Numerical Methods For Tracer Transport

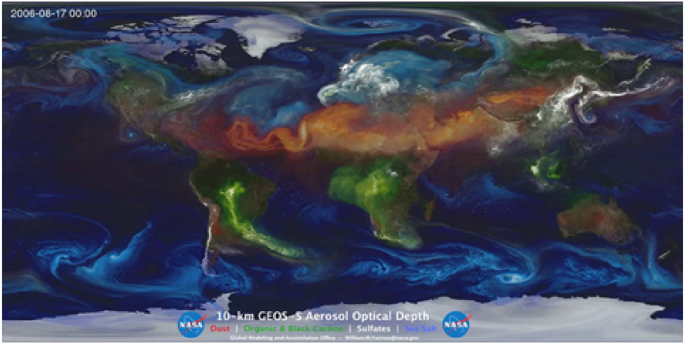
James Kent

University of South Wales

Outline

- The Advection Equation
- Finite-Difference Methods
- Finite-Volume Methods
- Multi-Dimensional Transport
- Testing Advection Schemes

Motivation



Bill Putman, NASA

The Advection Equation

In the absence of sources and sinks, tracer transport is governed by the continuity equation

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

and the tracer conservation equation

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

where ρ is density, $\mathbf{u}$ is the 3D velocity, and q is the tracer mixing ratio.

This leads to the advection equation

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

The Advection Equation

Eulerian or **Lagrangian** frame:

$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0 \qquad\qquad \frac{Dq}{Dt} = 0$$

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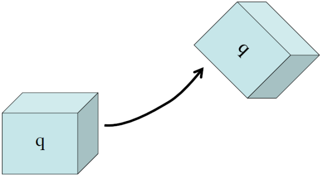
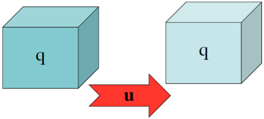
Lagrangian frame follows fluid parcel.



Eulerian frame needs rate of change of q.



Lagrangian Frame: Tracking rapidly deforming regions is difficult.

R. A. Pielke and M. Uliasz (1997)

We will focus on the Eulerian frame.

The Advection Equation

What does the advection equation tell us?

$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0 \text{ is a Lagrangian conservation law.}$$

Therefore q is conserved $\quad \left(\frac{d}{dt} \int_A q dA = 0 \right)$

$$\frac{\partial \rho q}{\partial t} + \nabla \cdot (\mathbf{u} \rho q) = 0 \text{ is a flux-form conservation law.}$$

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Therefore ρq is conserved $\left(\frac{d}{dt} \int_A \rho q dA = 0 \right)$

$\frac{Dq}{Dt} = 0$ tells us that q is bounded by initial conditions (monotonicity).

ρq is a density and so must be positive (positivity).

The Advection Equation

To begin with we will consider transport in 1D.

We have a tracer mixing ratio $q(x, t)$ and consider constant velocity u.

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

The Advection Equation

To begin with we will consider transport in 1D.

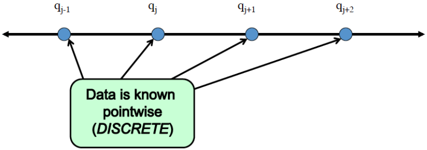
We have a tracer mixing ratio $q(x,t)$ and consider constant velocity u.

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

- q is conserved.
- Known solution $\quad q(x,t) = q(x - ut, 0)$.
- Can be written as $q_t + uq_x = 0$.

Finite-Difference Methods

Tracer, q, is stored at discrete grid points (with index j).



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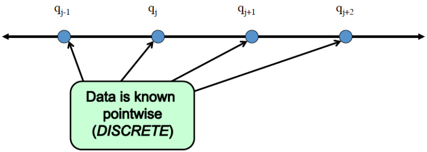

Approximate each term in the equations at these points

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0$$

Finite-Difference Methods

If q is smooth, with $q(x_j) = q_j$, we can expand using the Taylor series

$$q(x_j + \Delta x) = q_{j+1} = q_j + \Delta x \frac{\partial q_j}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 q_j}{\partial x^2} + \ldots$$

where Δx is the spacing between grid points.

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We can use this to approximate the first spatial derivative:

$$\frac{\partial q_j}{\partial x} = \frac{q_{j+1} - q_j}{\Delta x} - \frac{\Delta x}{2!} \frac{\partial^2 q_j}{\partial x^2} + \dots$$

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Use n as the temporal index, with $q(x_j, t_n) = q_j^n$, then the first temporal derivative becomes:

$$\frac{\partial q_j^n}{\partial t} = \frac{q_j^{n+1} - q_j^n}{\Delta t} - \frac{\Delta t}{2!} \frac{\partial^2 q_j^n}{\partial t^2} + \dots$$

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Finite-Difference Methods

A finite-difference approximation to the advection equation:

$$\frac{q_j^{n+1} - q_j^n}{\Delta t} + u\left(\frac{q_{j+1}^n - q_j^n}{\Delta x}\right) = 0 \qquad \text{(plus some error)}$$

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Rearranged to give us our numerical scheme:

$$q_j^{n+1} = q_j^n - u \frac{\Delta t}{\Delta x} \left(q_{j+1}^n - q_j^n \right)$$

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We can use a backwards approximation to the spatial derivative:

$$\frac{q_j^{n+1} - q_j^n}{\Delta t} + u\left(\frac{q_j^n - q_{j-1}^n}{\Delta x}\right) = 0 \qquad \text{(plus some error)}$$

Rearranged to give us our numerical scheme:

$$q_j^{n+1} = q_j^n - u\frac{\Delta t}{\Delta x}\left(q_j^n - q_{j-1}^n\right)$$

Finite-Difference Methods

Taylor Series:

$$q(x_j + \Delta x) = q_{j+1} = q_j + \Delta x \frac{\partial q_j}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 q_j}{\partial x^2} + \ldots$$

$$q(x_j - \Delta x) = q_{j-1} = q_j - \Delta x \frac{\partial q_j}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 q_j}{\partial x^2} + \ldots$$

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A more accurate approximation to the derivatives:

$$\frac{q_j^{n+1} - q_j^{n-1}}{2\Delta t} + u\left(\frac{q_{j+1}^n - q_{j-1}^n}{2\Delta x}\right) = 0 \qquad \text{(plus less error?)}$$

Rearranged to give us our numerical scheme:

$$q_j^{n+1} = q_j^{n-1} - u\frac{\Delta t}{\Delta x}\left(q_{j+1}^n - q_{j-1}^n\right)$$

Finite-Difference Methods

More Accurate? We can calculate the truncation error of a numerical method using Taylor expansions.

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$$q_j^{n+1} = q_j^n - u\frac{\Delta t}{\Delta x}\left(q_{j+1}^n - q_j^n\right)$$

$$q_t + uq_x = -\frac{u\Delta x}{2}\left(\frac{u\Delta t}{\Delta x} - 1\right)q_{xx} + \text{ H.O.T} \qquad \text{(first-order)}$$

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The *more accurate* approximation gives

$$q_j^{n+1} = q_j^{n-1} - u\frac{\Delta t}{\Delta x}\left(q_{j+1}^n - q_{j-1}^n\right)$$

$$q_t + uq_x = \frac{u\Delta x^2}{3}\left(\frac{u^2\Delta t^2}{\Delta x^2} - 1\right) q_{xxx} + \text{ H.O.T} \qquad \text{(second-order)}$$

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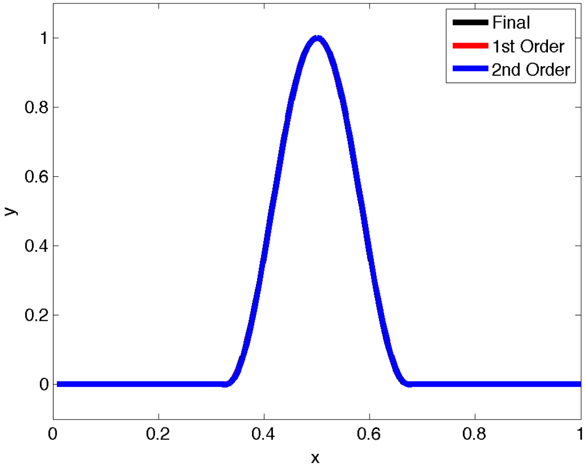
Finite-Difference Methods



Finite-Difference Methods

First-order or second-order (or nth-order) refers to the **formal order of accuracy** of the numerical scheme.

This is the rate at which the error tends to zero as the grid spacing is reduced.

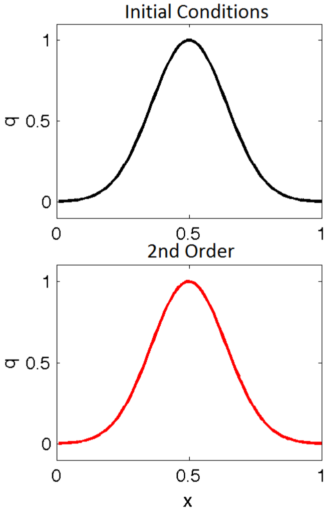
It is often written as $O(\Delta x)$ or $O(\Delta x^2)$.

Finite-Difference Methods

An Example

Second-order method $O(\Delta x^2)$:

Δx	error
1	≈ 1
$\frac{1}{2}$	?



Finite-Difference Methods

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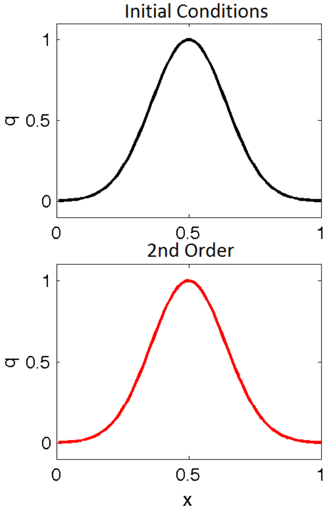
Second-order method $O(\Delta x^2)$:

Δx	error
1	≈ 1
$\frac{1}{2}$	$\approx \frac{1}{4}$



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Finite-Difference Methods

Another Example

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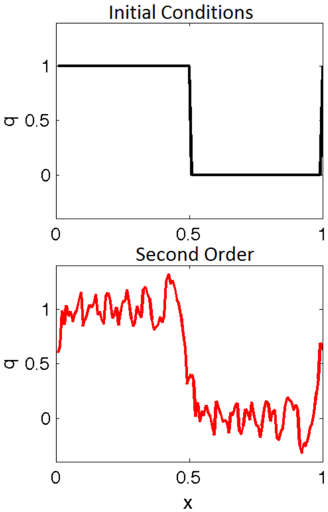

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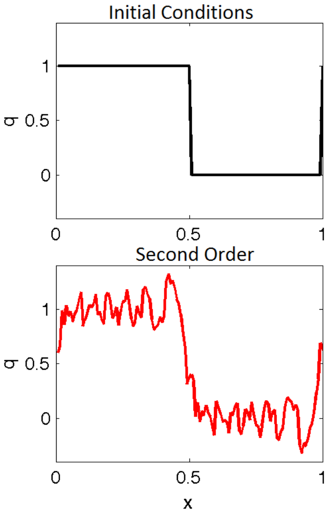

Finite-Difference Methods

More important than accuracy is **stability**.

Use von Neumann stability analysis: $q_j^n = A^n e^{ikx_j}$

Idea is we want the amplitude factor $|A| \leq 1$.

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Use von Neumann stability analysis: $q_j^n = A^n e^{ikx_j}$

Idea is we want the amplitude factor $|A| \leq 1$.

Substitute into our discretization and simplify to find conditions for stability.

Finite-Difference Methods

For our first-order scheme $$q_j^{n+1} = q_j^n - u\frac{\Delta t}{\Delta x}\left(q_{j+1}^n - q_j^n\right)$$

we get $-1 \leq \frac{u\Delta t}{\Delta x} \leq 0$.

Let ν be the **Courant Number**, $\nu = \frac{u\Delta t}{\Delta x}$, this can be written as $-1 \leq \nu \leq 0$.

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For the backwards-space first-order scheme we get $0 \leq \nu \leq 1$.

For the second-order Leapfrog scheme we get $-1 \leq \nu \leq 1$.

Finite-Difference Methods

Some schemes are unconditionally stable (e.g. implicit schemes)

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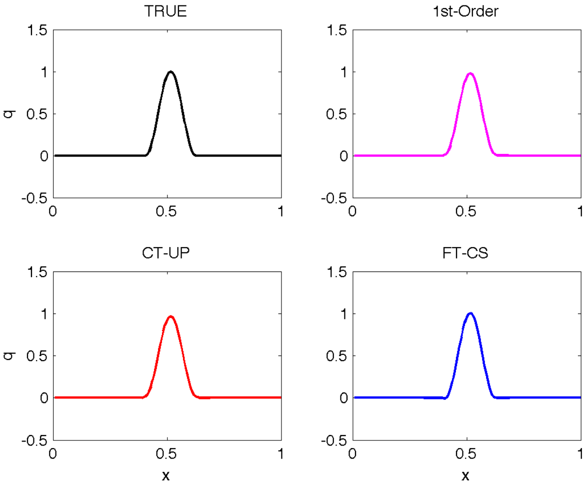
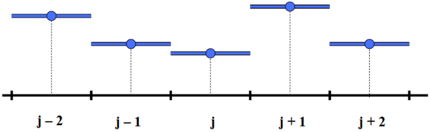
Finite-Difference Methods



Finite-Volume Methods

Tracers are stored as volume averaged values



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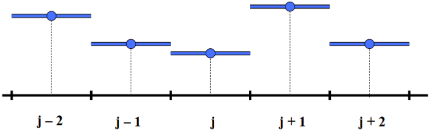

Idea is to take the equation in flux-form

$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{F} = 0$$

Integrate over the volume and apply the divergence theorem

$$\frac{\partial}{\partial t} \int_V q dV + \int_S \mathbf{F} \cdot d\mathbf{S} = 0$$

Finite-Volume Methods

For the advection equation in 1D we get

$$\frac{\partial q_j}{\partial t} + \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta x} = 0$$

where F is the flux at the grid cell boundaries ($F = uq$).

Finite-Volume Methods

For the advection equation in 1D we get

$$\frac{\partial q_j}{\partial t} + \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta x} = 0$$

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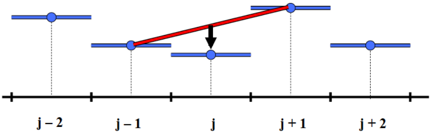
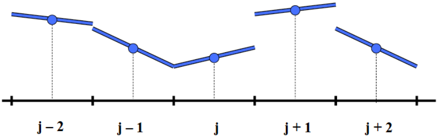
Use neighboring grid values to build a subgrid reconstruction





Finite-Volume Methods

Finite-volume methods are guaranteed to be conservative:

One cell's loss is another cell's gain

If we sum over all the cells then the F term will vanish.

Finite-Volume Methods

An example - the Lax-Wendroff Flux:

$$F_{j+\frac{1}{2}} = \frac{1}{2}\left(q_{j+1} + q_j\right) - \frac{u\Delta t}{2\Delta x}\left(q_{j+1} - q_j\right)$$

$$q_j^{n+1} = q_j^n - \frac{u\Delta t}{\Delta x}\left(F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}\right)$$

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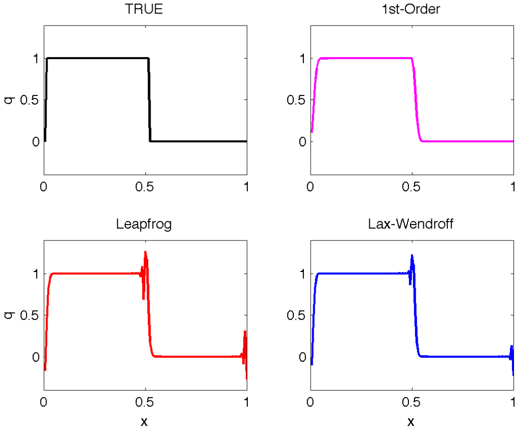
- Second-order accurate
- Stable for $-1 \leq \nu \leq 1$

Finite-Volume Methods

Lax-Wendroff is not very good at discontinuities:



Flux-Limiters

To enforce montonicity we use **limiters**:

- Slope limiters (limit subgrid reconstruction)
- Flux limiters (limit F)
- Flux Corrected Transport (correct F)

Flux-Limiters

Idea: Limit the flux to ensure monotonicity.

First-order is monotonic but low-order.

Lax-Wendroff is oscillatory but high(ish)-order.

Flux-Limiters

Idea: Limit the flux to ensure monotonicity.

First-order is monotonic but low-order.

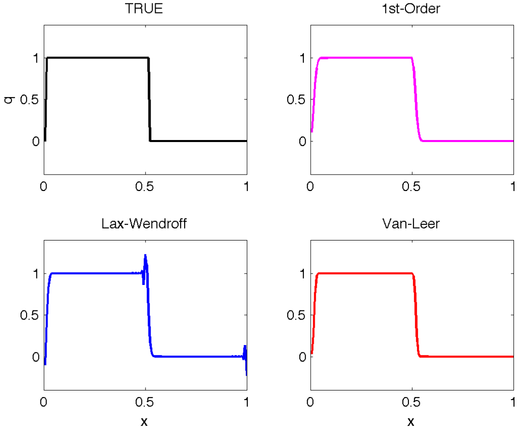
Lax-Wendroff is oscillatory but high(ish)-order.

Use Lax-Wendroff for smooth data and first-order for discontinuities. The **flux limiter** switches between them. Our new flux is:

$$F_{j+\frac{1}{2}} = F_{LOW} + \phi_j \left(F_{HIGH} - F_{LOW} \right)$$

where $\phi = \phi(r)$ and $r_j = \dfrac{q_j - q_{j-1}}{q_{j+1} - q_j}$

Flux-Limiters



2D Advection

Multi-dimensional flow. Assume u and v are constant (for now) and our domain is a doubly periodic 2D box:

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} = 0$$

We now need to consider **cross-terms**, i.e. flow into grid cell (i, j) from $(i-1, j-1)$ for example.

2D Advection

Consider Lax-Wendroff in 2D:

Expand $q_{i,j}^{n+1} = q + \Delta t q_t + \frac{\Delta t^2}{2!} q_{tt} + \ldots$

Using $q_t = -u q_x - v q_y \;\Rightarrow q_{tt} = u^2 q_{xx} + 2uv q_{xy} + v^2 q_{yy}$

Then $q_{i,j}^{n+1} = q - \Delta t \left(u q_x + v q_y \right) + \frac{\Delta t^2}{2!} \left(u^2 q_{xx} + 2uv q_{xy} + v^2 q_{yy} \right) + \ldots$

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Our discretization becomes:

$$q_{ij}^{n+1} = q_{ij}^n - \frac{u\Delta t}{\Delta x}\left(F_{i+\frac{1}{2}j} - F_{i-\frac{1}{2}j}\right) - \frac{v\Delta t}{\Delta y}\left(G_{ij+\frac{1}{2}} - G_{ij-\frac{1}{2}}\right)$$

where F and G must include the cross-terms.

2D Advection

Lin-Rood method captures cross-terms using multiple 1D fluxes:

$$q^x = q - \frac{u\Delta t}{2\Delta x}\left(F(q)_{i+\frac{1}{2}j} - F(q)_{i-\frac{1}{2}j}\right)$$
$$q^y = q - \frac{v\Delta t}{2\Delta y}\left(G(q)_{ij+\frac{1}{2}} - G(q)_{ij-\frac{1}{2}}\right)$$

$$q_{ij}^{n+1} = q_{ij}^n - \frac{u\Delta t}{\Delta x}\left(F(q^y)_{i+\frac{1}{2}j} - F(q^y)_{i-\frac{1}{2}j}\right) - \frac{v\Delta t}{\Delta y}\left(G(q^x)_{ij+\frac{1}{2}} - G(q^x)_{ij-\frac{1}{2}}\right)$$

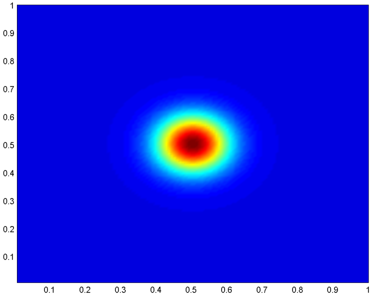
where F and G are 1D fluxes

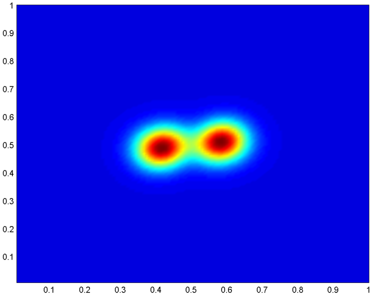
2D Advection

Lin-Rood uses 1D fluxes F and G: these fluxes can use limiters e.g. PPM.

Limiters must limit cross-terms to ensure monotonicity.

2D Advection





Advection on the Sphere

In spherical coordinates the advection equation becomes:

$$\frac{\partial q}{\partial t} + \frac{u}{a\cos\varphi}\frac{\partial q}{\partial \lambda} + \frac{v}{a}\frac{\partial q}{\partial \varphi} + w\frac{\partial q}{\partial z} = 0$$

where $\mathbf{u} = (u, v, w)$, λ and φ are longitude and latitude, and a is the radius of the Earth.

Advection on the Sphere

Latitude-longitude grid converges at poles:

$$\Delta x \to 0$$

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Stability of numerical methods we've looked at:

$$-1 \leq \frac{u\Delta t}{\Delta x} \leq 1$$

As $\Delta x \to 0$ then $\Delta t \to 0$

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Solution:

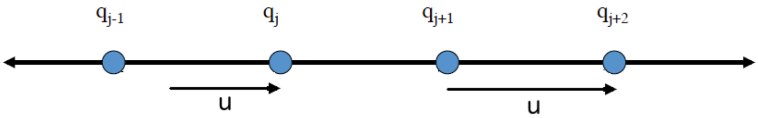
- Different grid
- Long time step permitting method

Semi-Lagrangian Methods

Semi-Lagrangian methods back-track along particle trajectories to update the value at a given grid point.

Uses the value of the tracer at the departure point.

If the departure point lies in between grid points then interpolation must be used.



Semi-Lagrangian Methods

- Semi-Lagrangian methods permit long time steps.
- Easy to make monotonic.
- In general they are not conservative.

Vertical Advection

For fully 3D flow we can either:

- Split the horizontal and vertical directions
- Expand our method to 3D

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In general these methods (FD, FV, SL) can be made fully 3D, but this is computationally costly.

Testing Transport Schemes

Constant velocity gives us a known solution.

$$\text{e.g.} \qquad q(x,t) = q(x-ut,0)$$

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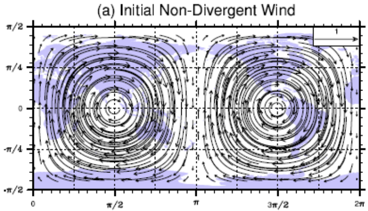
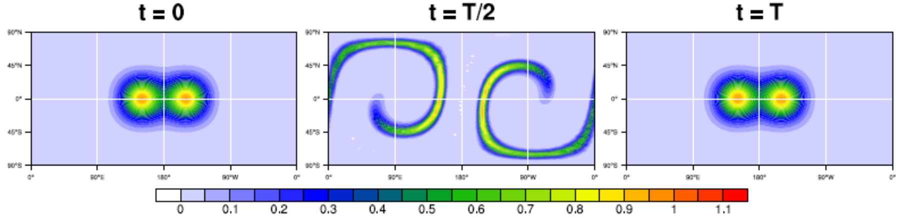
More complicated velocity with reversed flow.

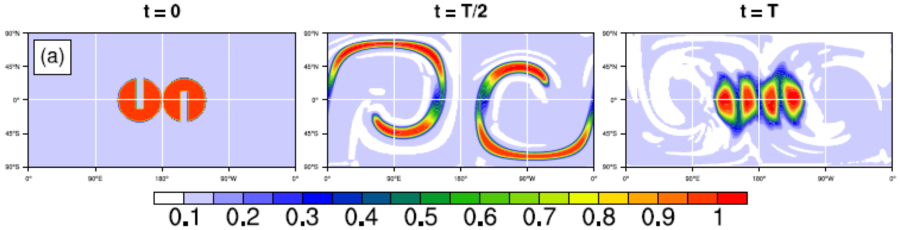


Testing Transport Schemes

Smooth initial conditions (Gaussian Hill)

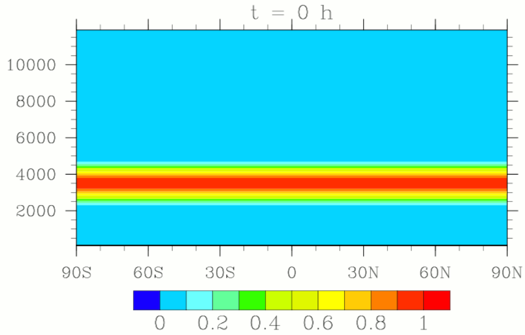


Discontinuous initial conditions (Slotted Cylinder)

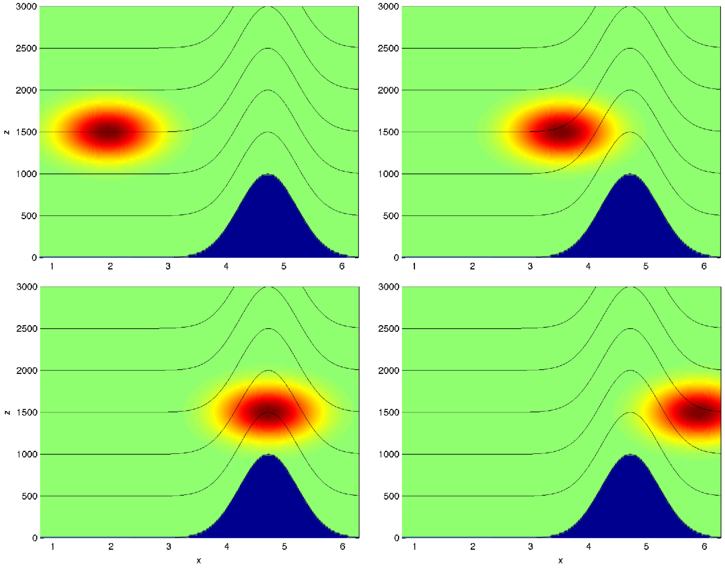


Testing Transport Schemes

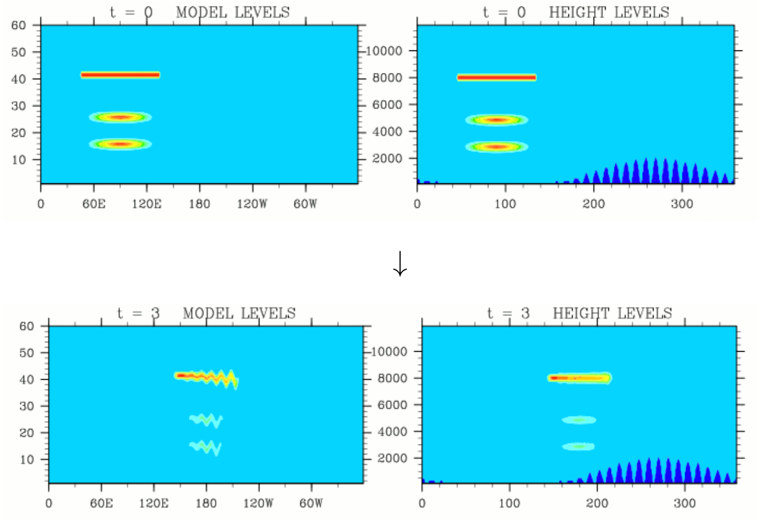
Testing horizontal-vertical coupling:



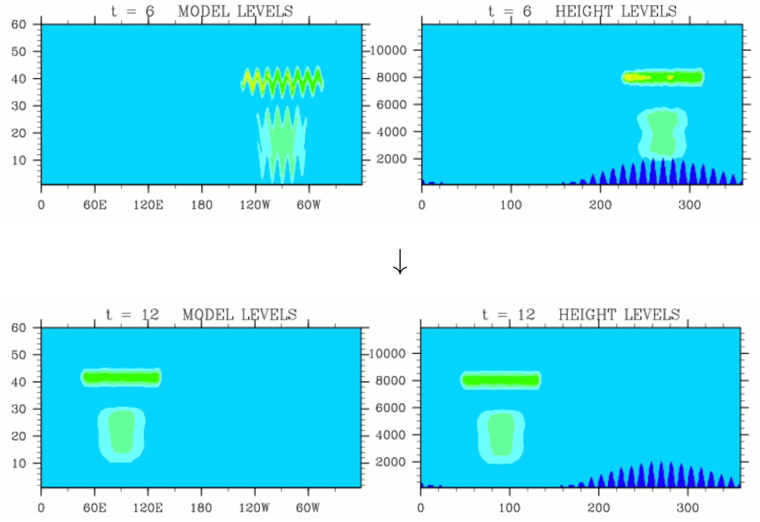
Testing Transport Schemes



Testing Transport Schemes



Testing Transport Schemes



Other Methods

There are other numerical methods for tracer transport, for example:

- Implicit time stepping
- Global spectral
- Finite (spectral) element
- Fully Lagrangian

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Other considerations for transport scheme:

- Computational efficiency
- Consistency with dynamics
- Non-orthogonal and unstructured grids

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Summary

Many different types of method for tracer transport.

Desirable properties: accuracy, conservation, monotonicity...

Essential property: stability!

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Active research into the development of numerical methods for tracer transport.

Questions?