Transport schemes for weather and climate

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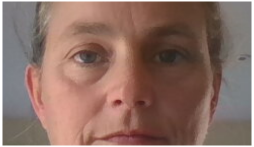


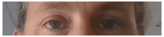
What is your favourite transport scheme?
http://www.met.reading.ac.uk/~sws02hs/talks/2020/ECMWFseminar/Weller_print.pdf

Atmospheric Transport/Advection

Pollution Plumes

- Constituents of the atmosphere are transported long distances by the winds
- Transport does not generate new extrema
- Transport does not create or destroy material
- Climate models need to transport hundreds of related species

A search on Google Scholar for “numerical advection schemes” returns 144,000 results



Numerical Methods for Advection

Two forms of the advection equation to find species ϕ

$$\frac{\partial \phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = 0 \qquad\qquad \frac{\partial \rho\phi}{\partial t} + \nabla\cdot(\rho\phi\mathbf{u}) = 0$$

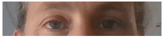
where $\mathbf{u}$ is the wind speed (given) and ρ is the air density. These are equivalent because of the continuity equation for ρ:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$$

Consistency with Continuity

If you use a different numerical method for ρ and $\rho\phi$ then ϕ can end up in the wrong place.

For example if temperature, moisture and density are advected inconsistently then it will rain in the wrong place.



Classes of Advection Scheme

Eulerian

Also called:
- Method of lines
- Split space-time

Discretise space and time separately

Spatial discretisation could be:

- FD: Finite difference
- FV: Finite volume
- FE: Finite element
- SE: Spectral Element
- DG: Discontinous Galerkin
- Spectral ...

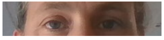
Time stepping could be:

- RK: Runge-Kutta (multi-stage) (implicit or explicit)
- Multi-step (implicit or explicit)

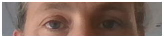
Semi-Lagrangian includes:

- Interpolating semi-Lagrangian
  - Values set by interpolating onto upstream points
  - not conservative
  - large time steps
  - usually finite difference
- Conservative mapping
  - map onto upstream departure volumes
- Flux-form semi-Lagrangian (FFSL or Forward in time or swept area or volume)
  - fluxes calculated over a swept upstream volume
  - usually finite volume

Who uses what? ...



Model/Modelling centre	**Version**	**Numerical method**
UK Met Office	Current	Semi-Lagrangian (not conservative)
	Next	Finite volume - FFSL or Eulerian?
ECMWF	Current	Semi-Lagrangian (not conservative)
	Next	?
Environment Canada		Semi-Lagrangian (not conservative)
NOAA		Flux form semi-Lagrangian (FV)
NCAR CAM	FV	Flux form semi-Lagrangian (FV)
	SE	Spectral Element (no upwinding, Eulerian)
FV3 (NOAA and GFDL)		Flux form semi-Lagrangian (FV)
NUMA-Neptune (US Navy)	Next	Discontinuous Galerkin (Eulerian)
NICAM (A Japanese model)		Flux form semi-Lagrangian (FV)
MPAS (to replace WRF)		Upwinded finite volume (Eulerian)
ICON		Flux form semi-Lagrangian (FV)
DYNAMICO		Flux form semi-Lagrangian (FV)
CSU		Upwinded finite volume (Eulerian)



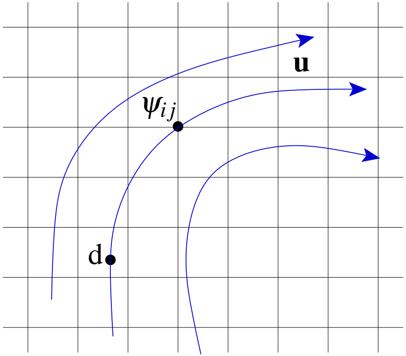
Semi-Lagrangian

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = 0$$

solved as

$$\psi_{ij}^{n+1} = \psi_d^n$$

where n is the time level, ij is the position on the grid and d is the departure point.
Interpolate to find ψ_d at the departure point from surrounding values on the grid.



Advantages and Disadvantages

☺ Stable and accurate for very long time steps

☺ Cost and accuracy not strongly related to time step

☹ ψ is not conserved

Conservative (or cell integrated) Semi-Lagrangian

$$\frac{\partial \rho \psi}{\partial t} + \nabla \cdot \rho \psi \mathbf{u} = 0$$

solved as

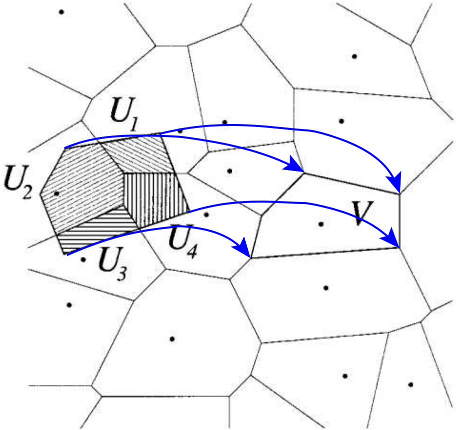
$$(\rho \psi)_V^{n+1} = \sum_i (\rho \psi)_{U_i}^n$$

Advantages and Disadvantages

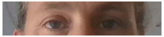
☺ Stable for very long time steps

☹ Not sure about accuracy

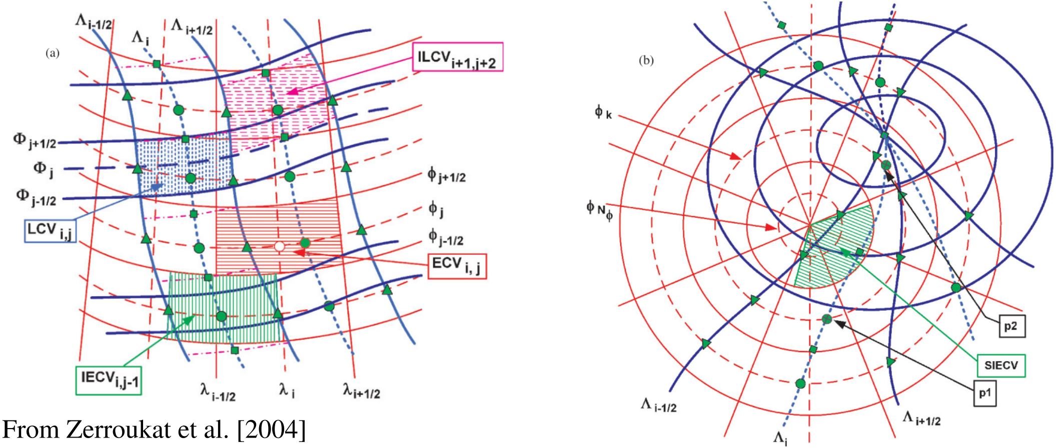
☹ complicated and expensive



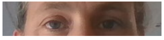
Adapted from Iske and Kaser [2004]



Conservative (cell integrated) Semi-Lagrangian



From Zerroukat et al. [2004]



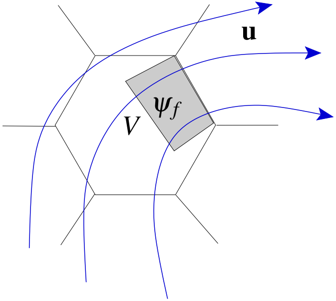
Flux Form Semi-Lagrangian

Also known as:

- Forward in time
- Swept area/volume
- Space-time

Examples:

- PPM (piecewise parabolic method)
- Lin and Rood
- COSMIC
- Lax-Wendroff.
- CSLAM Harris et al. [2011]



☺ Conservative

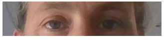
☹ Only used with small time-steps ($c < 1$)

$$\frac{\partial \psi}{\partial t} + \nabla \cdot \psi \mathbf{u} = 0$$

solved as

$$\psi^{n+1} = \psi^{n} - \frac{1}{V} \sum_{\text{faces}} \psi_f \mathbf{u} \cdot \mathbf{S}$$

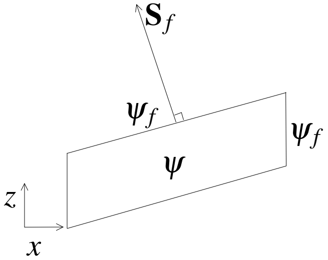
where ψ_f is integrated over the volume swept through the face during one time step.



Eulerian

- Combined any explicit or implicit time stepping scheme with any spatial discretisation
- Explicit $\implies$ time step restrictions

For Example Finite Volume Eulerian



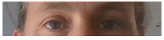
$$\frac{\partial \psi}{\partial t} = -\nabla \psi \mathbf{u} = -\frac{1}{V} \sum_{f \in \text{faces}} \psi_f \mathbf{u}_f \cdot \mathbf{S}_f$$

Calculate fluxes at faces, $\psi_f \mathbf{u}_f \cdot \mathbf{S}_f$ at any time, t, from values at cell centres, ψ, at exactly the same time:

$$\frac{1}{V} \sum_{f \in \text{faces}} \psi_f \mathbf{u}_f \cdot \mathbf{S}_f(t) \approx \sum_{\text{cells, } i} w_i \psi_i(t)$$

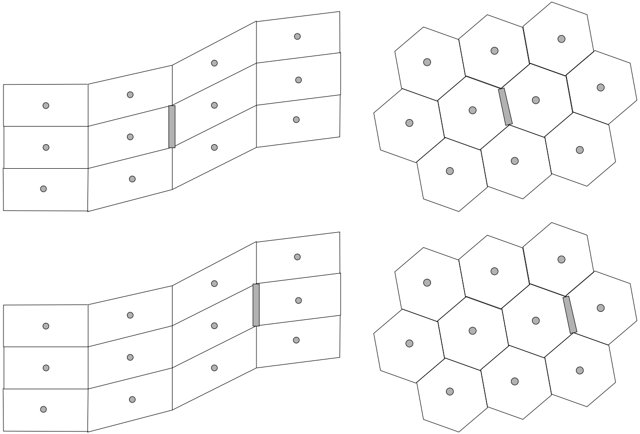
Then use a multi-step or multi-stage (RK) scheme to discretise the ordinary differential equation:

$$\frac{d\psi}{dt} = -\sum_{\text{cells, } i} w_i \psi_i(t)$$

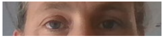


Centered or Upwinded Stencils for Spatial Eulerian discretisation

- Interpolate from cell centres onto faces by fitting a 1d or 2d polynomial over the stencil

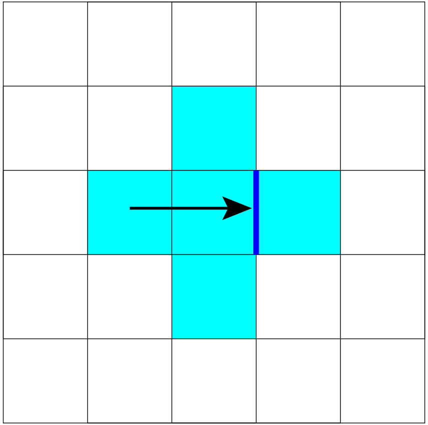


Eg. Shaw, Weller, Methven, and Davies [2017]

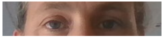


Quiz

For Eulerian advection in 2D on a grid of squares, for any edge, if the stencil consists of the upwind cell and all the edge neighbours of the upwind cell, how many possible stencils are there depending on the wind direction?

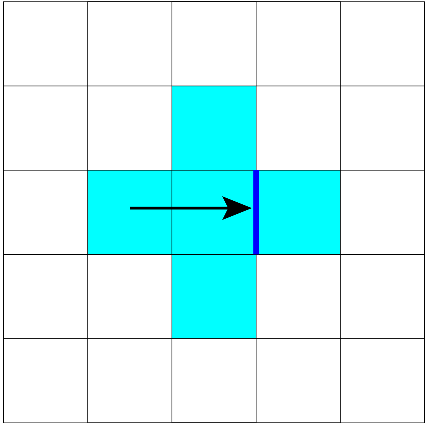


- 1
- 2
- 3
- 4
- 5
- more

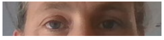


Quiz

For Eulerian advection in 2D on a grid of squares, for a stencil of 5 cells, how many multiplies are needed to interpolate onto the edge?

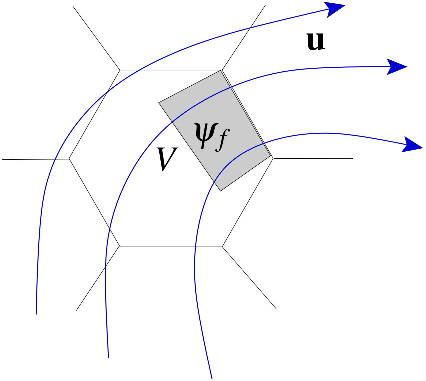


- 1
- 2
- 3
- 4
- 5
- more

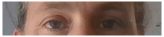


Quiz

For Flux for semi-Lagrangian advection in 2D on a grid of hexagons, for a stencil of 7 cells, how many multiplies are needed to interpolate map onto the edge?



- 7
- 14
- 21
- 8
- 49
- other



RK2 Explicit Time Stepping

To solve

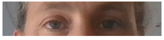
$$\frac{d\psi}{dt} = -F(\psi, t)$$

between time $t^n = n\Delta t$ and t^{n+1} with 2 iterations:

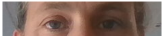
$$\begin{aligned} \psi' &= \psi^n - \Delta t F(\psi^n, t^n) \\ \psi^{n+1} &= \psi^n - \Delta t \left\{ (1-\alpha) F(\psi^n, t^n) + \alpha F\left(\psi', t^{n+1}\right) \right\} \end{aligned}$$

$\alpha = 1/2 \implies$ 2nd order accuracy.

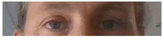
Use > 2 iterations for better stability.



Deformational Advection using Explicit Eulerian Advection - Cubic Centred

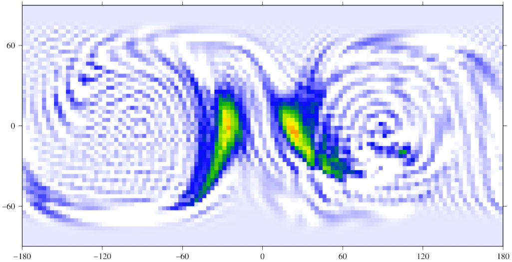


Deformational Advection using Explicit Eulerian Advection - Cubic Upwinded



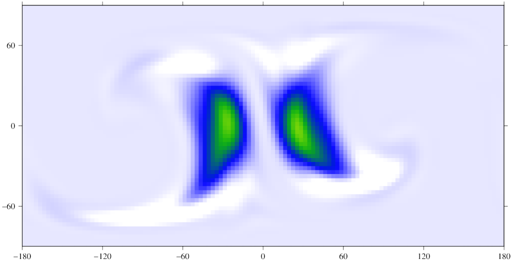
Deformational Advection using Explicit Eulerian Advection

Cubic centred



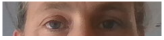
min = −0.515501   max = 0.857344

Cubic upwind



min = −0.0981133   max = 0.610054

The upwind stencil reduces dispersion errors but there are still undershoots.



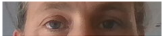
Linear and Non-linear Advection Schemes

Linear

- Values at the next time step linearly dependent on previous values
- Can be 1st, 2nd, 3rd ... order accurate
- Can be Eulerian, semi-Lagrangian, FD, FV, FE ...
- Can be implicit or explicit
- Godunov's theorem – New extrema will be generated if order > first

Non-linear

- Values at the next time step non-linearly dependent on previous values
- Order of accuracy locally reduced to avoid generating oscillations
- Accuracy depends on solution
- Can only be explicit



MPDATA [Smolarkiewicz and Margolin, 1998]

Multidimensional Positive Definite Advection Transport Algorithm

- First solve the advection equation

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(u\psi) = 0 \tag{1}$$

using first-order upwind (the solution is bounded but diffusive):

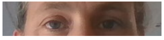
$$\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} + u\frac{\psi_j^n - \psi_{j-1}^n}{\Delta x} = 0 \tag{2}$$

- This is a second-order approximation to the advection diffusion equation:

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(u\psi) = \frac{\partial}{\partial x}\left(K\frac{\partial \Psi}{\partial x}\right) \tag{3}$$

where $K = u\frac{\Delta x - u\Delta t}{2}$. $K\frac{\partial \Psi}{\partial x}$ can be written as a flux of ψ:

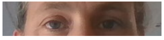
$$K\frac{\partial \Psi}{\partial x} = v\Psi \qquad \text{where v is the anti-diffusive velocity.} \tag{4}$$



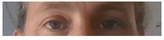
- Solve

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(v\psi) = 0 \tag{5}$$

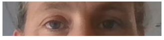
so that advection by the anti-diffusive velocity removes the diffusion. Solve with first-order upwind to ensure positivity.



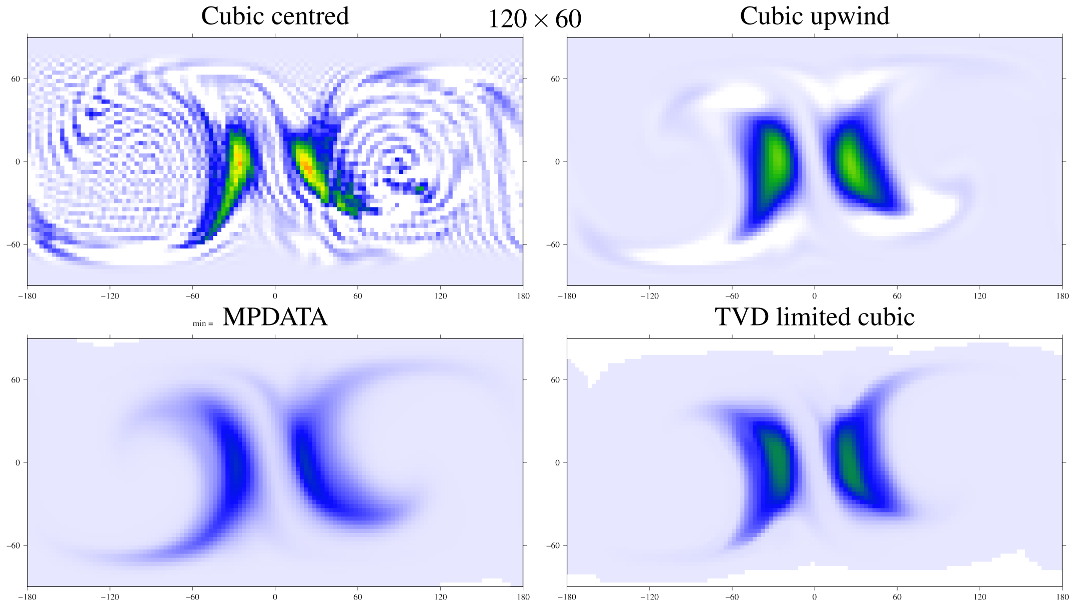
Deformational Advection using MPDATA



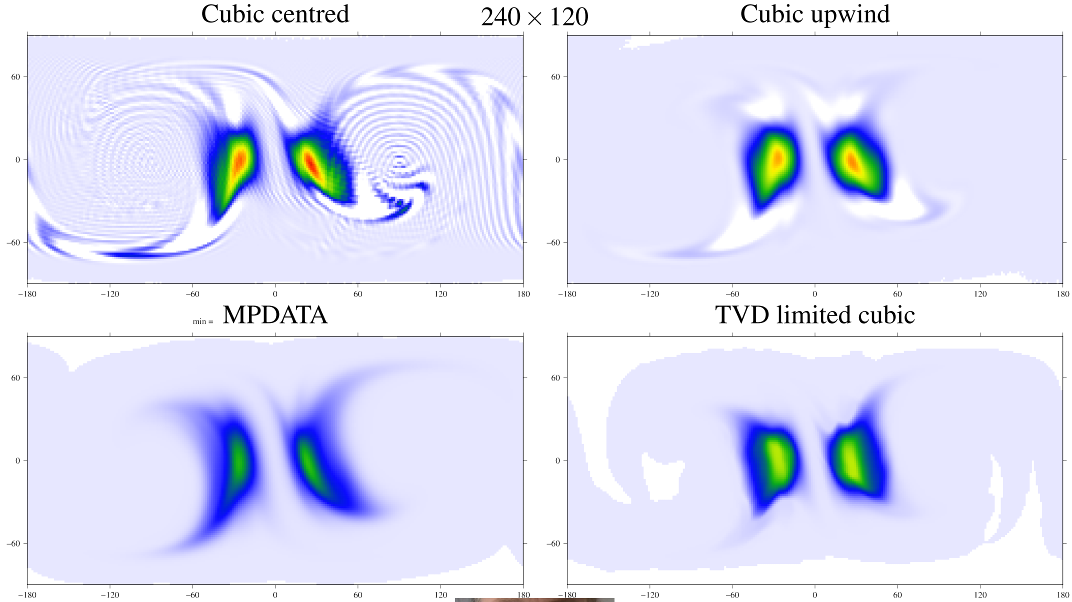
Deformational Advection using Explicit Eulerian Advection – cubic with a TVD limiter

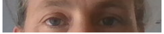


120×60


Cubic centred
Cubic upwind
MPDATA
TVD limited cubic
60
0
−60
−180
−120
−60
0
60
120
180
min =
min = 2.6809e−17 max = 0.304901
min = −1.13344e−11 max = 0.429408

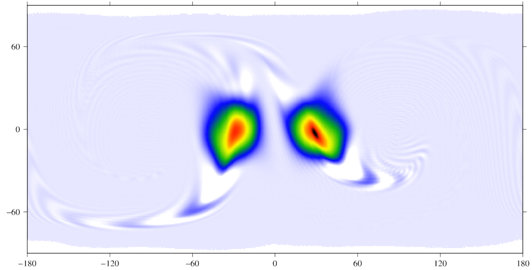
240 × 120


Cubic centred
Cubic upwind
MPDATA
TVD limited cubic
60
0
−60
−180
−120
−60
0
60
120
180
min =
min = 1.1192e−30 max = 0.536001
min = −3.16495e−13 max = 0.686534

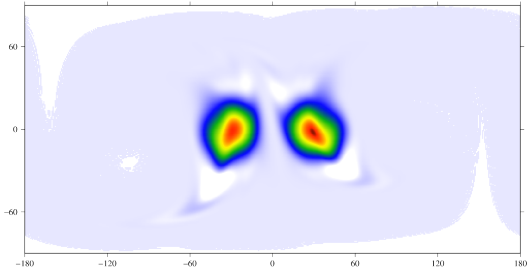


480 × 240

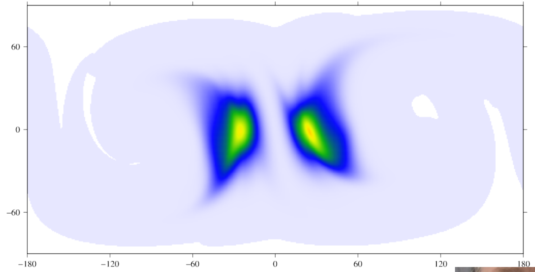
Cubic centred



Cubic upwind

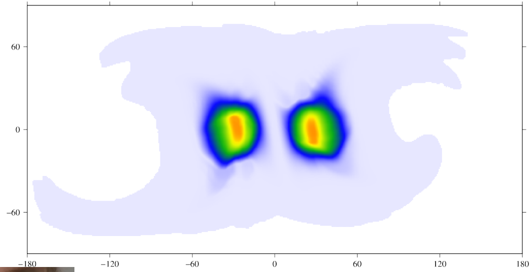


min = MPDATA



min = 1.98048e−55 max = 0.800021

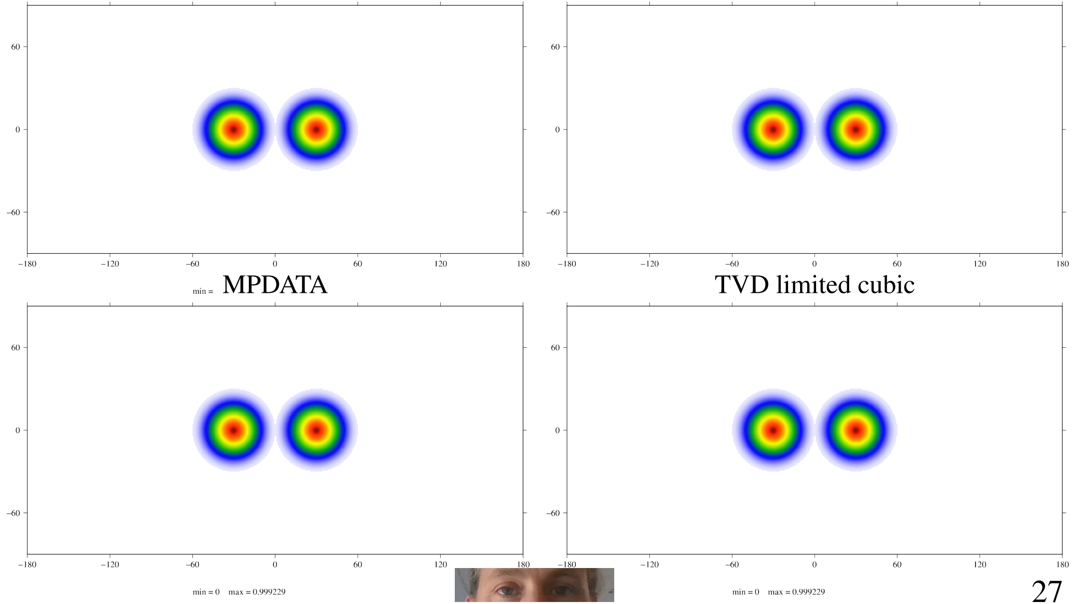
TVD limited cubic



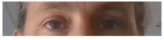
min = −3.18499e−17 max = 0.865926

Initial conditions

Cubic centred — Cubic upwind — MPDATA — TVD limited cubic

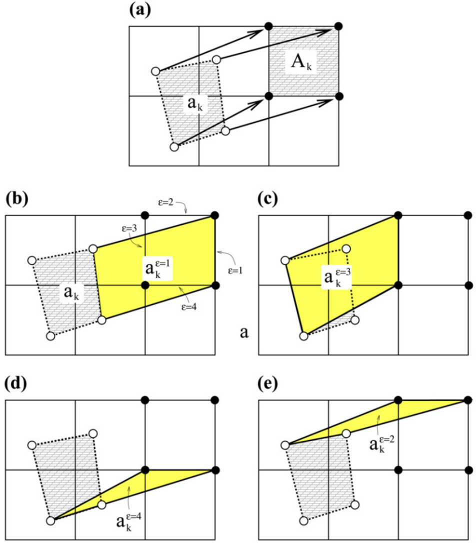


When the Time step is too large for an Explicit Scheme (Courant number = $u\Delta t/\Delta x < 2$)

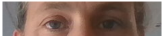


Stability for Long Time Steps

- Semi-Lagrangian
  - Not conservative
- Cell integrated semi-Lagrangian
  - Complicated and expensive
- Flux-form semi-Lagrangian
  - Ideal? On lat-lon grids
- Implicit Eulerian
  - Matrix solvers are expensive
  - Looses accuracy for large time steps
  - Largely ignored in atmospheric modelling
  - But
    - ∗ Conservative
    - ∗ Simple on any grid of the sphere
    - ∗ Cost may be manageable



From Harris et al. [2011]

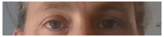


Order Barriers for Implicit Runge-Kutta Methods

Implicit time-stepping for advection may be unconditionally stable (stable for all time steps) BUT

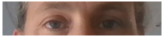
- Only linear schemes can be solved implicitly
- If Courant number $c \gtrsim 1$ and spatial discretisation order > 1 then matrix is not diagonally dominant
- Theorem of Spijker: Any Runge–Kutta method of order $p > 1$ has a finite radius of absolute monotonicity
  - ie if temporal order > 1 then oscillations will be generated for large Courant number c

$\therefore$ **My conclusion:** A non-linear, bounded spatio-temporal discretisation needs to be an explicit correction on first-order upwind in space, first-order implicit in time.



Use of Implicit Advection in Atmospheric Models

- Chen, Weller, Pring, and Shaw [2017] compared Implicit Eulerian with FFSL linear advection on a 2D vertical slice and a distorted 2d mesh.
- Jähn et al. [2015] used implicit advection in small cut cells and explicit elsewhere
- May and Berger [2017] used implicit advection in small cut cells and explicit elsewhere
- Wicker and Skamarock [2020] use implicit advection in the vertical only where needed (vigorous convection)



Implicit/Explicit Runge-Kutta Time Stepping (Deferred Correction)

To solve

$$\frac{\partial \psi}{\partial t} = -\nabla \cdot \psi \mathbf{u}$$

define two spatial discretisations:

$$\begin{aligned} \nabla \cdot \psi \mathbf{u} &= L + O(\Delta x) \\ \nabla \cdot \psi \mathbf{u} &= H + O(\Delta x^p) = L + H_{\text{corr}} + O(\Delta x^p) \end{aligned}$$

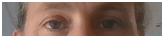
then

$$\begin{aligned} \psi' &= \psi^n - \Delta t L' \\ \psi^{n+1} &= \psi' - \Delta t \left\{ (1-\alpha) H^n_{\text{corr}} + \alpha H'_{\text{corr}} \right\} \end{aligned}$$

$\alpha = 1/2 \implies$ 2nd order accuracy.

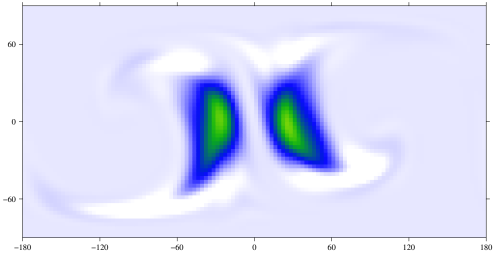
Use > 2 iterations for better stability.

[Chen et al., 2017]

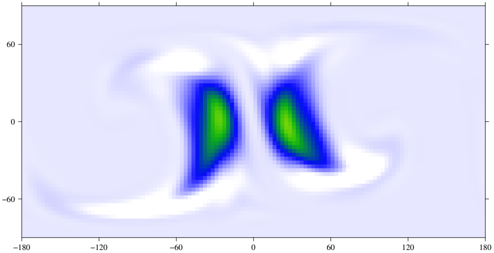


Implicit and Explicit in Time with cubic upwind in space

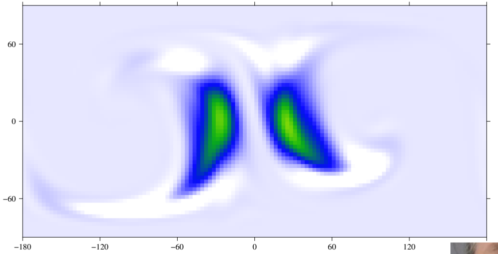
Explicit, $c < 1$



Implicit, $c < 1$

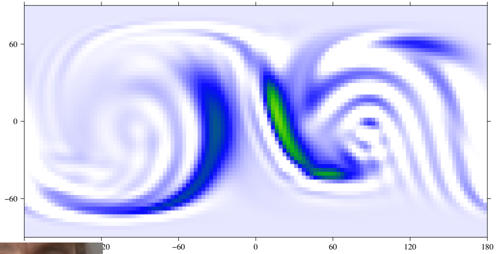


Implicit, $c < 2$

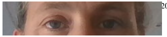


min = −0.126137 max = 0.618706

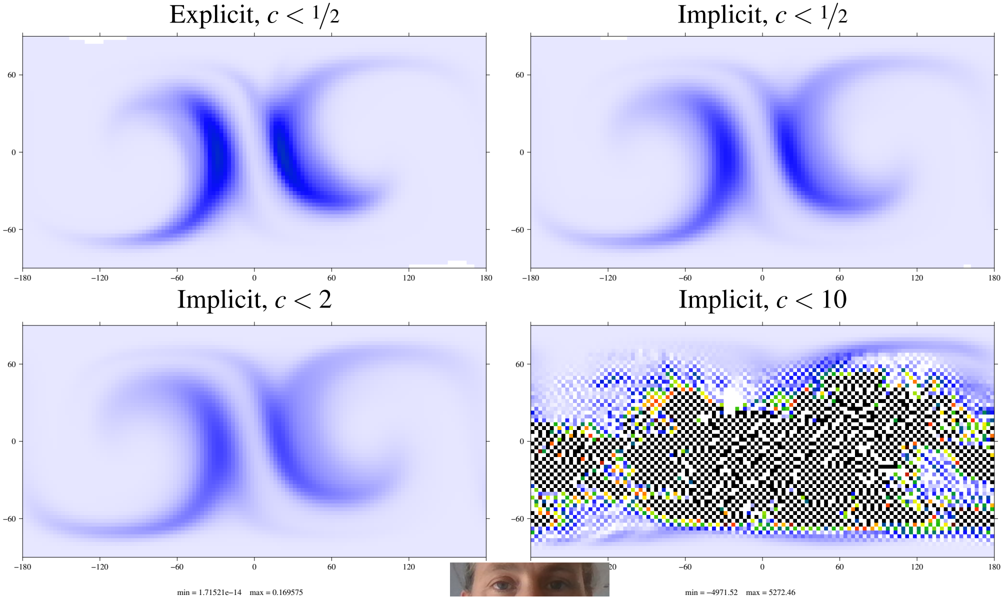
Implicit, $c < 10$



min = −0.243359 max = 0.612264

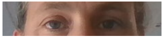


Implicit and Explicit in Time with MTDATA

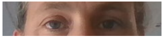


Implicit Time-Stepping - ongoing work

- Reduce the size of the corrections so that monotonicity is not violated
- Use implicit time stepping only in regions of the domain that need it

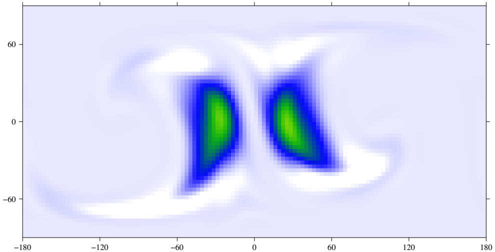


James ...

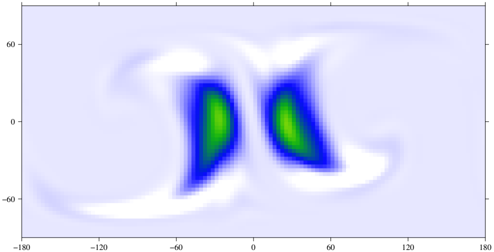


With implicit advection, can you increase spatial resolution without decreasing the time step?

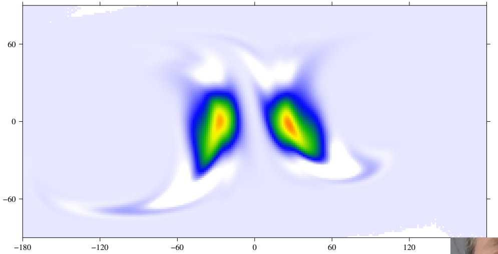
Explicit, 120×60, $\Delta t = 0.01$, $c < 1$



Implicit, 120×60, $\Delta t = 0.01$, $c < 1$

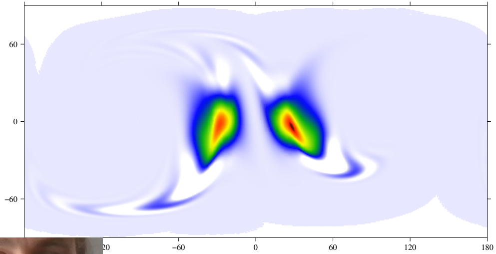


Implicit, 240×120, $\Delta t = 0.01$, $c < 2$

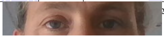


min = −0.205298   max = 0.878891

Implicit, 480×240, $\Delta t = 0.01$, $c < 4$



min = −0.338209   max = 1.00764

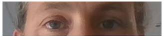


Non-linear Advection – Burgers Equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = K\frac{\partial^2 u}{\partial x^2}$$

$$\Delta x = \frac{1}{40}, \Delta t = \frac{1}{60}, c \leq 0.8$$

$$\Delta x = \frac{1}{40}, \Delta t = \frac{1}{20}, c \leq 2.4$$

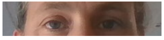


Non-linear Advection – Burgers Equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = K\frac{\partial^2 u}{\partial x^2}$$

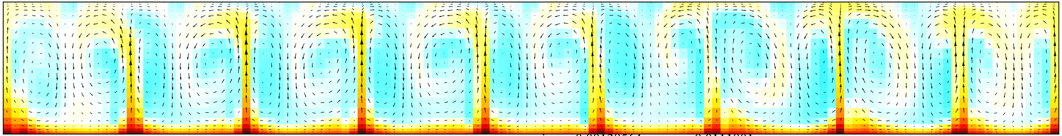
$$\Delta x = \frac{1}{40}, \Delta t = \frac{1}{60}, c \leq 0.8$$

$$\Delta x = \frac{1}{120}, \Delta t = \frac{1}{60}, c \leq 2.4$$



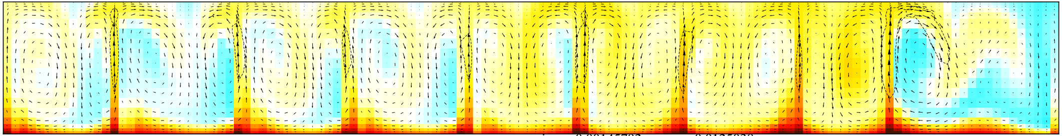
Radiative-Convective Equilibrium - Boussinesq Equations

Explicit, $\Delta t = 100$, $c < 1$



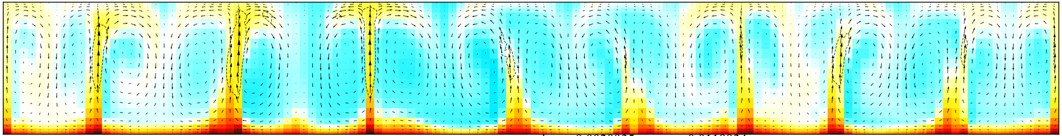
min = −0.00138564   max = 0.0111801

Explicit, $\Delta t = 200$, $c < 2$. Dashed contour shows $c = 1$

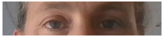


min = −0.00145792   max = 0.0125038

Implicit, $\Delta t = 200$, $c < 2$

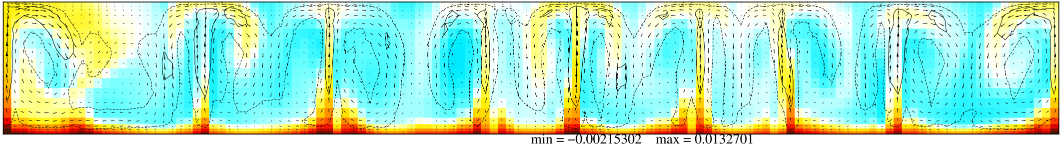


min = −0.0020935   max = 0.0118834

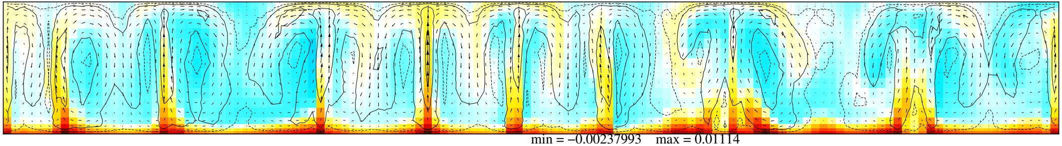


Radiative-Convective Equilibrium - Boussinesq Equations

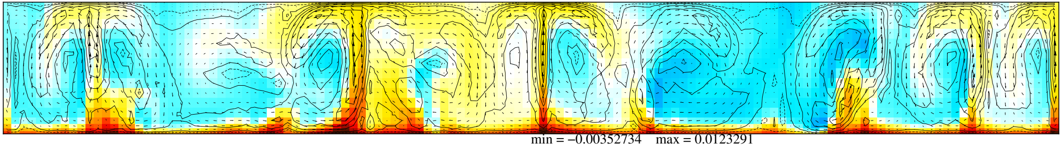
Implicit, $\Delta t = 500$, $c < 5$. Dashed contour shows $c = 1$, solid contours at $c = 2, 4, 6, \ldots$

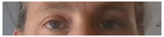


Implicit, $\Delta t = 1000$, $c < 10$.



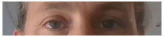
Implicit, $\Delta t = 2000$, $c < 20$





Conclusions

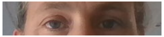
- Classes of advection schemes
  - Flux-form semi-Lagrangian (time step limits) and interpolating semi-Lagrangian (not conservative) are commonly use in atmospheric models
  - Explicit Eulerian schemes are also used but have strict time-step limits
  - Implicit Eulerian schemes have hardly been used
    - expensive matrix solutions
    - cost increases with time step (but not much)
    - looses accuracy as time step increases
    - conservative
    - suitable for any mesh structure
    - loss of accuracy may not be a problem if localised
    - needs care to maintain monotonicity
    - implicit advection allows you to increase spatial resolution alone



- Non-linear advection
  - semi-Lagrangian $\rightarrow$ big conservation errors
  - implicit solution of linearised equations $\rightarrow$ stable solutions
- Radiative-convective equilibrium (Boussinesq)
  - stable and $\sim$ accurate solutions for $c \rightarrow 20$!

Further Work

- Limit application of accuracy corrections with implicit to maintain monotonicity
- Maintain monotonicity and accuracy with locally implicit
- Share pre-conditions between multiple tracers to gain multi-tracer efficiency



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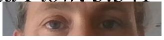

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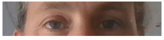

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