The semi-Lagrangian technique: current status and future developments

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ECMWF

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(thanks to: Adrian Simmons, Niels Borman and Richard Forbes)

Outline

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1. Semi-Lagrangian technique and history
2. Semi-Lagrangian numerics in the upper atmosphere
   - Trajectory equation and numerical noise
   - Extratropical tropopause cold bias
3. The mass conservation .... headache
4. Concluding

Semi-Lagrangian modeling in NWP

Semi-Lagrangian: an established numerical technique for solving the *atmospheric transport equations*.

Many global and regional weather & climate prediction models use a semi-Lagrangian semi-implicit numerical formulation (SLSI):

- ARPEGE(MeteoFrance)/IFS(ECMWF)/ALADIN, UM(UKMO), HIRLAM, SL-AV(Russia)
- GEM(Environment Canada), GFS(NCEP)
- GSM(JMA)
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What is the reason for this?

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A very stable formulation

Semi-Lagrangian advection:

- Unconditionally stable
- Good phase speeds with little numerical dispersion
- Simplicity: the nonlinear advective terms are “absorbed” by the Lagrangian derivative operator and essentially the advection problem is turned to an interpolation one!
- Combines virtues of Lagrangian and Eulerian approach

Semi-implicit timestepping:

- Wide (unconditional) stability for fast forcing terms: gravity + acoustic waves (in non-hydrostatic models)

SL+SI: Δt determined by desired accuracy and not limited by stability

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- there is a fixed (Eulerian) grid to keep parcels evenly distributed and to accurately calculate spatial derivatives
- air parcels arrive always at fixed grid points at the end of each timestep

1960s Robert develops semi-implicit time integration for HPE NWP models

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The “economics” behind the introduction of SLSI ...

At the beginning of 1991 IFS is a spectral Eulerian model on a full Gaussian grid running at T106/L19 resolution

Resolution increase and super-computer upgrade

- A 4×CPU computer upgrade is planned
- It was estimated then that increasing resolution to T213/L31 would require 12×CPU. That was a serious underestimate!

A numerical analysis miracle

Change to SLSI numerics and to a reduced Gaussian grid came to rescue

- the planned resolution/model upgrade was made possible at the given hardware
- with the new model elapsed time for a 10d forecast at new increased resolution was reduced from $>$ 24hrs to 4 hours!

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Semi-Lagrangian advection

Let ρ be the air density and ρ_χ the density of a tracer transported by a wind field $\mathbf{V}$

Continuity equation in non-conservative form

$$\frac{D\rho_\chi}{Dt} = -\rho_\chi \nabla \cdot \mathbf{V}, \quad \frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{V}, \qquad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$$

Using specific ratios $\phi_\chi = \rho_\chi / \rho$:

$$\frac{D\phi_\chi}{Dt} = 0 \Rightarrow \frac{\phi_\chi^{t+\Delta t} - \phi_{\chi,d}^t}{\Delta t} = 0 \Rightarrow \phi_\chi^{t+\Delta t} = \phi_{\chi,d}^t$$

d: departure point (d.p.), i.e. spatial location of field at time t

- A simplified linear equation: non-linear advection terms absent
- To compute $\phi^{t+\Delta t}$: (i) find d (ii) interpolate ϕ^t to d

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Basic steps in Semi-Lagrangian algorithm

Solve $\frac{D\phi}{Dt} = 0$ given a grid $\mathbf{r}$ and a velocity field $\mathbf{V}$

1. Fluid parcels are always assumed to "arrive" on $\mathbf{r}$ at $t + \Delta t$
2. For each grid-point solve backward trajectory equation for the d.p.:

$$\frac{D\mathbf{r}}{Dt} = \mathbf{V}(\mathbf{r}, t) \Rightarrow \underbrace{\mathbf{r}^{t+\Delta t}}_{arrival\ g.p.} - \underbrace{\mathbf{r}_d^t}_{unknown\ d.p.} = \int_t^{t+\Delta t} \mathbf{V}(\mathbf{r}, t) dt$$

3. Remap (interpolate) ϕ to $\mathbf{r_d}$ (Lagrangian grid) to obtain

$$\phi^{t+\Delta t} = \phi_d^t$$

Usual techniques employed

- Midpoint rule and fixed point iteration for solving trajectory equation
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Computing trajectories

"Classic" scheme: midpoint using time extrapolation

Midpoint discretization:

$$\mathbf{r} - \mathbf{r_d} = \Delta t\, \mathbf{V}\left(\frac{\mathbf{r}+\mathbf{r_d}}{2}, t + \frac{\Delta t}{2}\right), \quad \mathbf{V} = (u, v, \dot{\eta})$$

1. Extrapolate velocity field: $\mathbf{V}^{t+\Delta t/2} = 1.5\mathbf{V}^{t} - 0.5\mathbf{V}^{t-\Delta t}$

2. $$\left\{\begin{array}{l} \mathbf{r_d}^{(0)} = \mathbf{r} \\ \text{Interpolate } \mathbf{V}^{t+\Delta t/2} \text{ to } \mathbf{r_M} \equiv 0.5[\mathbf{r} + \mathbf{r}_\mathbf{d}^{(\ell-1)}] \\ \text{Update: } \mathbf{r_d}^{(\ell)} = \mathbf{r} - \Delta t\, \mathbf{V}^{t+\Delta t/2}\big|_{\mathbf{r_M}} \end{array}\right\}, \ \ell = 1, 2, \ldots$$

SLSI time-stepping in IFS

General adiabatic prognostic equation

$$\frac{DX}{Dt} = F. \quad \text{Let} \;\; F = N + L, \;\; N \equiv F - L \;\; \text{where,}$$

L: fast terms linearised on a reference state, N: nonlinear slow terms

- Fast linear terms L are treated implicitly
- Non-linear terms can be extrapolated at $t + \Delta t/2$ using:

$$N^{t+\Delta t/2} \approx 1.5N^{t} - 0.5N^{t-\Delta t}$$

2nd order two time-level discretization

$$\frac{X^{t+\Delta t} - X_d^t}{\Delta t} = \frac{1}{2}\left(L_d^t + L^{t+\Delta t}\right) + N_M^{t+\Delta t/2}, \quad M: \text{trajectory midpoint}$$

- Prognostic variables are eliminated to derive a constant coefficient Helmholtz equation for D: *cheap and easy to solve in spectral space*

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Iterative Centred Implicit SLSI solver

- Extrapolation results to a weak instability Durran & Reinecke (MWR 2003), Cordero et al (QJRMS, 2005)
- This is mostly noticed in strong jet areas in the stratosphere

- An iterative approach (P. Bénard, MWR 2003) can be used to obtain a stable semi-implicit formulation:
  - Once a predictor for prognostic variable X becomes available

$$X^{(P)} \approx X^{t+\Delta t}, \quad X^{(P)} : \text{solution at the end of an iteration}$$

then time-interpolation can be used instead of extrapolation:

Use $\mathbf{V}^{t+\Delta t/2} = 0.5 \left[\mathbf{V}^{(P)} + \mathbf{V}^{t} \right]$ in trajectory iterations

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SETTLS: stable extrapolation (Hortal, QJRMS 2002)

Assume $\dfrac{dX}{dt} = R$ and expand:

$$X(t+\Delta t) \approx X_d(t) + \Delta t \overbrace{\left(\frac{dX}{dt}\right)_d}^{R_d(t)} + \frac{\Delta t^2}{2} \overbrace{\left(\frac{d^2X}{dt^2}\right)_{AV}}^{\frac{R(t)-R_d(t-\Delta t)}{\Delta t}}$$

$$\Downarrow$$

$$X(t+\Delta t) = X_d(t) + \frac{\Delta t}{2}\{R(t) + [2R(t) - R(t-\Delta t)]_d\}$$

Use same formula for:

- Trajectories: $r_d^{(\ell)} = r - 0.5\Delta t \left[V^t + \left(2V^t - V^{t-\Delta t}\right)\Big|_{d^{(\ell-1)}} \right]$
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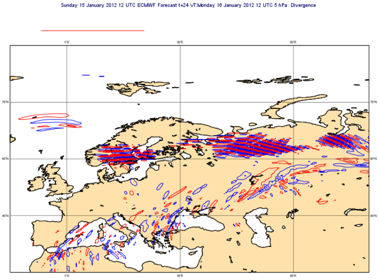
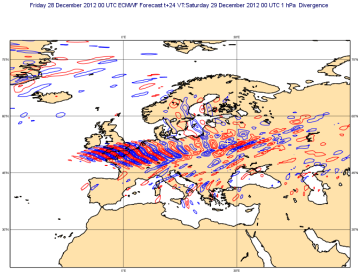
Stratospheric noise

- SETTLS greatly improves stability, however, occasionally, solution becomes noisy in the upper atmosphere (near strong jets)
- Testing shows that noise originates from the calculation of the vertical component of the departure point
- Until recently solution used “smoothing of vertical velocities” (least square interpolation)



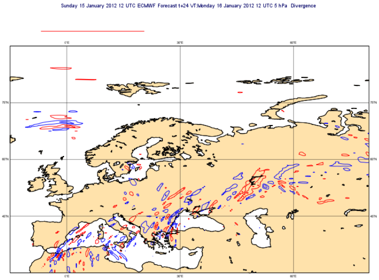
(a) 5hPa D at T+24 (16/01/12)



(b) 1hPa D at T+24 (29/12/12)

Techniques to solve stratospheric noise problem

- Iterative scheme (ICI) - too expensive
- Off-centring - damps gravity waves/impact on accuracy
- Smoothing vertical velocities - impact on accuracy (temperature)
- Using "at selected grid-points" non-extrapolated trajectory scheme (SETTLS limiter) for computing vertical component of the d.p.



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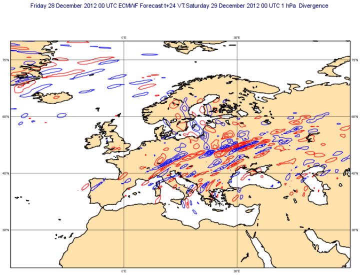
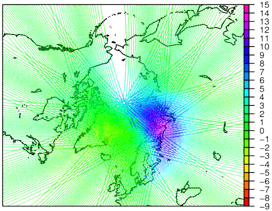


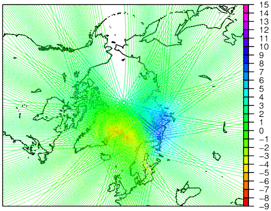
(d) 1hPa D at T+24 (29/12/12)

Sudden stratospheric warming episode 15/01/2012

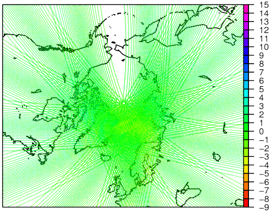
instabilities → noisy solution upper atmosphere → rejection of satellite obs



(e) Control FC



(f) Smoothing $\dot{\eta}$



(g) SETTLS traj limiter

SETTLS Limiter:

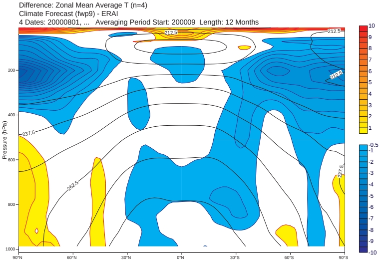
$$\eta_d = \begin{cases} \eta - \frac{\Delta t}{2}\left(\dot{\eta}^t + \dot{\eta}_d^t\right), & \left|\nabla_t \dot{\eta}^t\right| > \beta \overline{|\dot{\eta}|}^{\,t,t-\Delta t} \\ \text{SETTLS}, & \text{otherwise} \end{cases}$$

$$0 < \beta < 2, \quad \nabla_t \dot{\eta}^t = \dot{\eta}^t - \dot{\eta}^{t-\Delta t}$$

Outline

Extra-tropical cold bias

{Results from cubic QM
RMS norm FC-ERAI} →



Stenke et all (Clim Dyn 2008)

- Water vapor (q) overestimation by SL models in lower extratropical stratosphere leads to radiative cooling and noticeable cold bias
- "Considerable numerical meridional diffusion in presence of sharp gradients"
  - Interpolation in the horizontal is acting on model levels intersecting downward sloping tropopause (from tropics to extra-tropics)
- No bias in pure Lagrangian models (non-diffusive)

Cold bias investigations with IFS

A dynamically sensitive problem

Dynamical model components affecting cold bias

- Large sensitivity to (horizontal part) of q-interpolation
  - the more diffusive the interpolation the worst
  - switching on/off quasi-monotone limiter
- Large sensitivity wrt to d.p. calculation
- Moderately sensitive wrt to timestep
- Moderately sensitive wrt to semi-implicit options (ICI, off-centring)
- Problem persists at low and high resolution

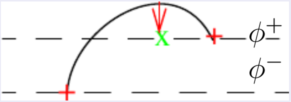
Current results suggest that bias can be reduced by improving interpolation scheme and accuracy of d.p. calculation

Quasi-monotone limiting in cubic interpolation

Bermejo & Staniforth limiter (MWR, 1992)

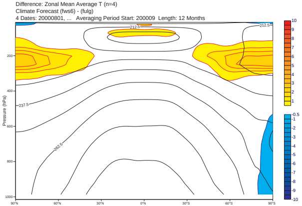
$$\phi_d = \max(\min(\phi_d, \phi^+), \phi^-), \quad \phi^+ = \max_{i \in \{N_i\}} \{\phi_i\},\ \phi^- = \min_{i \in \{N_i\}} \{\phi_i\}$$

$$N_i = \{\text{set of neighbouring points surounding d}\}$$

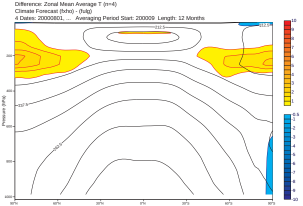


- IFS qm-interpolation in (λ, θ, η) coordinates:
  Interp in λ and limit $\rightarrow$ Interp in θ and limit $\rightarrow$ Interp in η and limit
- The limiter can also be applied at the very end of interpolation:
  Interp in λ $\rightarrow$ Interp in θ $\rightarrow$ Interp in η $\rightarrow$ limit in (λ, θ, η)
- Limiting at the end seems to be beneficial for the cold bias

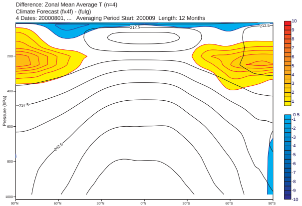
Differences from control FC: testing QM limiter



(h) QM off / neg fixer on



(i) Bermejo & Staniforth QM

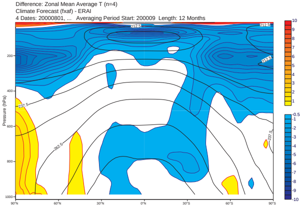


←

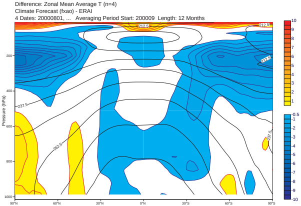
1. Point i at lev k is limited.
2. Mass removed/added by limiter added/removed at point i, $k+1$
3. Point $i, k+1$ is limited ...

(j) QM + vert quasi-conserv filter

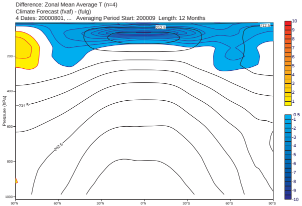
Trajectory sensitivities



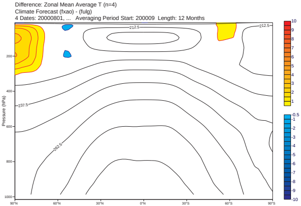
(k) smoothing $\dot{\eta}$ - ERAI



(l) SETTLS lim - ERAI



(m) smoothing $\dot{\eta}$ - CNTL fc



(n) SETTLS limiter - CNTL fc

Outline

Mass Conservation

Mass conservation becomes increasingly important

- Has always been for long (climate) integrations
- Moist tracer conservation important for microphysics/convection
- Increasing importance of "environmental/chemical" forecasts

Eulerian flux-form models

Conservation straightforward: change of mass in volume ΔA = total flux through its faces ΔS from neighbouring grid-boxes

$$\frac{\partial}{\partial t}\int_{\Delta A}\rho dV = -\int_{\Delta A}\nabla\cdot(\rho\mathbf{U})dV \Rightarrow \overline{\rho}^{t+\Delta t} - \overline{\rho}^{t} = \frac{\Delta t}{\Delta A}\int_{\Delta S}\rho\mathbf{U}\cdot\eta dS$$

Semi-Lagrangian schemes are not formally conserving: equations applied on grid-points rather than volumes - there is no flux-counting

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Accurate continuity discretization in IFS

$$\frac{D}{Dt}(\ln p_s) = RHS,$$

Split

$$\ln p_s = l' + l^*$$

where $l^* = \phi_s / \left(R_d \overline{T}\right)$ the orography time-independent part and solve

$$\frac{Dl'}{Dt} = [RHS] + \frac{1}{R_d \overline{\overline{T}}} \mathbf{V}_h \cdot \nabla \phi_s$$

Benefits of this formulation:

- Advected field is smoother and therefore better air mass conservation due to reduced interpolation error
- Aleviates orographic resonance problem

Global mass conservation error in IFS

In NWP forecasts we have been not paying too much attention in mass conservation. Why?

- An accurate numerical scheme may not be mass conserving but its mass conservation error should be small
- In a 10 day IFS forecast at T1279 horizontal resolution total air mass approximately increasing by 0.015% of its initial value.

- Global conservation errors in tracer advection are larger and depend on the smoothness of the field, i.e. smoother fields such as ozone and specific humidity have much smaller conservation errors than fields with sharp features such as cloud fields
- Global tracer-mass conservation error reduces with increasing resolution
- Not reduced when timestep is reduced

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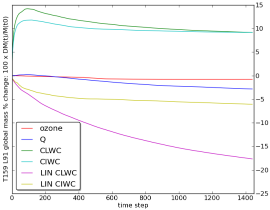
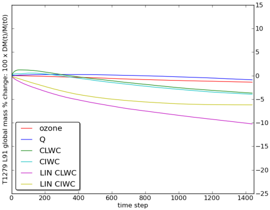
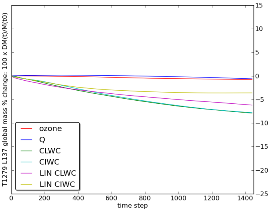
Timeseries of global tracer-mass conservation error



(o) T159 L91



(p) T1279 L91



(q) T1279 L137

Approaches in improving mass conservation

How to improve mass conservation error, particularly for tracers?

Interpolation

- Improving interpolation schemes. In IFS quasi-cubic Lagrange with a quasi-monotone filter is used. Alternative ones have been recently tested:
  - cubic splines in the vertical: very good for smooth fields such as ozone but worst for rough fields
  - cubic Hermite in the vertical with derivative limiting: improved conservation in specific humidity
  - improving quasi-monotone limiters can also have positive impact

Mass conservative advection schemes

- mass fixers
- inherently conserving schemes

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SL mass conservative advection schemes

Global Mass Fixers

- Low cost algorithms
- Easy to implement in existing models: no need to change model formulation
- a-posterior fixes: diagnose global mass conservation error and correct the interpolated field to ensure total mass remains unchanged
- Criticism: they are somewhat ad-hoc and global in nature

Inherently conserving

- Theoretically desirable schemes: both local and global conservation is achieved for tracers and air mass without inserting artificial fixes
- They can be very expensive and implementation in an operational model is a complex task

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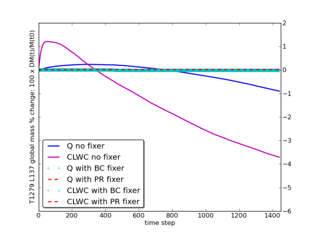
Mass Fixers

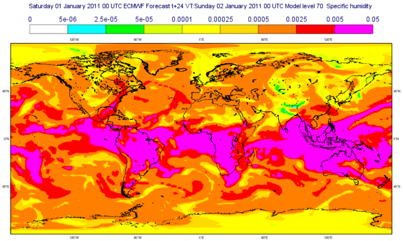
- Proportional fixers: adjust each g.p. value by the same proportion
- There are more sophisticated approaches which correct locally (very small corrections when solution is smooth, larger when not):
  - quasi-monotone Bermejo & Conde fixer (MWR 2002)
  - quasi-monotone Priestley fixer (MWR 1993)
  - Mac Gregor's fixer (C-CAM, CSIRO Tech Rep 70)
  - Zerroukat fixer (JCP, 2010)

The above fixers have been recently implemented in IFS

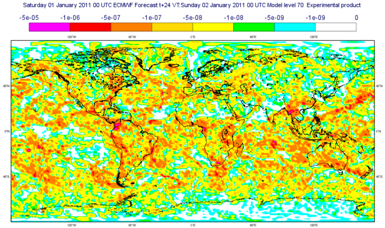


Mass Fixer	CPU overhead (5 tracers)
BC	1%
PRqm	2%
PR	3.5%
JMG	0.75%
Ze	0.85%

Local behaviour of Bermejo & Conde fixer



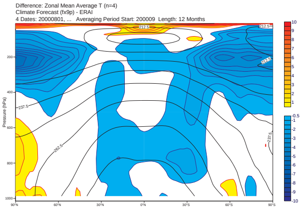
(r) T+24 q field at ≈ 700 hPa



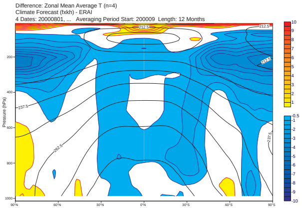
(s) BC fixer correction

- Corrections are concentrated in areas of large gradients
- The quality of forecast is maintained (verification scores neutral)

Long integrations with fixers



(t) Control - no fixer



(u) BC fixer on all

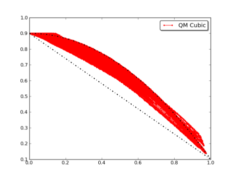
RMS norm of FC-ERAI

EXP ID	TR 200	TR 700	TR 925
CNTL	1.4085	0.7214	0.7881
BC fixer	1.2825	0.6812	0.7795
MacGregor fixer	1.3006	0.6778	0.7596

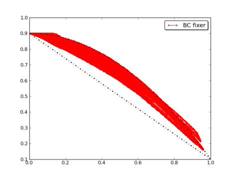
EXP ID	NH 200	NH 700	SH 200	SH 700
CNTL	1.9332	0.9664	1.7280	0.8341
BC fixer	1.9730	0.9414	1.6726	0.8258
MacGregor fixer	2.0665	0.9645	1.6120	0.7906

Preserving functional relationships between tracers

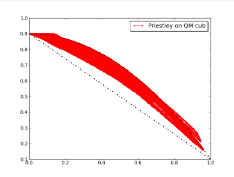
3-d version of DCMIP case 11: $q_2 = 0.9 - 0.8q_1^2$



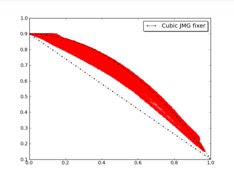
(v) qm cubic



(w) BC fixer



(x) PR fixer



(y) JMG fixer

- Adding the fixers didn't distort functional relationship

Summary on mass fixers

- Global mass conservation at low cost and no deterioration of forecast quality
- They correct locally where interpolation error is *expected* to be larger
  - difference between high order and low order interpolation scheme is used to construct a weight which determines how much to correct
- They can preserve monotonicity or positive-definitiness
- When applied on point sources they can be diffusive (they remove mass due to large gains)
- Work underway to determine impact on other chemical tracers
- No matter how good a fixer algorithm can be will never be "perfect":
  - cannot be truly locally conserving
  - inconsistent transport of different species

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Inherently conserving schemes: SLICE

Finite volume semi-Lagrangian continuity:

$$\frac{D}{Dt}\int_{A(t)} \psi dA = 0 \Rightarrow \int_{A} \overline{\psi}^{n+1} dA = \int_{A_d} \overline{\psi}^{n} dA, \quad \psi = \text{air/tracer density}$$

SLICE-3D (Zerroukat & Allen QJRMS, 2012)

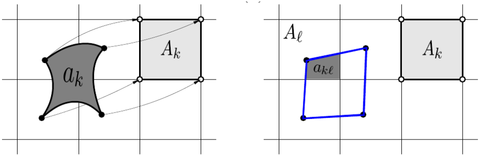
$$\overline{\psi}^{n+1} = \frac{M_d^t}{A}, \quad M_d^t = \int_{A_d} \overline{\psi}^{n} dA$$

No need to compute Lagrangian (departure) volume A_d. Instead:

1. Compute departure points as usual to define Lagrangian control volumes (CV) corresponding to Eulerian CVs
2. Remap: compute mass M_d^n of LCVs using 1-dimensional cascade interpolation at each direction

SLICE is available as an option in new UKMO ENDGame model

CSLAM (Lauritzen, JCP 2010)



$$\alpha_{k\ell} = \alpha_k \cap A_\ell, \quad \ell = 1, 2, \ldots, L_k$$

$$\overline{\psi}_k^{n+1} = \frac{1}{A_k} \overline{\psi_{k,d}}^n \alpha_k, \quad \overline{\psi}_{k,d}^n \alpha_k = \sum_{\ell=1}^{L_k} \int\int_{\alpha_{k\ell}} f_\ell dA = \sum_{\ell=1} \sum_{i+j\leq 2} c_\ell^{(i,j)} w_{k\ell}^{(i,j)}$$

- For each Eulerian grid cell find corresponding departure (Lagrangian) grid cell by computing departure points of Eulerian vertices
- Continuous sub-grid-scale representation f_ℓ of ψ with mass conservation as an integral constraint:

$$\int\int_{A_\ell} f_\ell dA = \overline{\psi}_\ell A_\ell, \quad \ell = 1, 2, \ldots, L_k$$

The difficulty with inherently conserving schemes

- Computational expense is a limiting factor for their application in operational meteorology
- However, they may be competitive for the multiple-tracer advection problem
  - e.g. CSLAM is currently developed as an offline transport package for multi-tracer advection in climate model CAM-SE
  - also see LMCSL 3-D (Sorensen, GeoSci. Model Dev. 2013) for HIRLAM
- Performance of such schemes in presence of complex terrain
  - Departure volumes are computed using simple algorithms not coupled with continuity: along the trajectory the gas volume may deform/compress/expand
  - Alternative (expensive) trajectory calculations: Thuburn et al (QJRMS, 2010), Cossette & Smolarkiewicz (Computer & Fluids 2011)
  - Accurate (no staright line) representations of departure cell boundaries are even more expensive to compute

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Outline

1. Semi-Lagrangian technique and history
2. Semi-Lagrangian numerics in the upper atmosphere
   - Trajectory equation and numerical noise
   - Extratropical tropopause cold bias
3. The mass conservation .... headache
4. Concluding

A view of the future of SLSI techniques

High resolution global NWP models on massively parallel machines

- Efficiency of (any) advection scheme on a regular lat/lon grid on the sphere deteriorates: convergence of meridionals, anisotropy near poles
- SLSI and Eulerian SI advection schemes on quasi-uniform grids (cubed sphere, icosahedral, reduced Gaussian etc) are in better position provided that:
  - For semi-implicit types efficient elliptic solver is available (multigrid?)
  - They are mass conservative
- For multi-tracer applications even expensive inherently conserving SL may be more efficient comparing to Eulerian flux-form
- Spectral transform SLSI: critical issue cost of transpositions + mass conservation

Climate models

- Likely that existing climate models built on SLSI techniques will continue being used in climate modeling for long time

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Future work plans for the ECMWF SL scheme

- Efforts to improve the IFS SLSI scheme continue
- Focusing on areas such as:
  - Mass conservation
  - Investigating interpolation techniques and limiters
  - Numerical schemes for solving SL trajectory equations
  - Model biases due to dynamics such as the cold bias

Thank you for your attention!

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  - Mass conservation
  - Investigating interpolation techniques and limiters
  - Numerical schemes for solving SL trajectory equations
  - Model biases due to dynamics such as the cold bias

Thank you for your attention!