{k}^{n+1} \Delta A_{k} = \overline{\psi}_{k}^{n} \Delta a_{k},
\]

\[
\overline{\psi}_{k}^{n+1} \Delta A_{k} = \sum_{\ell=1}^{L_{k}} \int_{a_{k\ell}} \psi_{n}^{n}(x, y) \, dA.
\]

where \( a_{k\ell} \) is the non-empty overlap area

\[a_{k\ell} = a_{k} \cap A_{\ell}, \quad a_{k\ell} \neq \emptyset; \quad \ell = 1, \ldots, L_{k},\]

where \( N \) is the number of cells in the domain and \( L_{k} \) number of overlap areas.

**Eulerian (flux-form) form**

\[
\overline{\psi}_{k}^{n+1} \Delta A_{k} = \overline{\psi}_{k}^{n} \Delta A_{k} - \sum_{\tau=1}^{4} F_{k}(\tau),
\]

\[
F_{k}(\tau) = \frac{4}{\Delta t} \int_{a_{k\ell}} \psi_{n}(x, y) \, dA.
\]
Finite-volume approach:

- **semi-Lagrangian form**

\[
\frac{\psi^{n+1}}{\psi^n} \Delta A_k = \frac{\psi^n}{\psi^n} \Delta a_k,
\]

\[
\frac{\psi^{n+1}}{\psi^n} \Delta A_k = \sum_{\ell=1}^{L_k} \int_{a_{k\ell}} \psi^n(x, y) \, dA.
\]

where \(a_{k\ell}\) is the non-empty overlap area

\[
a_{k\ell} = a_k \cap A_\ell, \quad a_{k\ell} \neq \emptyset; \quad \ell = 1, \ldots, L_k,
\]

where \(N\) is the number of cells in the domain and \(L_k\) number of overlap areas.

- **Eulerian (flux-form) form**

\[
\frac{\psi^{n+1}}{\psi^n} \Delta A_k = \frac{\psi^n}{\psi^n} \Delta A_k - \sum_{\tau=1}^{4} F_k^{(\tau)},
\]

\[
F_k^{(\tau)} = \sum_{\ell=1}^{L_k^{(\tau)}} \int_{a_{k\ell}} \psi^n(x, y) \, dA,
\]

where \(L_k^{(\tau)}\) is number of non-empty ‘flux’ overlap areas for face \(\tau\).

Note that in general: \(L_k \ll \sum_{\tau=1}^{4} L_k^{(\tau)}\)
Finite-volume approach: Conditions for inherent mass-conservation

**semi-Lagrangian form**

\[ \psi_{k}^{n+1} \Delta A_{k} = \psi_{k}^{n} \Delta a_{k}, \]

- \( a_{k} \)'s span \( \Omega \) without gaps/overlaps
  \[
  \bigcup_{k=1}^{N} a_{k} = \Omega, \text{ and } a_{k} \cap a_{\ell} = \emptyset \forall k \neq \ell.
  \]
- Sub-grid-scale representation of \( \psi \) must integrate to cell-average mass
  \[
  \int_{A_{k}} \psi_{k}^{n}(x, y) \, dA = \psi_{k}^{n} \Delta A_{k},
  \]

**Eulerian (flux-form) form**

\[ \psi_{k}^{n+1} \Delta A_{k} = \psi_{k}^{n} \Delta A_{k} - \sum_{\tau=1}^{4} F_{k}(\tau), \]

- Fluxes for ‘shared’ faces must cancel, e.g.,
  \[
  F_{k}^{(3)} = -F_{k-1}^{(1)}
  \]

Any flux, even highly inaccurate fluxes, will NOT violate mass-conservation!
The only direct way of enforcing shape-preservation is to filter the sub-grid-scale distribution $\psi^n_k(x, y)$:

- fully 2D filters (Barth and Jespersen, 1989)
- 1D filters for cascade schemes (Colella and Woodward, 1984; Zerroukat et al., 2005; Lin and Rood, 1996)

Shape-preservation can be enforced by

- blending monotone and high-order fluxes (e.g., Flux-Corrected Transport Zalesak, 1979)
- making $\psi^n_k(x, y)$ shape-preserving (Barth and Jespersen, 1989)
Finite-volume approach: Area approximation

(a) Exact
(b) Straight lines (Rančić, 1992; Lauritzen et al., 2010)
(c) Step-functions for ‘North/South’ faces & straight lines parallel to ‘longitudes’ for ‘East/West’ faces (Nair and Machenhauer, 2002).
(d) Cascade (flow-split) (Nair et al., 2002; Zerroukat et al., 2002)

(g-k) Quadrilateral flux-areas (Dukowicz and Baumgardner, 2000; Harris et al., 2010)
(l) ‘Effective’ departure area
Finite-volume approach: Area approximation

(a) Exact
(b) Straight lines (Rančić, 1992; Lauritzen et al., 2010)
(c) Step-functions for ‘North/South’ faces & straight lines parallel to ‘longitudes’ for ‘East/West’ faces (Nair and Machenhauer, 2002).
(d) Cascade (flow-split) (Nair et al., 2002; Zerroukat et al., 2002)

(g-k) ‘Curved’ (parabolic) flux-areas (Ullrich et al., 2012)
(l) ‘Effective’ departure area
Finite-volume approach: Area approximation

(a) Exact
(b) Straight lines (Rančić, 1992; Lauritzen et al., 2010)
(c) Step-functions for ‘North/South’ faces & straight lines parallel to ‘longitudes’ for ‘East/West’ faces (Nair and Machenhauer, 2002).
(d) Cascade (flow-split) (Nair et al., 2002; Zerroukat et al., 2002)

(g-k) Parallelogram flux-areas (Miura, 2007; Skamarock and Menchaca, 2010)
(l) ‘Effective’ departure area
Finite-volume approach: Area approximation

(a) **Exact**

(b) **Straight lines** (Rančić, 1992; Lauritzen et al., 2010)

(c) **Step-functions for ‘North/South’ faces & straight lines parallel to ‘longitudes’ for ‘East/West’ faces** (Nair and Machenhauer, 2002).

(d) **Cascade (flow-split)** (Nair et al., 2002; Zerroukat et al., 2002)

(a-c) **Dimensionally split scheme** (Lin and Rood, 1996): Flux-areas area combinations of rectangles aligned with grid lines

(d) ‘Effective’ departure area

**Figure from Machenhauer et al. (2009)**
Finite-volume approach: Geometric and reconstruction errors

- **Geometric error**: how well is the upstream Lagrangian area / flux areas approximated
- **Reconstruction error**: how well is the sub-grid-scale distribution approximated

(methods for reconstructions was discussed in P.A. Ullrich’s lecture 1)

Typically:
- for lower-order reconstruction functions the ‘reconstruction error’ $\gg$ ‘geometric error’
- the smaller the Courant number ($\Delta t$) the smaller the ‘geometric error’
- for higher-order reconstruction functions and shear flows (deformational) the ‘geometric error’ can be significant (Ullrich et al., 2012)
Further simplifications for flux-form approaches (Margolin and Shashkov, 2003)

Recall: we can do anything we want with the fluxes as long as $F_k^{(3)} = -F_{k-1}^{(1)}$

‘Rigorous’ flux for face 1 ($\tau = 1$):

$$F_k^{(1)} = \sum_{\ell=1}^{3} \int_{a_{k\ell}} \psi_n^\ell(x, y) \, dA.$$ 

For $\Delta t$ sufficiently small:

$$\Delta a_{k2} \gg \Delta a_{k1} \text{ and } \Delta a_{k2} \gg \Delta a_{k3}$$

→ simplify flux-integration by only using one upstream reconstruction function:

$$F_k^{(1)} \approx F_k^{(1)} = \int_{a_{k1} \cup a_{k2} \cup a_{k3}} \psi_2^n(x, y) \, dA.$$ 

$\psi_2^n$ is extrapolated over $a_{k1}$ and $a_{k3}$.

- note: the search for overlap areas has almost been eliminated in $F_k^{(1)}$
- $F_k^{(1)}$ stable for Courant numbers approximately less than $\frac{1}{2} (\Delta a_{k2} > \Delta a_{k1} + \Delta a_{k3})$ (Lauritzen et al., 2011a)
- $F_k^{(1)}$ can be slightly more accurate than $F_k^{(1)}$ (Lauritzen et al., 2011a)
The $\eta$-coordinate atmospheric primitive equations, neglecting dissipation and forcing terms:

\[
\frac{\partial \vec{v}}{\partial t} + (\zeta + f) \hat{k} \times \vec{v} + \nabla \left( \frac{1}{2} \vec{v}^2 + \Phi \right) + \dot{\eta} \frac{\partial \vec{v}}{\partial \eta} + \frac{RT_v}{\rho} \nabla p = 0 \tag{1}
\]

\[
\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T + \dot{\eta} \frac{\partial T}{\partial \eta} - \frac{RT_v}{c_p^* \rho} \omega = 0 \tag{2}
\]

\[
\frac{\partial}{\partial t} \left( \frac{\partial p}{\partial \eta} \right) + \nabla \cdot \left( \frac{\partial p}{\partial \eta} \vec{v} \right) + \frac{\partial}{\partial \eta} \left( \dot{\eta} \frac{\partial p}{\partial \eta} \right) = 0 \tag{3}
\]

\[
\frac{\partial}{\partial t} \left( \frac{\partial q}{\partial \eta} \right) + \nabla \cdot \left( \frac{\partial q}{\partial \eta} \vec{v} \right) + \frac{\partial}{\partial \eta} \left( \dot{\eta} \frac{\partial q}{\partial \eta} \right) = 0. \tag{4}
\]

- Continuity equation for air is coupled with momentum and thermodynamic equations:
  - thermodynamic variables and other prognostic variables feed back on the velocity field
  - which, in turn, feeds back on the solution to the continuity equation.
  - Hence the continuity equation for air can not be solved in isolation and one must obey the maximum allowable time-step restrictions imposed by the fastest waves in the system.

- The passive tracer transport equation can be solved in isolation given prescribed winds and air densities, and is therefore not susceptible to the time-step restrictions imposed by the fastest waves in the system.
Continuity equation for air density \( \rho \)

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0, \tag{1}
\]

and a tracer with mixing ratio \( q \)

\[
\frac{\partial (\rho q)}{\partial t} + \nabla \cdot (\rho q \vec{v}) = 0, \tag{2}
\]

- In continuous space:
  \[ q = 1 \Rightarrow \text{continuity equation for } (\rho q) \text{ reduces to continuity equation for air } (\rho) \]

- It is considered desirable that discretization schemes obey this relation:
  \[ \text{‘free-stream’ preserving or ‘consistent’ tracer transport.} \]

- Note: ‘complete consistency’ is obtained if air density and tracer mass continuity equations are solved using the same numerical method, on the same discretization grid, and using the same time-steps (everything is ‘in sync’!).
Time-stepping and coupling:

- semi-Lagrangian form
- Eulerian (flux-form) form
Time-stepping and coupling: mass-conservative semi-implicit approach

Traditionally: semi-Lagrangian advection of $\rho$ is combined with semi-implicit time-stepping:

$$
\rho_k^{n+1} = (\rho_k^{n+1})_{\text{exp}} - \frac{\Delta t}{2} \rho_{00} (\nabla \cdot \tilde{v}_k^{n+1} - \nabla \cdot \tilde{v}_k^{n+1}),
$$

where

- $\rho_{00}$ a constant reference density
- $(\cdot)_{\text{exp}}$ is the explicit prediction
- $\tilde{v}^{n+1}$ velocity extrapolated to time-level ($n + 1$)

What about tracers?

- Solving continuity equation for $(\rho q)$ explicitly

$$
\rho q_k^{n+1} \Delta A_k = \rho q_k^n \Delta a_k
$$

is NOT ‘free-stream’ preserving!

- Using ‘traditional’ semi-implicit approach for tracers

$$
\rho q_k^{n+1} \Delta A_k = \rho q_k^n \Delta a_k - \frac{\Delta t}{2} (\rho q)_{00} (\nabla \cdot \tilde{v}_k^{n+1} - \nabla \cdot \tilde{v}_k^{n+1}).
$$

is problematic (Lauritzen et al., 2008).
Traditionally: semi-Lagrangian advection of $\rho$ is combined with semi-implicit time-stepping:

$$\rho^n_{k+1} = (\rho^n_k)_{exp} - \frac{\Delta t}{2} \left\{ \nabla \cdot \left[ (\rho^n_{k+1})_{exp} \vec{v}^{n+1}_k \right] - \nabla \cdot \left[ (\rho^n_k)_{exp} \vec{v}^{n+1}_k \right] \right\}. $$

where

- $\rho_{00}$ a constant reference density
- $(\cdot)_{exp}$ is the explicit prediction
- $\tilde{v}^{n+1}$ velocity extrapolated to time-level ($n + 1$)

What about tracers?

- A solution is to formulate the semi-implicit terms in flux-form

$$\rho q^n_{k+1} = (\rho q^n_k)_{exp} - \frac{\Delta t}{2} \left\{ \nabla \cdot \left[ (\rho q^n_{k+1})_{exp} \vec{v}^{n+1}_k \right] - \nabla \cdot \left[ (\rho q^n_k)_{exp} \vec{v}^{n+1}_k \right] \right\}. $$

so that reference states are eliminated (Wong et al., 2012)
Time-stepping and coupling: Eulerian flux-form

For efficiency, sub-cycle dynamics with respect to tracers:

- Solve continuity equation for air $\rho$ together with momentum and thermodynamics equations.
- Repeat $k_{split}$ times
- Brown area = average flow of mass through cell face.
- Compute time-averaged value of $q$ across brown area using flux-form scheme: $\langle q \rangle$.
- Flux of tracer mass: $\langle q \rangle \times \sum_{i=1}^{k_{split}} \rho^{n+i/k_{split}}$
- Yields ‘free stream’ preserving solution!
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References


