

ATM 265, Spring 2019

Lecture 3

Numerical Methods:

Horizontal Discretizations

April 8, 2019

Paul A. Ullrich (HH 251)

paullrich@ucdavis.edu

Outline

- 1. Introduction / Motivation**
- 2. Finite Difference Methods**
- 3. Finite Volume Methods**
- 4. The Spectral Transform Method**
- 5. Spectral Element / Discontinuous Galerkin**

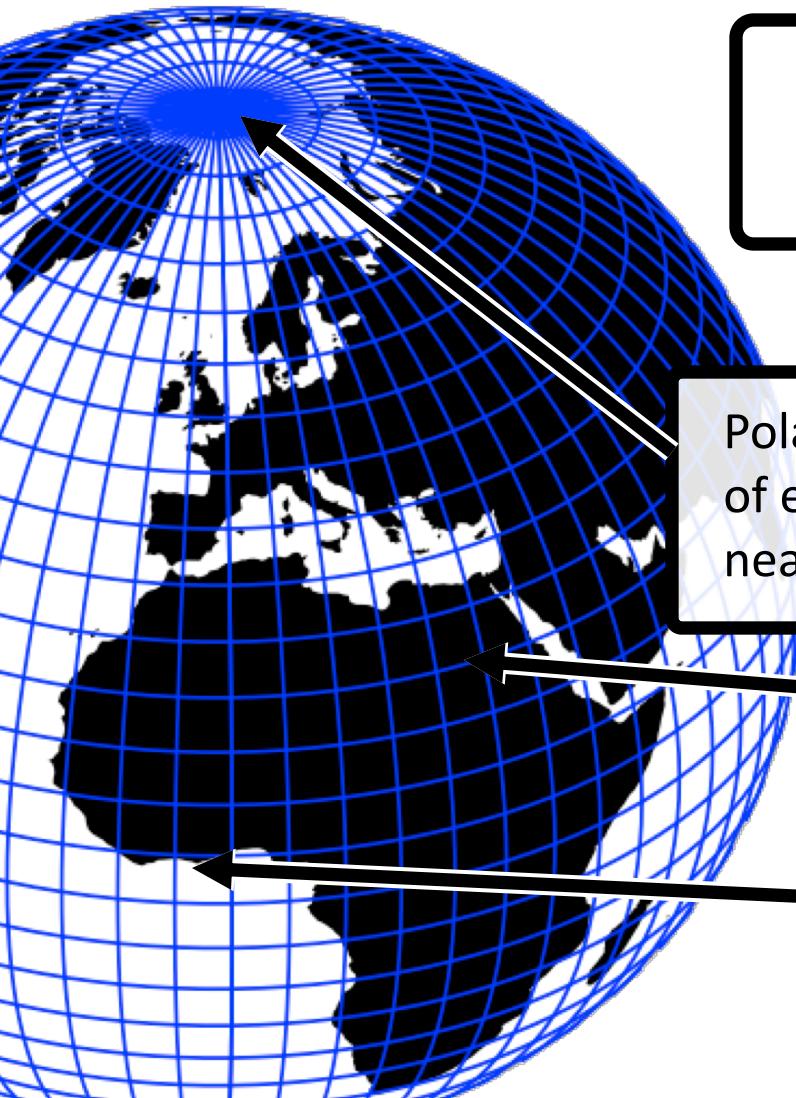
Introduction

Continuous vs. Discrete

Atmospheric Modeling – Question Number One

- How do we best represent continuous data when only a (very) limited amount of information can be stored?
- Equivalently, what is the best way to represent continuous data discretely?

The Regular Latitude-Longitude Grid



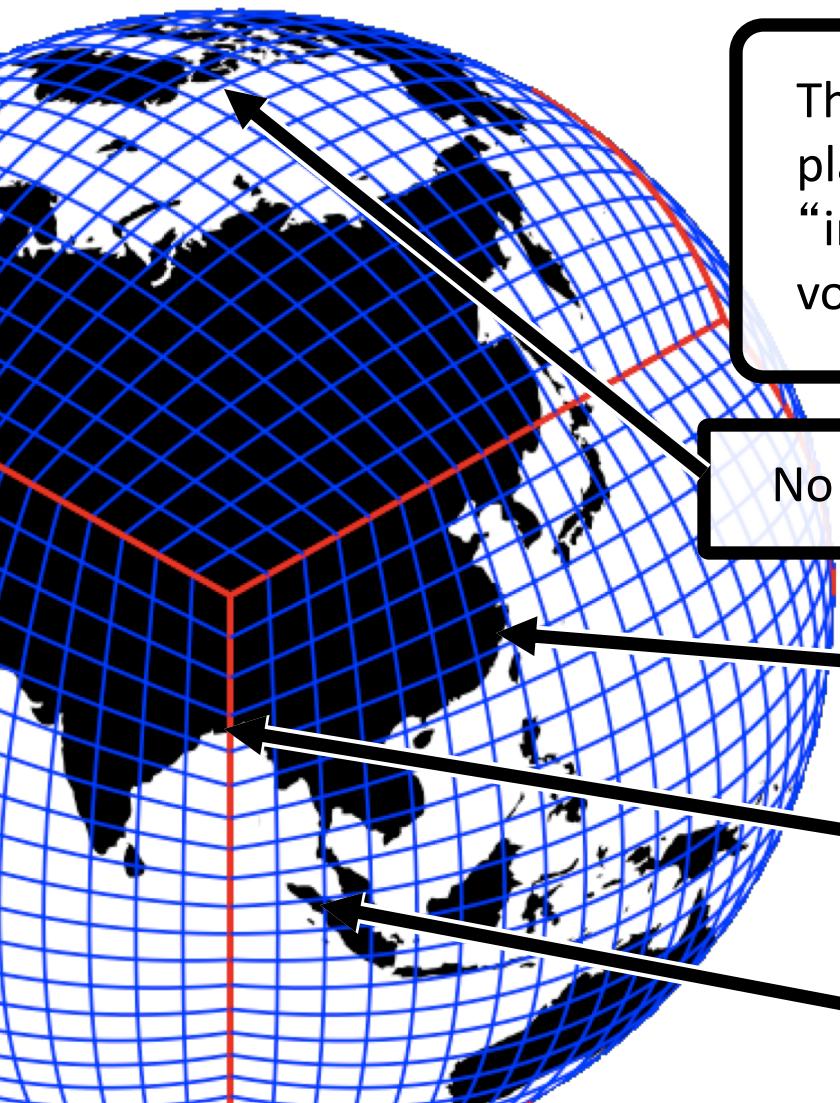
Grid lines are represented by lines of constant latitude and longitude.

Polar singularity leads to accumulation of elements and increase of resolution near the pole.

Grid faces individually regular

Orthogonal coordinate lines

The Cubed-Sphere



The cubed-sphere grid is obtained by placing a cube inside a sphere and “inflating” it to occupy the total volume of the sphere.

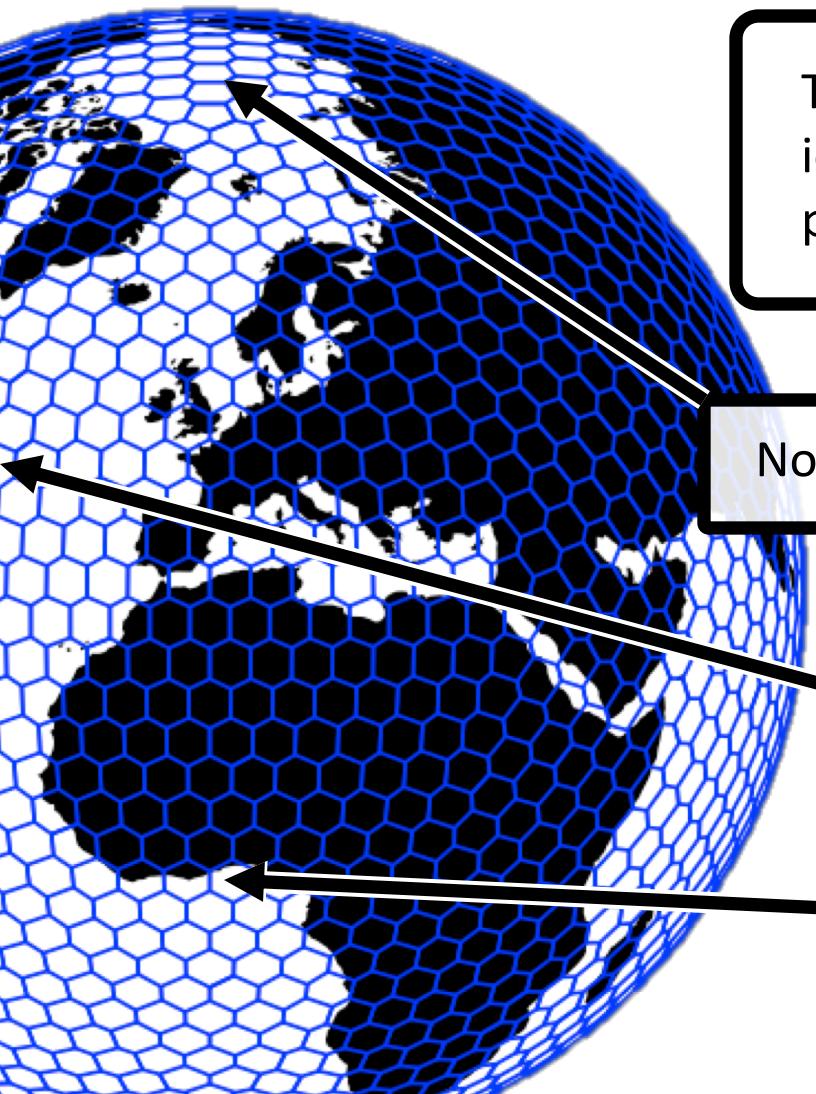
No polar singularities

Grid faces individually regular

Some difficulty at panel edges

Non-orthogonal coordinate lines

The Icosahedral Geodesic Grid



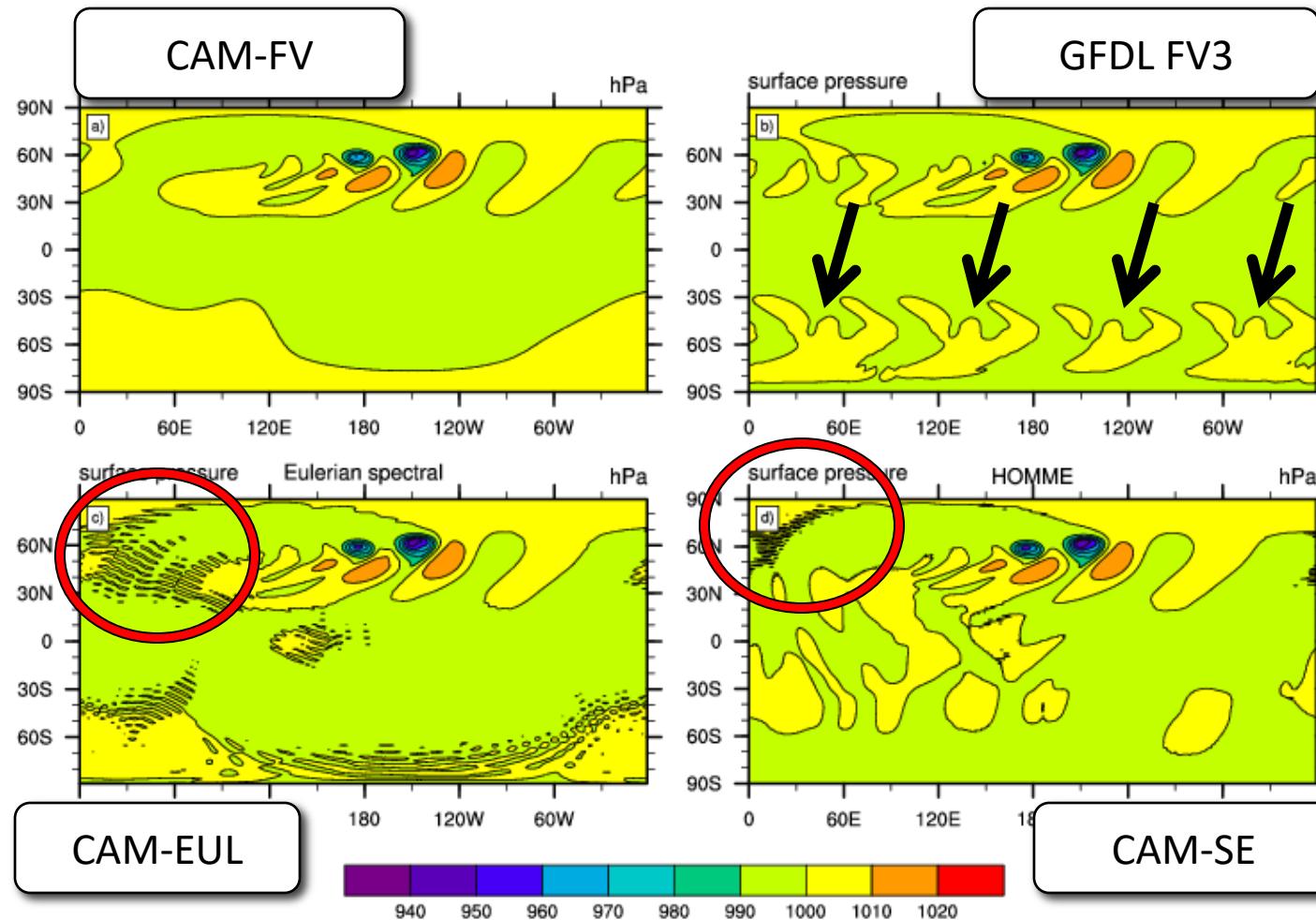
The grid is the “dual” grid of the refined icoahedron, consisting of hexagonal and pentagonal elements.

No polar singularities

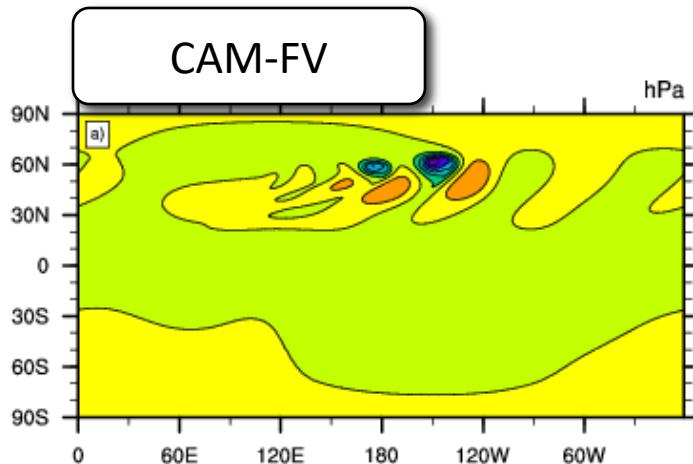
Grid largely unstructured

Most uniform element spacing

Numerical Methods: Issues



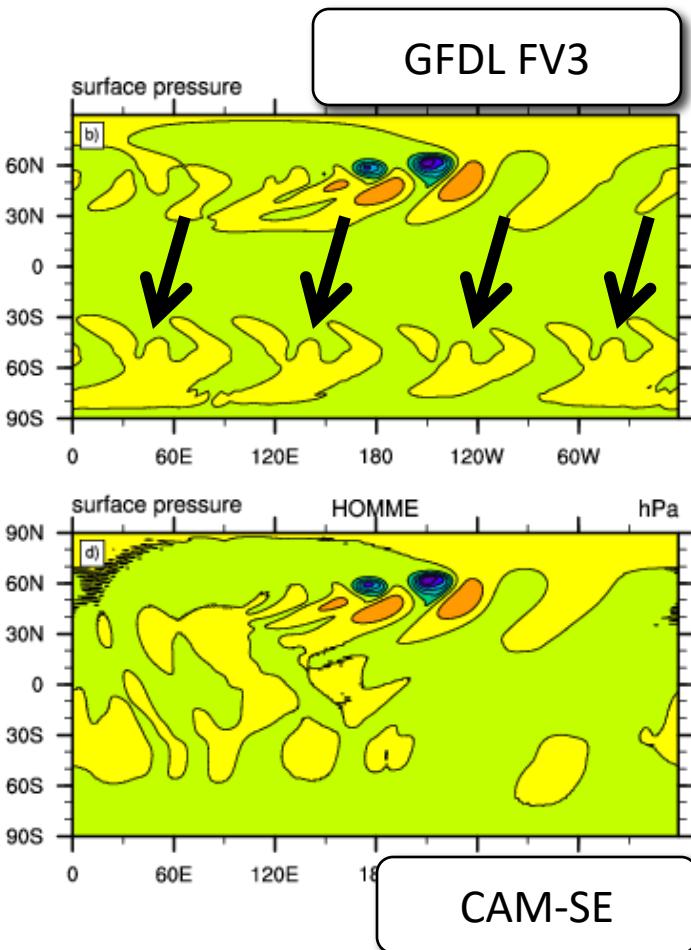
Numerical Methods: Issues



Although it is a standard in climate modeling, the CAM-FV model is known to possess a strong diffusive signature. Diffusion is enhanced as one approaches the poles in order to maintain stability.

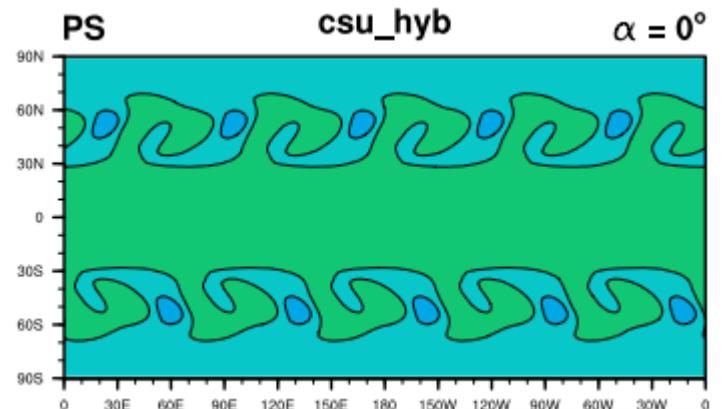
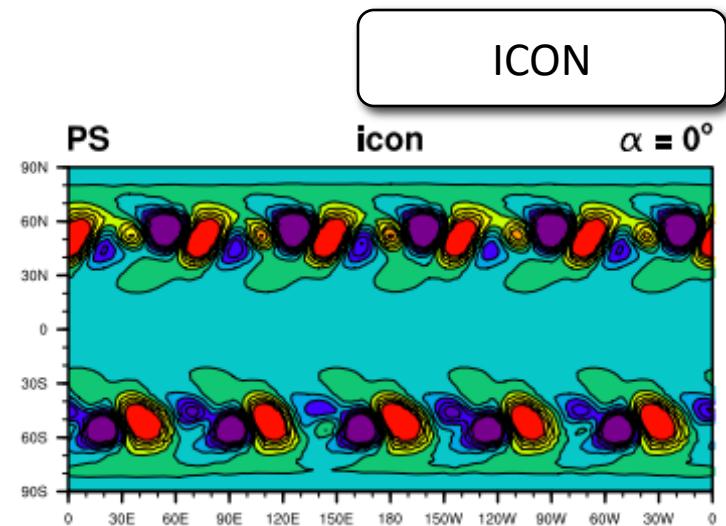
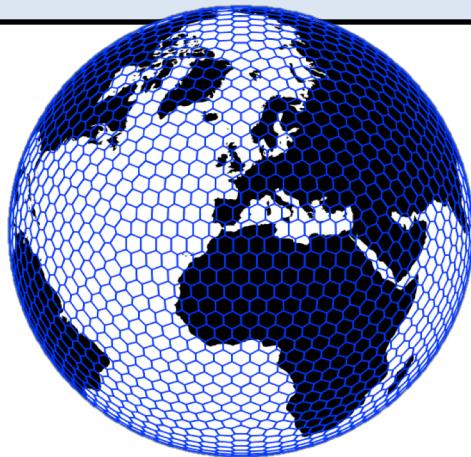
Numerical Methods: Issues

Both the GFDL FV3 (FVcubed) model and CAM-SE (spectral element) model are built on the cubed-sphere. This leads to an enhancement of the $k=4$ wave mode. The use of high-order numerics in CAM-SE is more effective at repressing this mode.



Numerical Methods: Issues

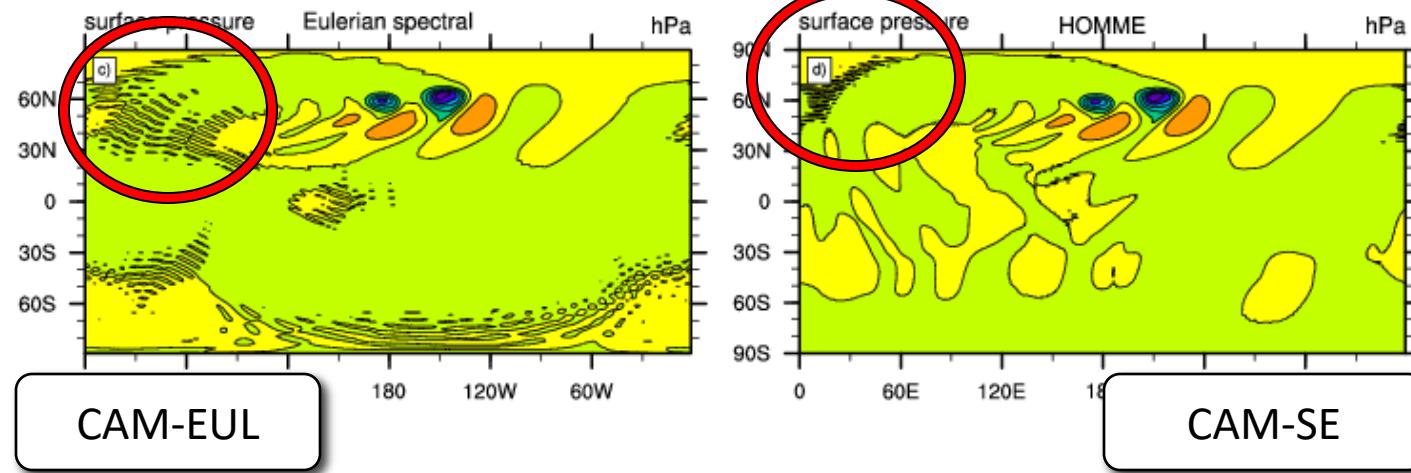
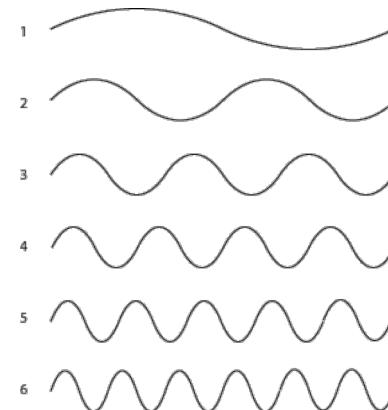
Both the ICON model CSU model are built on an icosahedral grid (results from 2008 workshop). This leads to an enhancement of the $k=5$ wave mode.



CSU

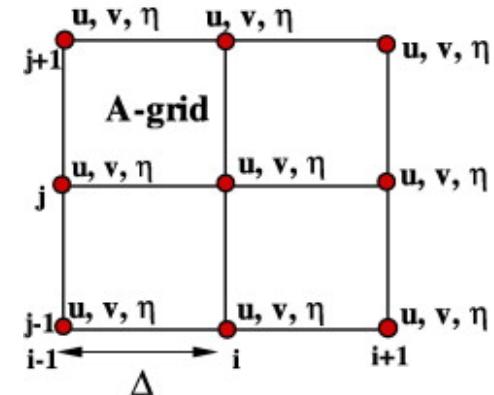
Numerical Methods: Issues

CAM-EUL (Eulerian) and CAM-SE (spectral element) use spectral methods, which are known to be prone to spectral ringing. This ringing is characterized by rapid oscillations due to enhancement of the high-frequency mode.



Numerical Methods: Staggering

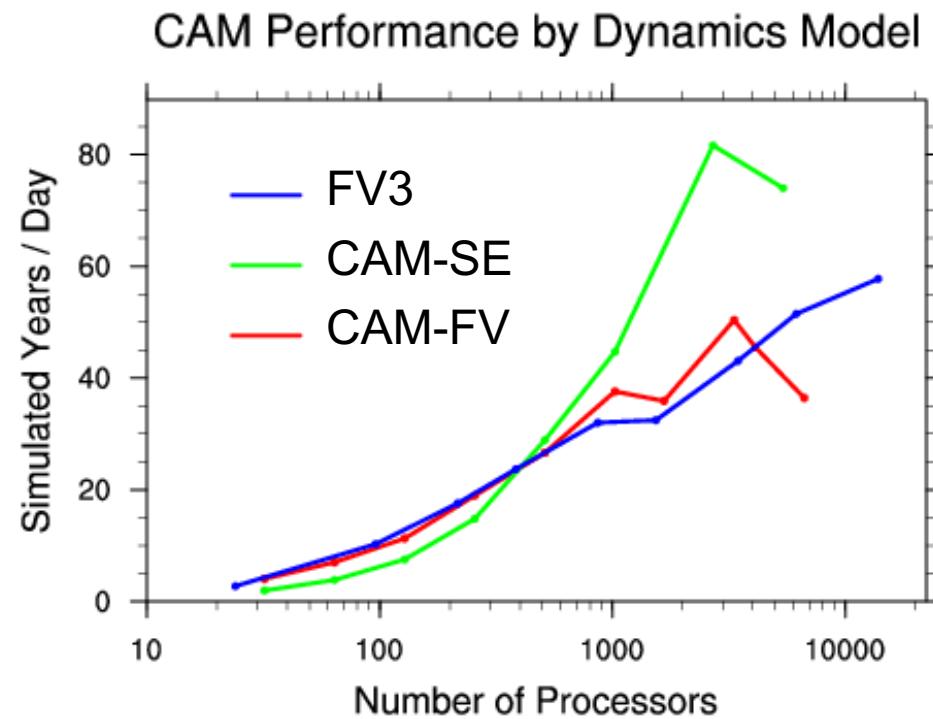
Unstaggered (Arakawa A-grid) finite-difference and finite-volume methods are known to support artificially support high-frequency modes. Additional diffusion is typically required to eliminate high-frequency imprinting.



Summary: When it comes to designing discretizations, there's no free lunch!

Parallel Performance

Methods which make the most use of local data will perform better on massively parallel computers (compact schemes). Conversely, methods which make use of global data (spectral transform) tend to perform more poorly in parallel.



10-day adiabatic runs with 1 tracer on Cray machine Jaguar XT4 (#4). The resolution is ~ 1 degree in the horizontal with 26 vertical levels. Source: Art Mirin (LLNL)

The Atmospheric Equations

$$\frac{Du}{Dt} - \frac{uv \tan \phi}{r} + \frac{uw}{r} = -\frac{1}{\rho r \cos \phi} \frac{\partial p}{\partial \lambda} + 2\Omega v \sin \phi - 2\Omega w \cos \phi + \nu \nabla^2 u$$

$$\frac{Dv}{Dt} + \frac{u^2 \tan \phi}{r} + \frac{vw}{r} = -\frac{1}{\rho r} \frac{\partial p}{\partial \phi} - 2\Omega u \sin \phi + \nu \nabla^2 v$$

$$\frac{Dw}{Dt} - \frac{u^2 + v^2}{r} = -\frac{1}{\rho} \frac{\partial p}{\partial r} - g + 2\Omega u \cos \phi + \nu \nabla^2 w$$

$$\frac{D\rho}{Dt} = -\rho \cdot \nabla \mathbf{u}$$

$$c_p \frac{DT}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} = J$$

$$p = \rho R_d T$$

$$\frac{Dq_i}{Dt} = S_i$$

Material derivative:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$$

Finite Difference Methods

Advection of a Tracer

We are interested in solving the advection equation:

$$\frac{Dq}{Dt} = 0$$

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

For now, we only consider 1D:

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

q represents the mixing ratio of a certain tracer species.

Temporal component
(next lecture)

Spatial component
(this lecture)

Advection of a Tracer

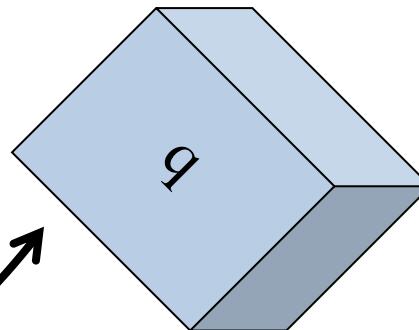
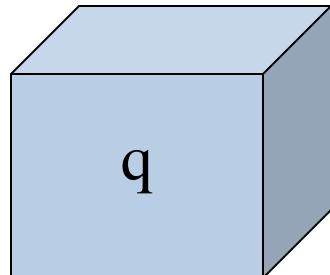
Lagrangian Frame

$$\frac{Dq}{Dt} = 0$$

Eulerian Frame

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

What does this mean?



Tracer mixing ratio is constant following a fluid parcel.

Advection of a Tracer

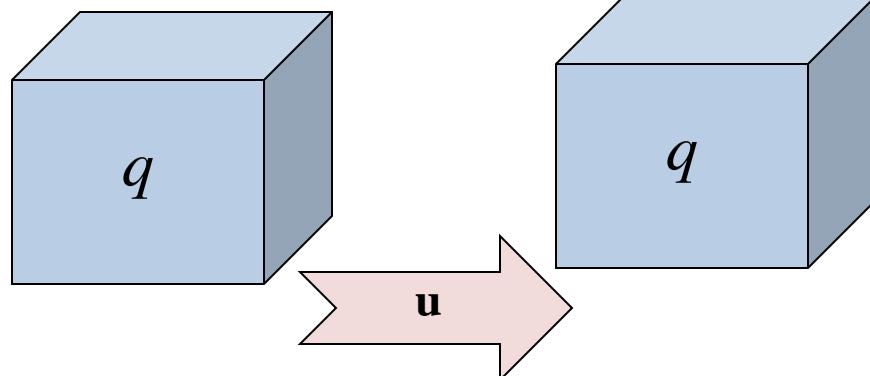
Lagrangian Frame

$$\frac{Dq}{Dt} = 0$$

Eulerian Frame

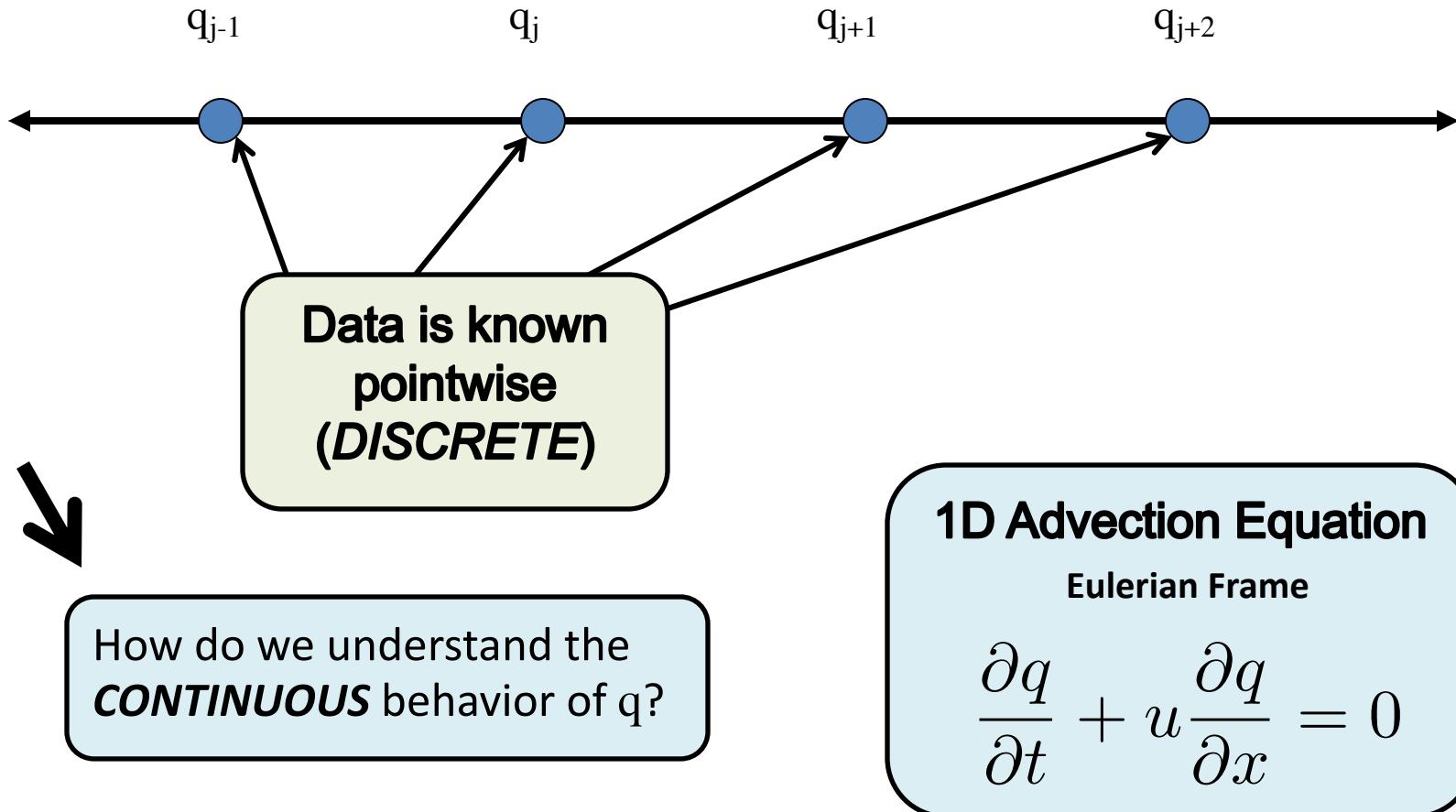
$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0$$

What does this mean?



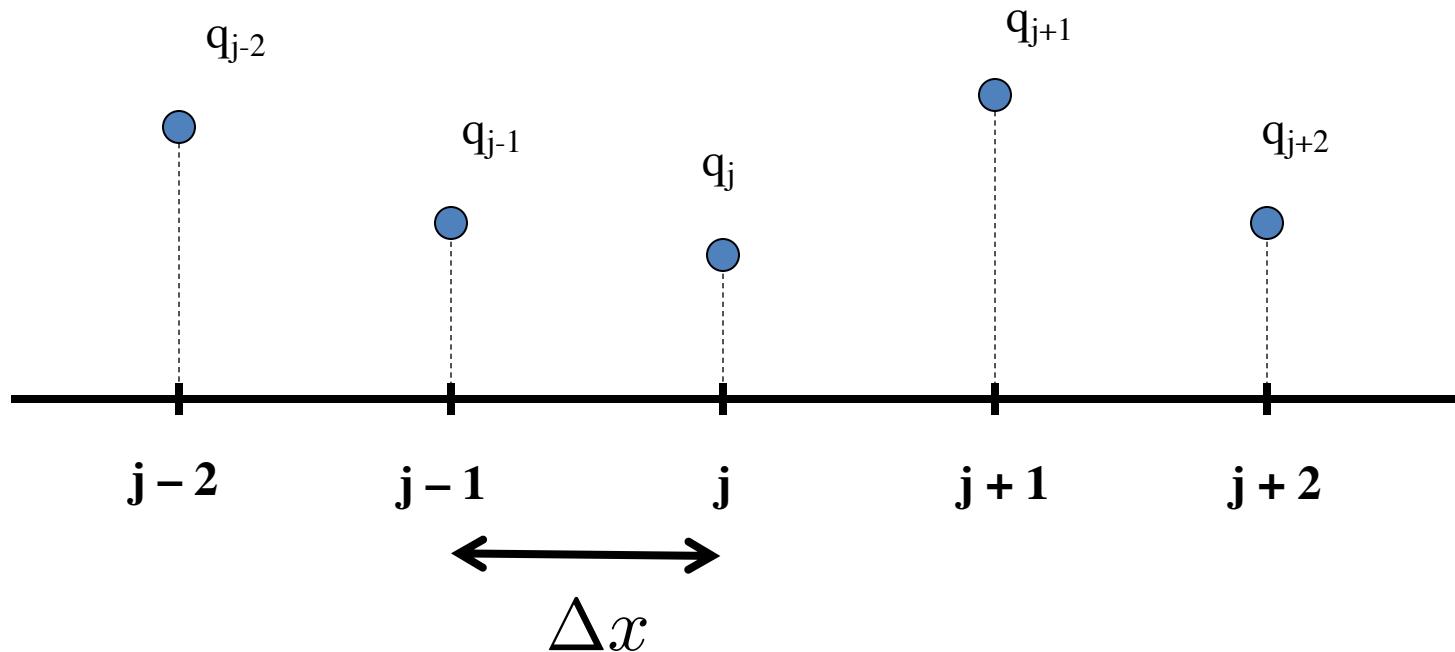
Local change in mixing ratio is determined by “rate of change” of q in the upstream wind direction.

Basic Finite Differences



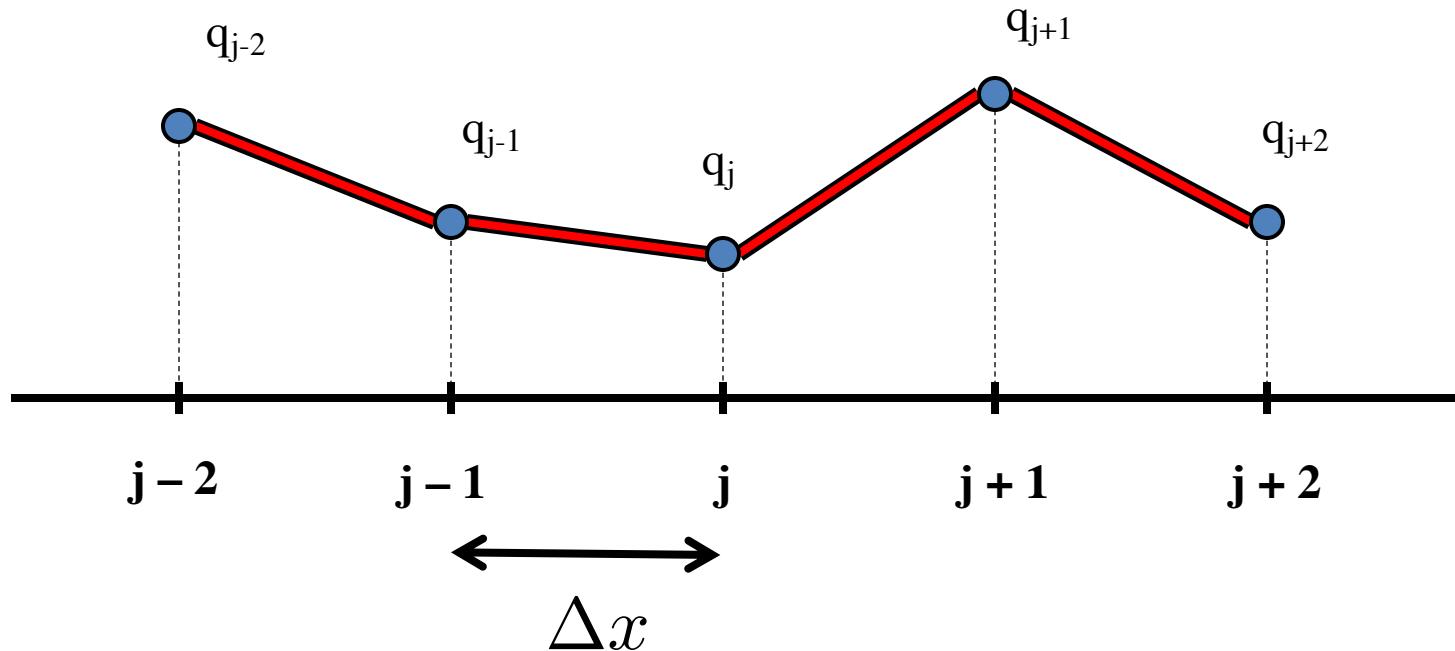
Basic Finite Differences

Consider some arbitrary values associated with q at each point. Grid points are distance Δx apart.



Basic Finite Differences

- The simplest approximation to the continuous field is obtained by connecting nodal points by straight lines.



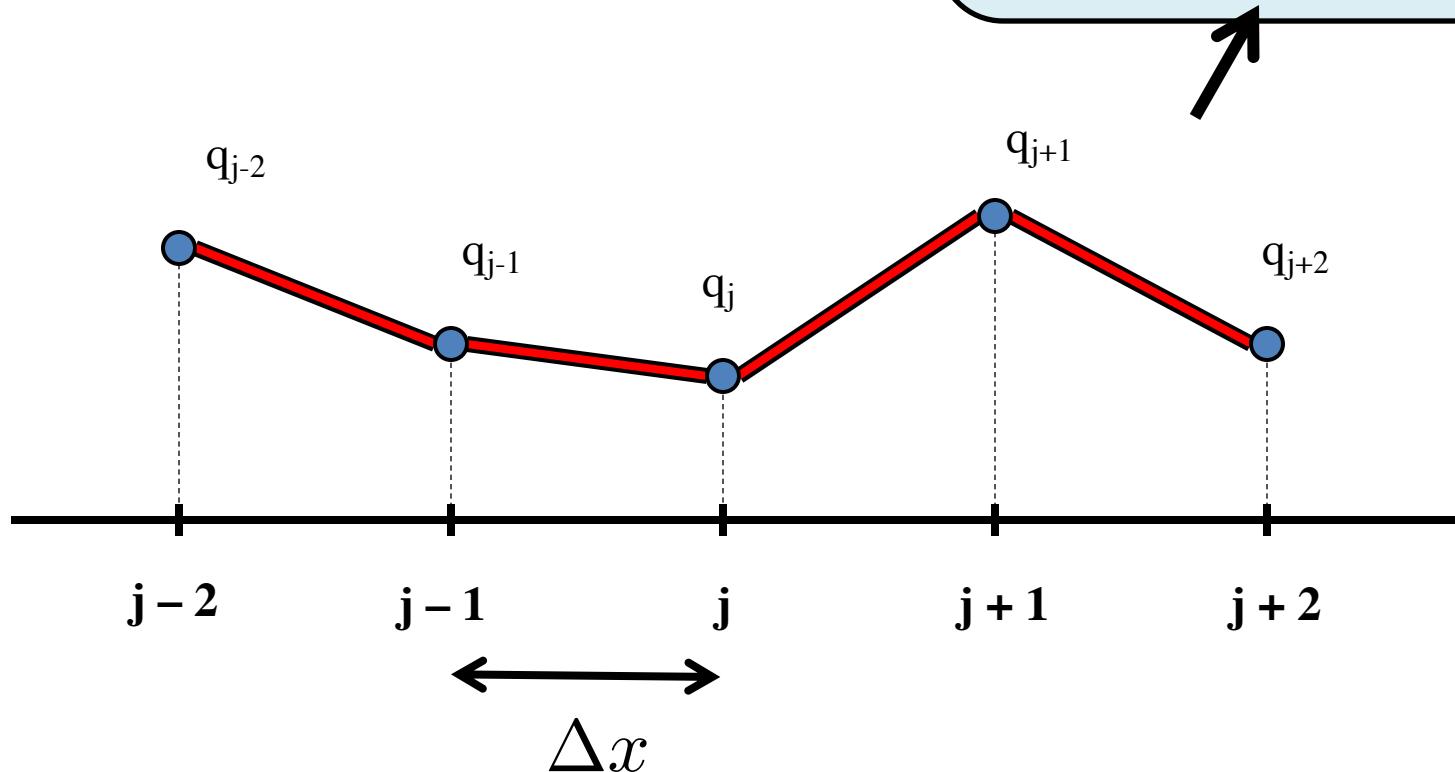
Basic Finite Differences

- We need first derivatives in space to approximate the advection equation

1D Advection Equation

Eulerian Frame

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



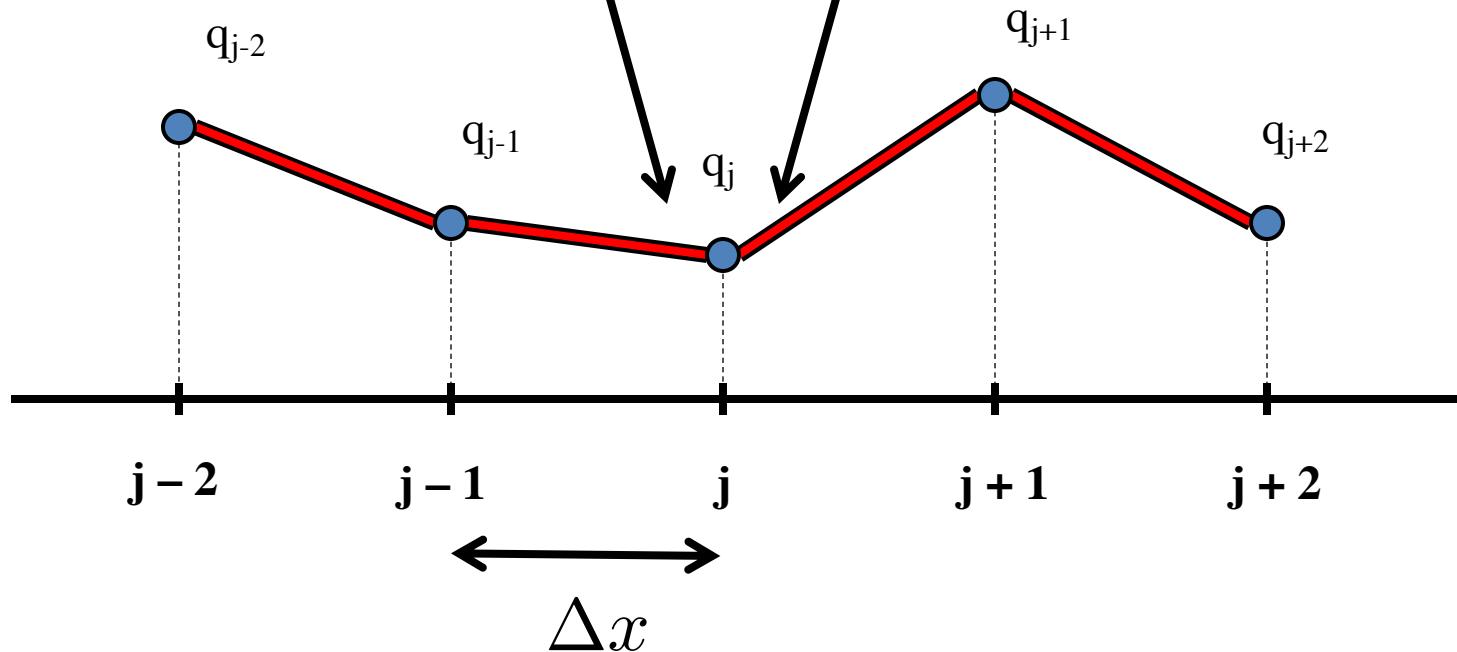
Basic Finite Differences

“Left” Derivative

$$\left(\frac{\partial q}{\partial x} \right)_j^- = \frac{q_j - q_{j-1}}{\Delta x}$$

“Right” Derivative

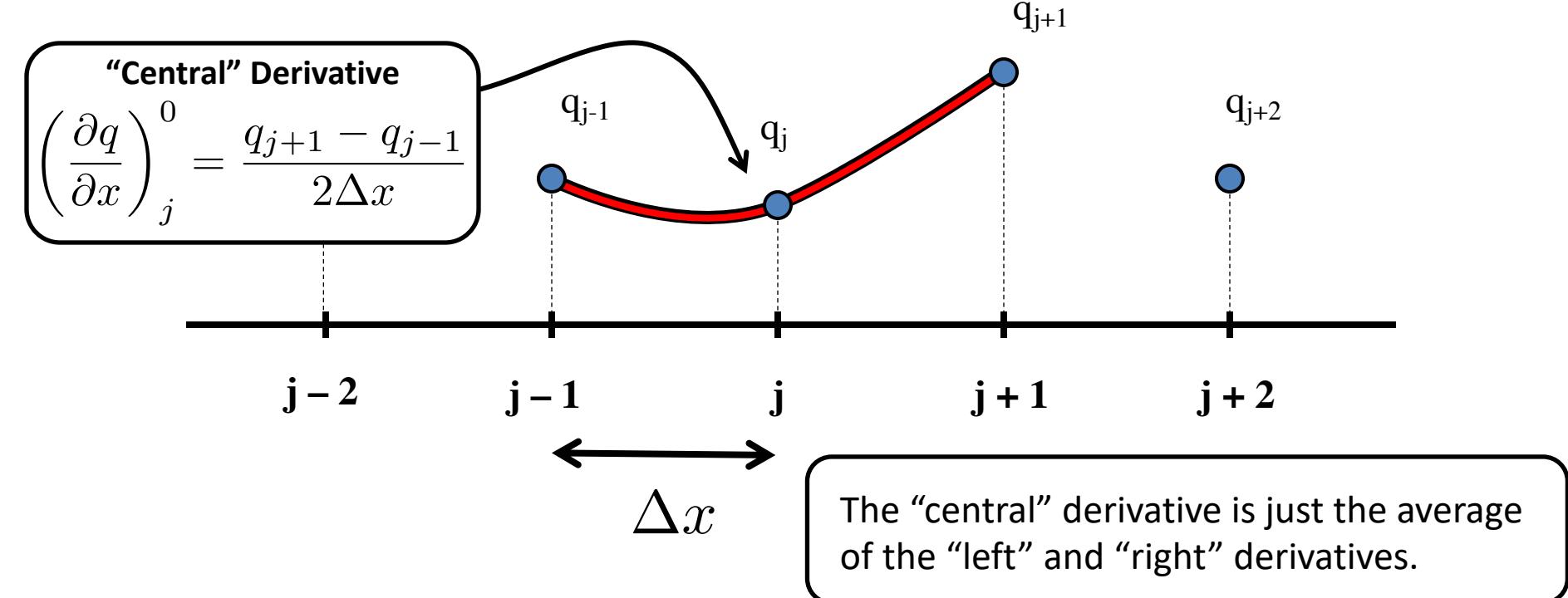
$$\left(\frac{\partial q}{\partial x} \right)_j^+ = \frac{q_{j+1} - q_j}{\Delta x}$$



Basic Finite Differences

A more accurate approximation can be made by fitting a parabola through three neighboring points.

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



Basic Finite Differences

The previously mentioned discrete derivatives then lead to two discrete approximations of the advection equation.

1D Advection Equation

Eulerian Frame

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

$$\frac{\partial q_j}{\partial t} = -u_j \left(\frac{q_j - q_{j-1}}{\Delta x} \right)$$

Upwind Scheme

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

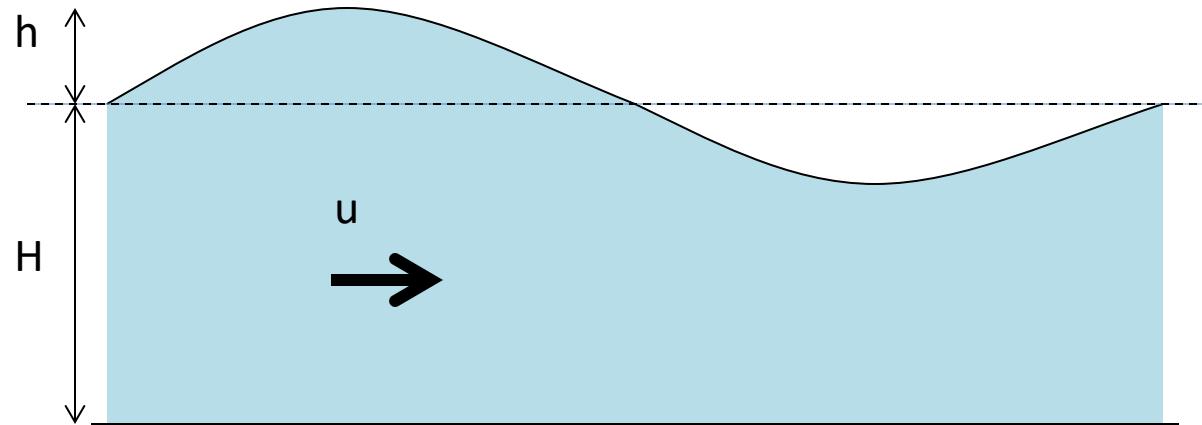
Central Scheme

1D Wave Equation

A bit more complicated (two coupled equations):

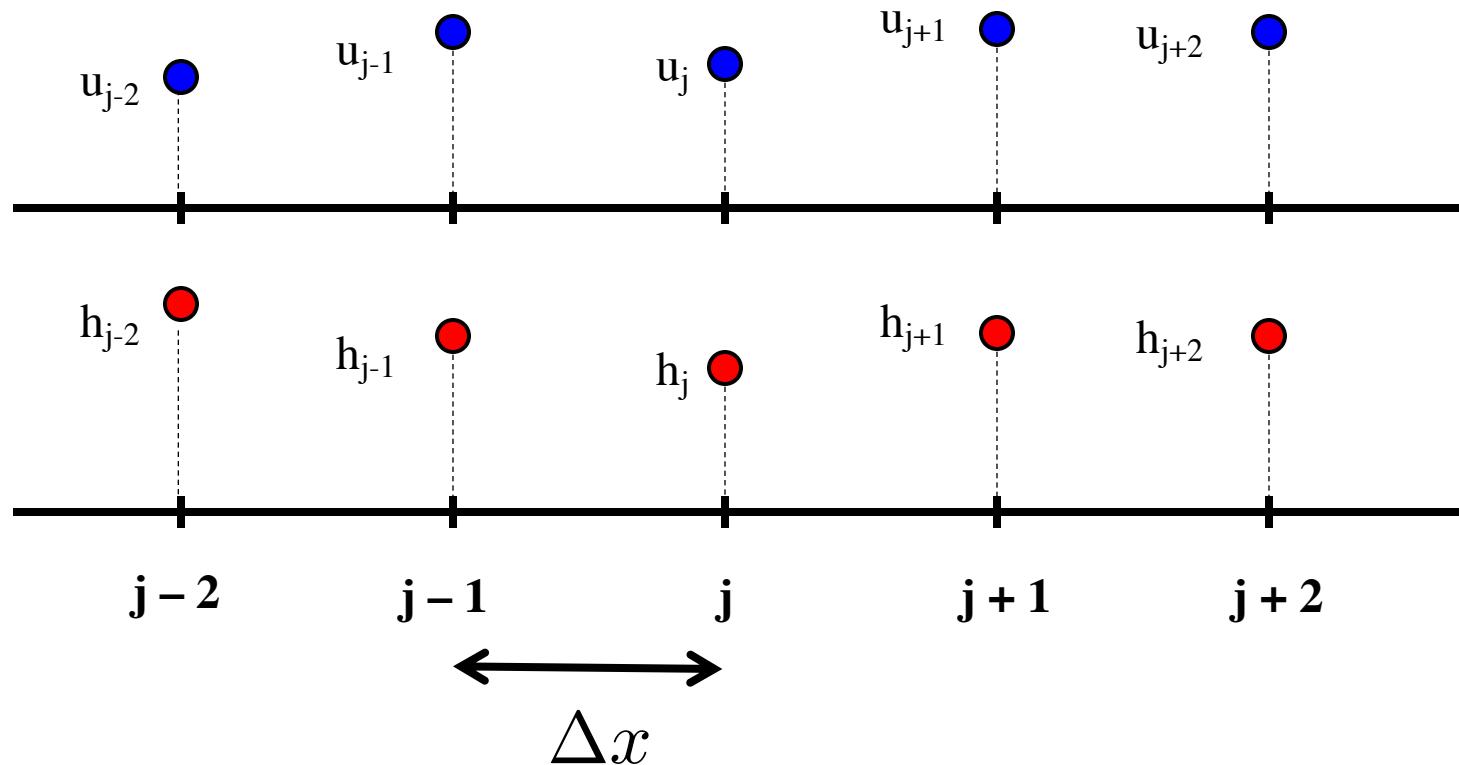
$$\frac{\partial h}{\partial t} + H \frac{\partial u}{\partial x} = 0 \quad \frac{\partial u}{\partial t} + g \frac{\partial h}{\partial x} = 0$$

Used to model small amplitude gravity waves in a shallow ocean basin.



1D Linear Wave Equation

Assume h and u are both stored at the same points (Arakawa A-grid)



1D Linear Wave Equation

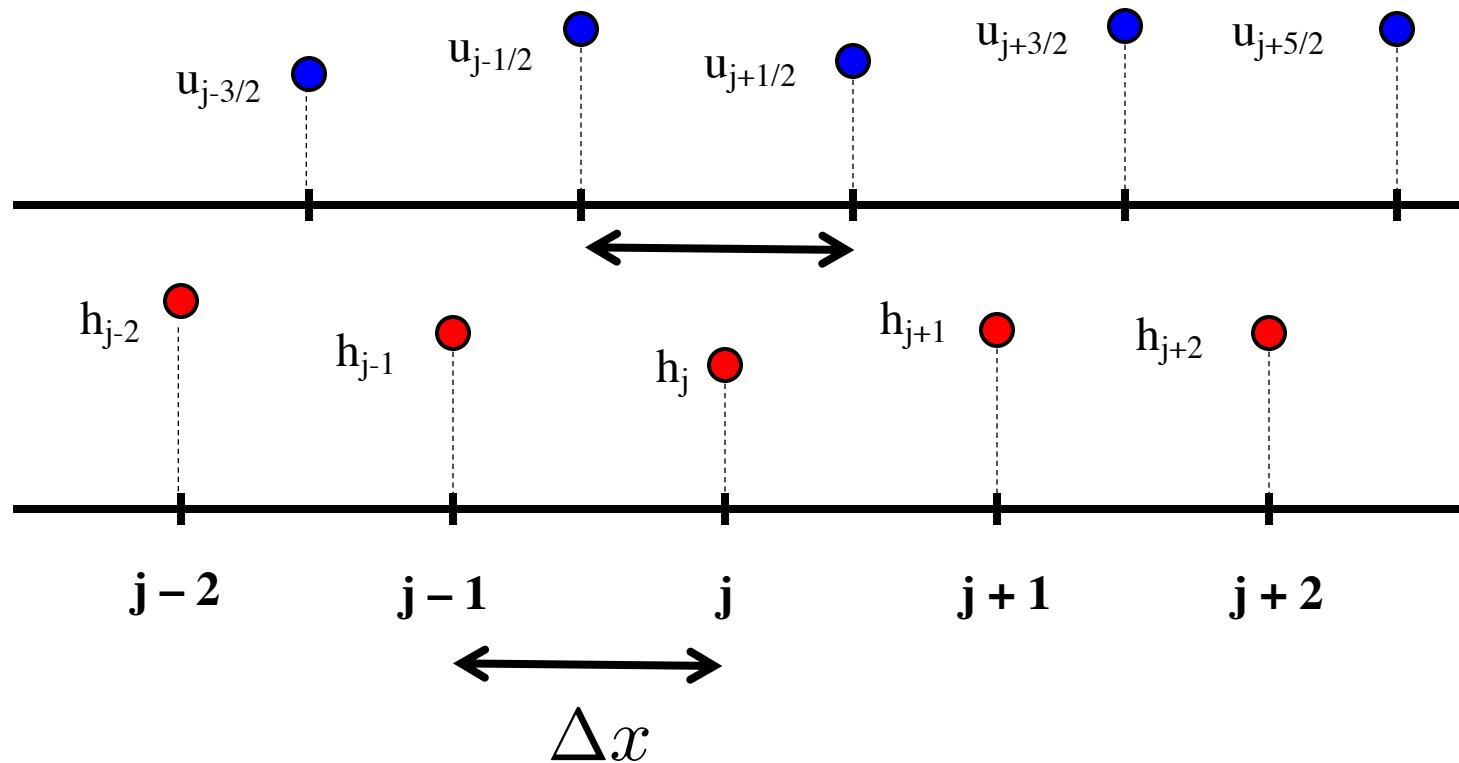
Again using the central difference approximation we derived earlier, the wave equation takes the following discrete form:

$$\frac{\partial h_j}{\partial t} + H \frac{u_{j+1} - u_{j-1}}{2\Delta x} = 0$$

$$\frac{\partial u_j}{\partial t} + g \frac{h_{j+1} - h_{j-1}}{2\Delta x} = 0$$

1D Linear Wave Equation

Other arrangements of h and u nodes are possible (Arakawa C-grid)



1D Linear Wave Equation

With staggered velocities, we can tighten the discretization:

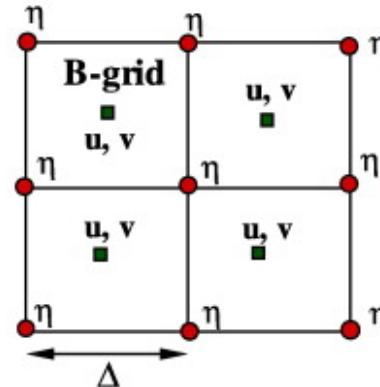
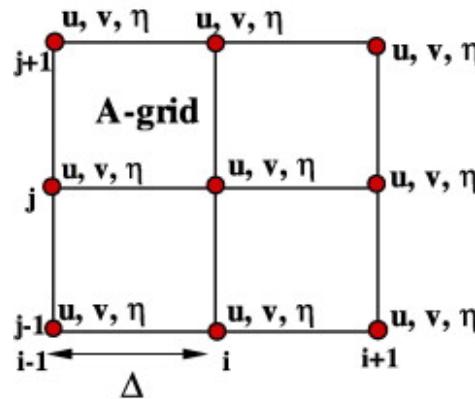
$$\frac{\partial h_j}{\partial t} + H \frac{u_{j+1/2} - u_{j-1/2}}{\Delta x} = 0$$

$$\frac{\partial u_{j+1/2}}{\partial t} + g \frac{h_{j+1} - h_j}{\Delta x} = 0$$

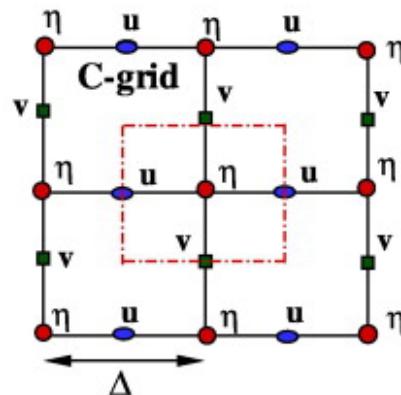
This choice tends to greatly improve errors associated with the discretization.

Arakawa Grid Types (2D)

**CAM-SE
NICAM**



**WRF
MPAS**



CAM-FV

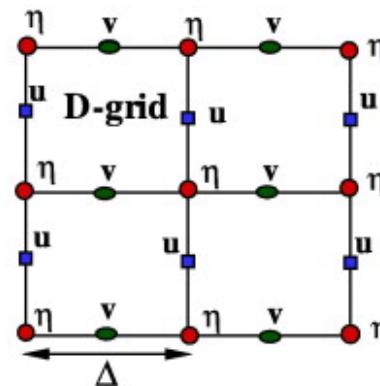


Image: <http://trac.mcs.anl.gov/projects/parvis/wiki/Discretizations>

Finite Difference Methods

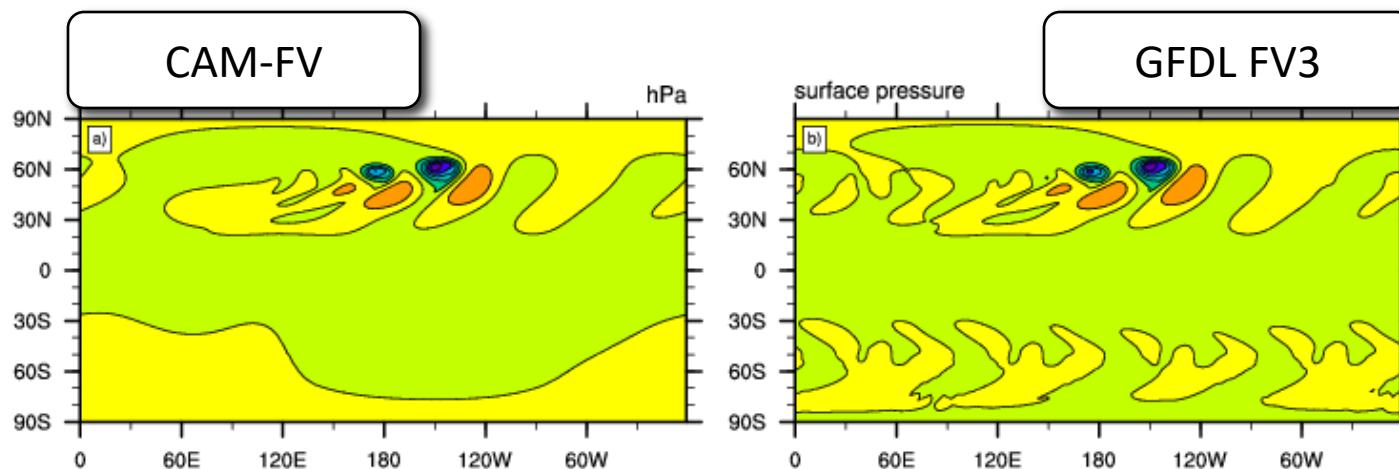
- Finite-difference methods are easy to implement, and consequently are typically fast.
- These methods are very easy to implement implicitly or semi-implicitly (to avoid issues with fast wave).
- One needs to be careful to ensure conservation (not guaranteed by the finite-difference method) and avoid spurious wave solutions.

Finite Volume Methods

CAM-FV
GFDL
FV3
MPAS

Finite Volume Methods

- Scalar variables (density, energy, tracers) are stored as element-averaged values (conservation)
- Velocities can be stored as pointwise values or as element-averaged momentum.



Conservative Shallow Water Eqn's

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

$$\frac{\partial h\mathbf{u}}{\partial t} + \nabla \cdot (h\mathbf{u} \otimes \mathbf{u} + \frac{1}{2}gh^2) = \mathbf{S}$$

h Fluid height

\mathbf{u} Fluid velocity vector

p Fluid pressure

\mathbf{S} Source terms (geometry, Coriolis, topography)

Finite Volume Methods

Given conservation law

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{1}{J} \nabla \cdot \mathbf{F} = \mathbf{S}$$

Integrate over an element \mathcal{Z} with boundary $\partial\mathcal{Z}$ and apply Gauss' divergence theorem. This gives

$$\underbrace{\frac{d\bar{\mathbf{q}}}{dt}}_{\text{Time evolution of element-averaged state}} + \underbrace{\oint_{\partial\mathcal{Z}} \mathbf{F} \cdot \mathbf{n} ds}_{\text{Flux through element boundary}} = \underbrace{\int_{\mathcal{Z}} \mathbf{S} dV}_{\text{Element-averaged source term}}$$

Time evolution of element-averaged state

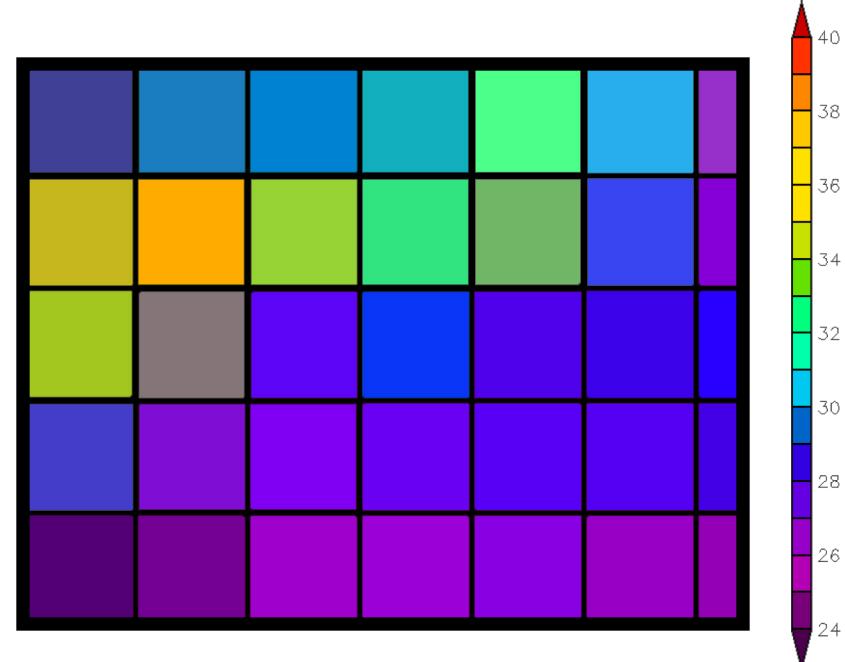
Flux through element boundary

Element-averaged source term

Sub-Grid Scale Reconstruction

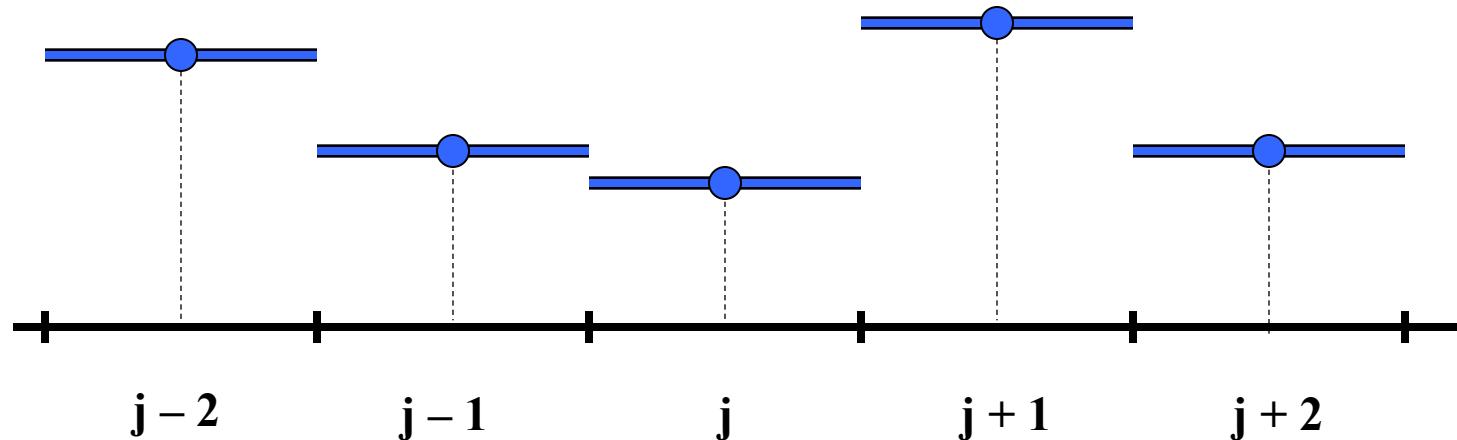
- Scalar variables (density, energy, tracers) are stored as element-averaged values.
- Neighboring values are needed to build a sub-grid-scale reconstruction.

Example: Surface temperature data



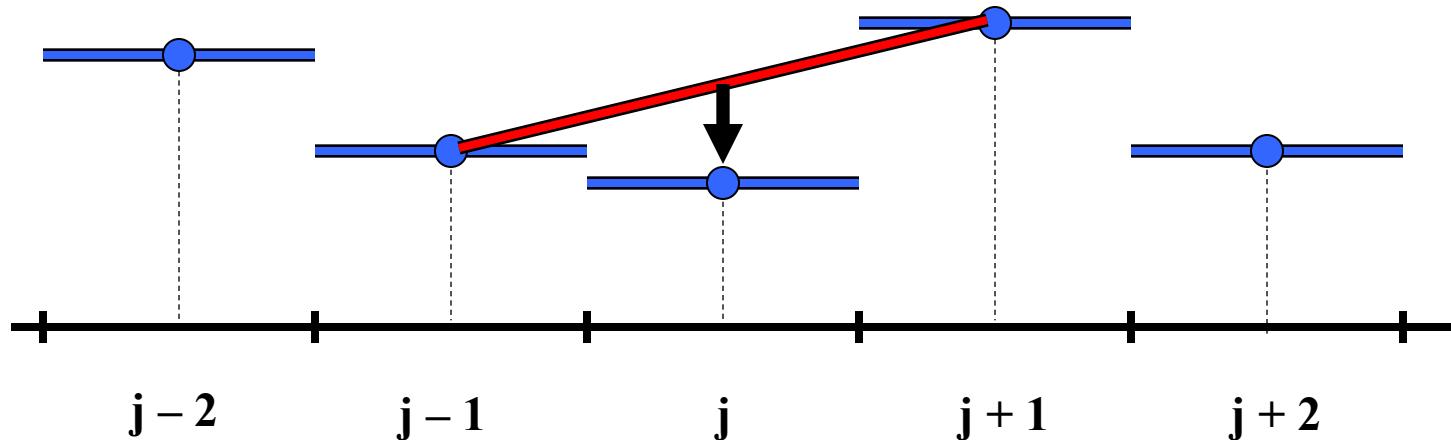
Sub-Grid Scale Reconstruction

- State variables (density, energy, tracers) are stored as element-averaged values.
- Neighboring values are needed to build a sub-grid-scale reconstruction.



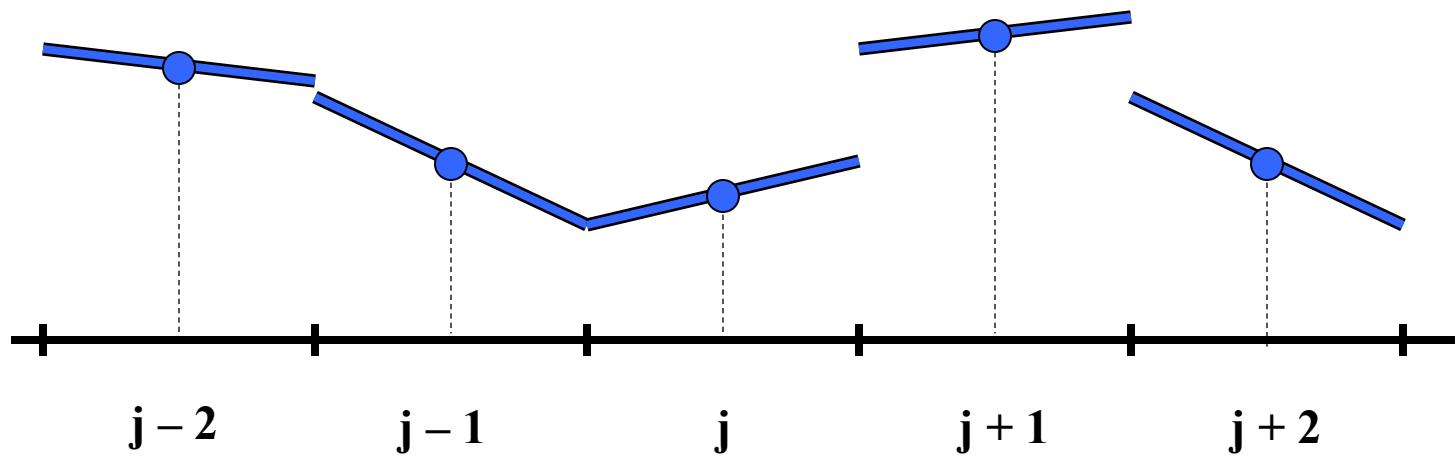
Sub-Grid Scale Reconstruction

- A linear profile: $\phi_j(x) = \bar{\phi}_j + \left(\frac{\partial \phi}{\partial x} \right)_j (x - x_j)$
- An approximation to the slope in element j can be obtained by differencing neighboring elements.

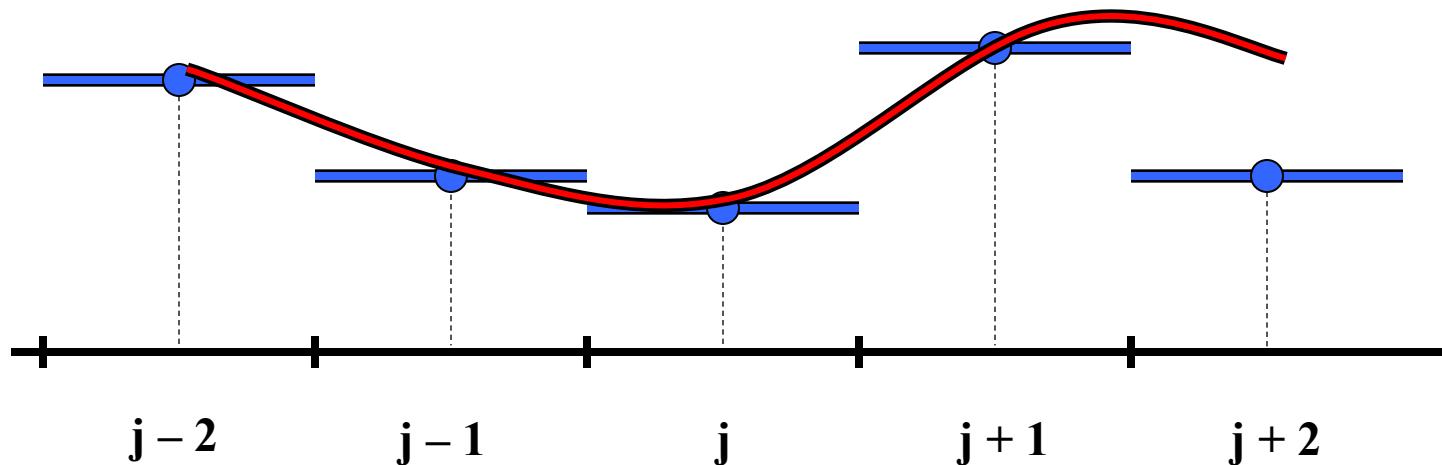


Sub-Grid Scale Reconstruction

When applied to all elements, our sub-grid scale reconstruction captures features which are not apparent at the grid scale.



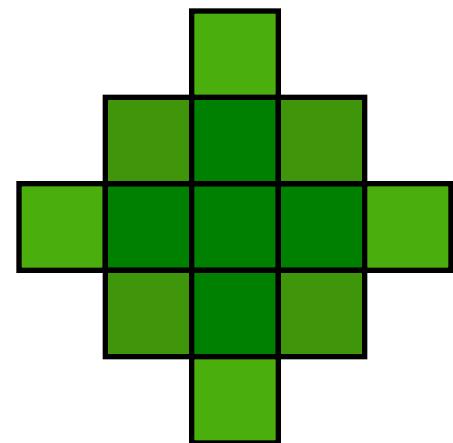
Sub-Grid Scale Reconstruction



A reconstructed cubic polynomial through an element and its four nearest neighbors provides very accurate sub-grid accuracy.

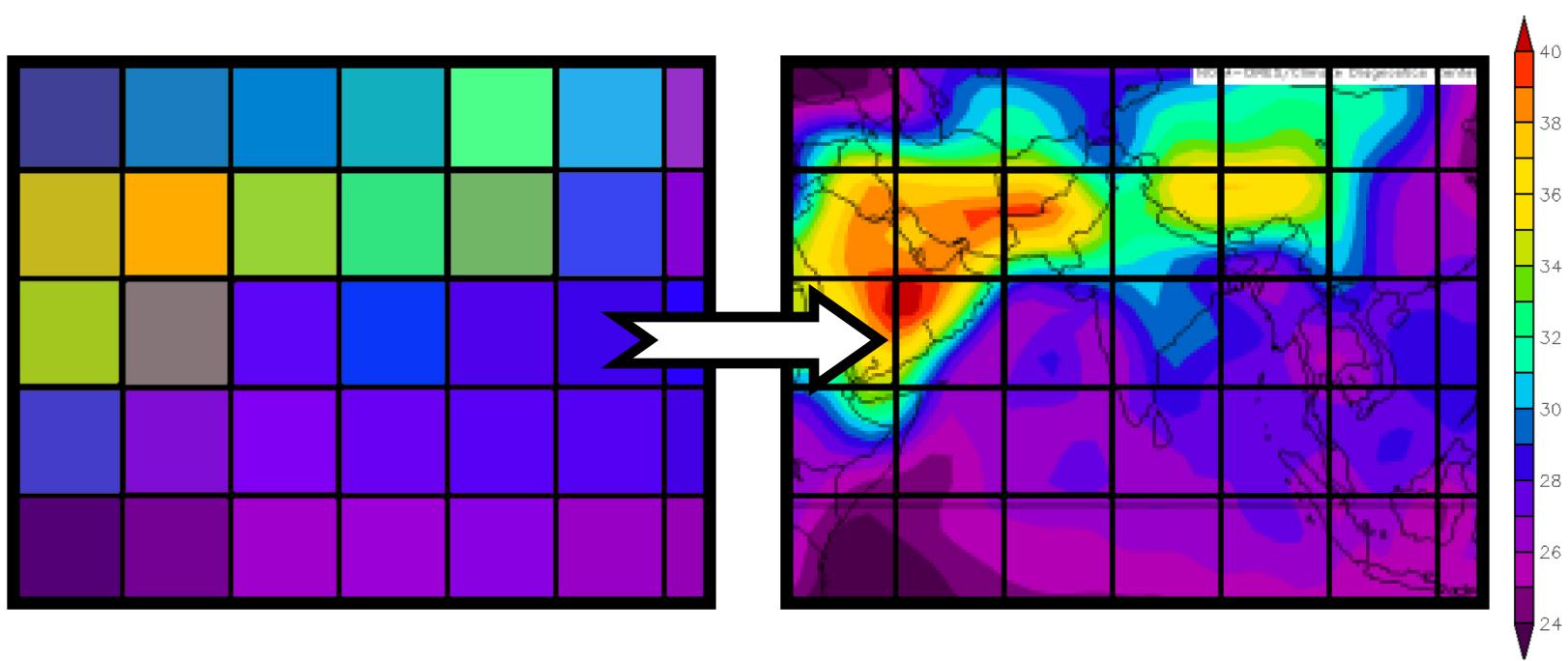
2D Stencil

In higher dimensions the reconstruction stencil incorporates neighboring elements in both directions.



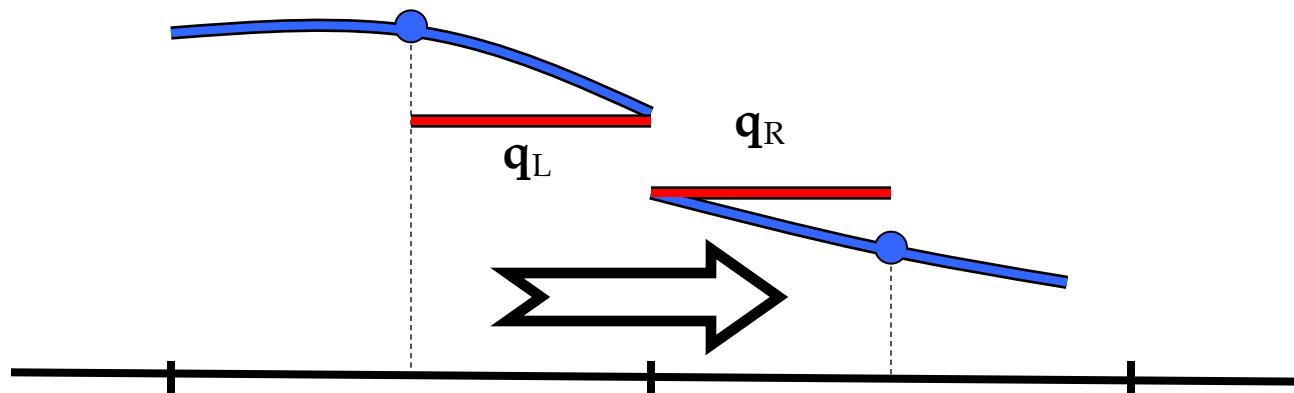
Sub-Grid Scale Reconstruction

Using polynomials information on the sub-grid-scale
(continuous) behavior of each state variable is recovered.



Solving for Fluxes

Since the sub-grid reconstruction can be discontinuous at cell interfaces (we have a left value q_L and right value q_R), we have several options for computing the flux (Riemann solver).



$$\mathbf{q}(x, t = 0) = \begin{cases} \mathbf{q}_L & \text{if } x < 0, \\ \mathbf{q}_R & \text{if } x > 0. \end{cases}$$

Finite Volume Methods

- With appropriately defined fluxes, finite-volume methods do not generally suffer from “spectral ringing” and generally only realize physically attainable states (diffusive errors are dominant)
- Finite-volume methods can be easily made to satisfy monotonicity and positivity constraints (i.e. to avoid negative tracer densities)
- These methods are generally very robust, and are heavily used in other fields.

2D Shallow Water Equations

Continuous Equations (Flux Form)

$$\frac{\partial h}{\partial t} = -\frac{\partial U}{\partial x} - \frac{\partial V}{\partial y}$$

$$\frac{\partial U}{\partial t} = -\frac{\partial}{\partial x}(U^2/h + gh^2/2) - +\frac{\partial}{\partial y}(UV/h)$$

$$\frac{\partial V}{\partial t} = -\frac{\partial}{\partial x}(UV/h) - \frac{\partial}{\partial y}(V^2/h + gh^2/2)$$

Semi-Discrete Equations

$$\frac{\partial h_{i,j}}{\partial t} = F_h$$

$$\frac{\partial U_{i,j}}{\partial t} = F_u$$

$$\frac{\partial V_{i,j}}{\partial t} = F_v$$

Flux terms

$$F_h = -\frac{U_{i+1,j} - U_{i-1,j}}{2\Delta x} - \frac{V_{i,j+1} - V_{i,j-1}}{2\Delta x},$$
$$F_u = -\frac{1}{2\Delta x} [U_{i+1,j}^2/h_{i+1,j} + gh_{i+1,j}^2/2 - U_{i-1,j}^2/h_{i-1,j} - gh_{i-1,j}^2/2]$$
$$- \frac{1}{2\Delta x} [U_{i,j+1}V_{i,j+1}/h_{i,j+1} - U_{i,j-1}V_{i,j-1}/h_{i,j-1}],$$
$$F_v = -\frac{1}{2\Delta x} [U_{i+1,j}V_{i+1,j}/h_{i+1,j} - U_{i-1,j}V_{i-1,j}/h_{i-1,j}]$$
$$- \frac{1}{2\Delta x} [V_{i,j+1}^2/h_{i,j+1} + gh_{i,j+1}^2/2 - V_{i,j-1}^2/h_{i,j-1} - gh_{i,j-1}^2/2]$$

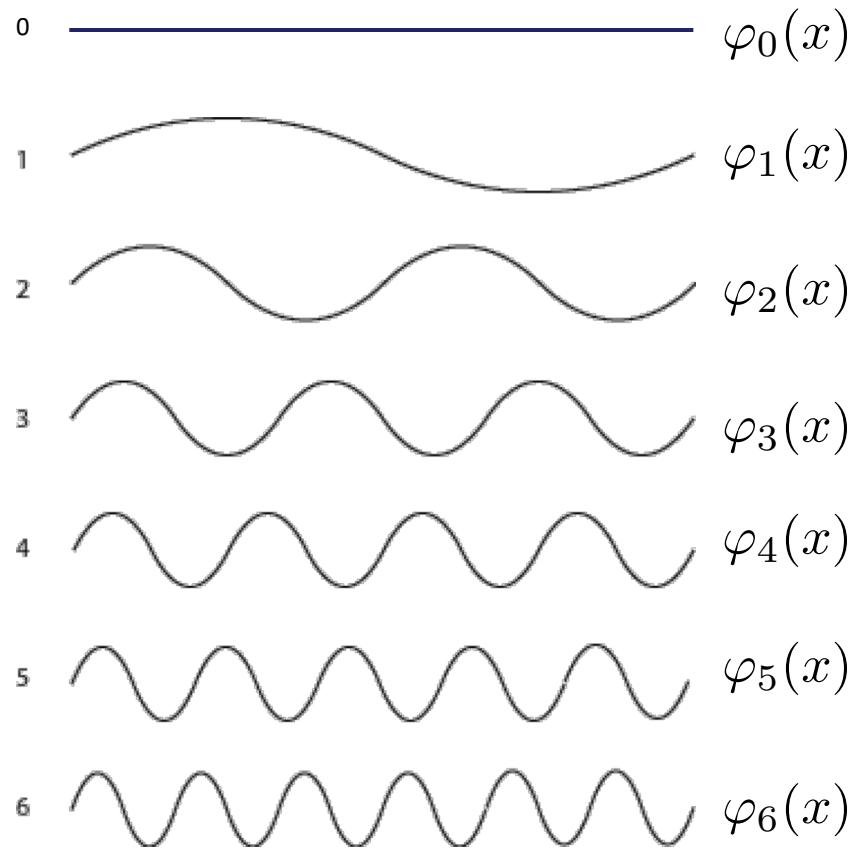
Spectral Methods

CAM-EUL
ECMWF

Linear Harmonics

Instead of writing state variables as pointwise quantities, we can instead write the continuous field as a linear combination of modes:

$$\phi(x, t) = \sum_{k=1}^N a_k(t) \varphi_k(x)$$



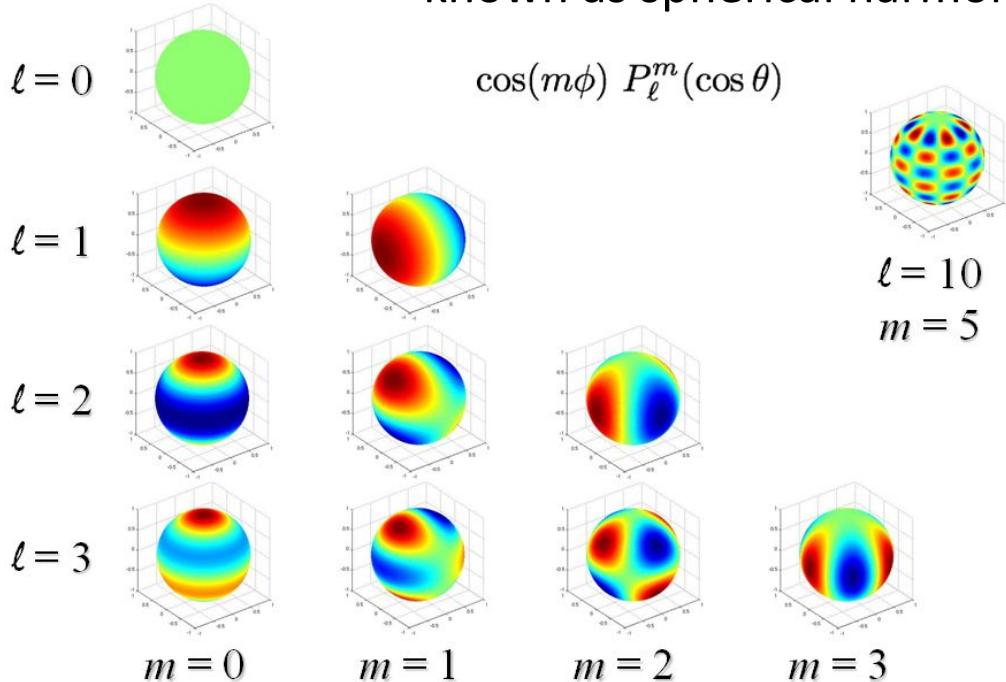
Linear Harmonics: Orthogonality

$$\psi_k(x) = \exp(ikx)$$

$$\int_S \psi_k \psi_n dS = \begin{cases} 2\pi, & \text{if } m = n \\ 0, & \text{if } m \neq n \end{cases}$$

Spherical Harmonics

On the sphere there is a natural basis of modes known as spherical harmonics.



Spherical Harmonics: Orthogonality

$$\int_S \varphi_{\ell,m} \varphi_{k,n} dS = \begin{cases} I_{\ell,m}, & k = \ell \text{ and } m = n \\ 0, & k \neq \ell \text{ or } m \neq n \end{cases}$$

Spectral Methods: Advection

Expand q in terms of basis functions:

$$q(x, t) = \sum_{n=1}^N a_n(t) \psi_n(x)$$

1D Advection Equation

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

Substitute into the 1D advection equation:

$$\sum_{n=1}^N \frac{da_n}{dt} \psi_n = -u \sum_{n=1}^N a_n \frac{\partial \psi_n}{\partial x}$$

Multiply by $\bar{\psi}_k$ and integrate over domain :

$$\sum_{n=1}^N \frac{da_n}{dt} \int_{\mathcal{S}} \psi_n \bar{\psi}_k dx = -u \sum_{n=1}^N a_n \int_{\mathcal{S}} \frac{\partial \psi_n}{\partial x} \bar{\psi}_k dx$$

Spectral Methods: Advection

Use orthogonality. For a linear differential equation, this leads to an exact separation of wave modes:

$$\frac{da_n}{dt} = -inua_n$$

$$\psi_k(x) = \exp(ikx)$$

Observe for exact time integration:

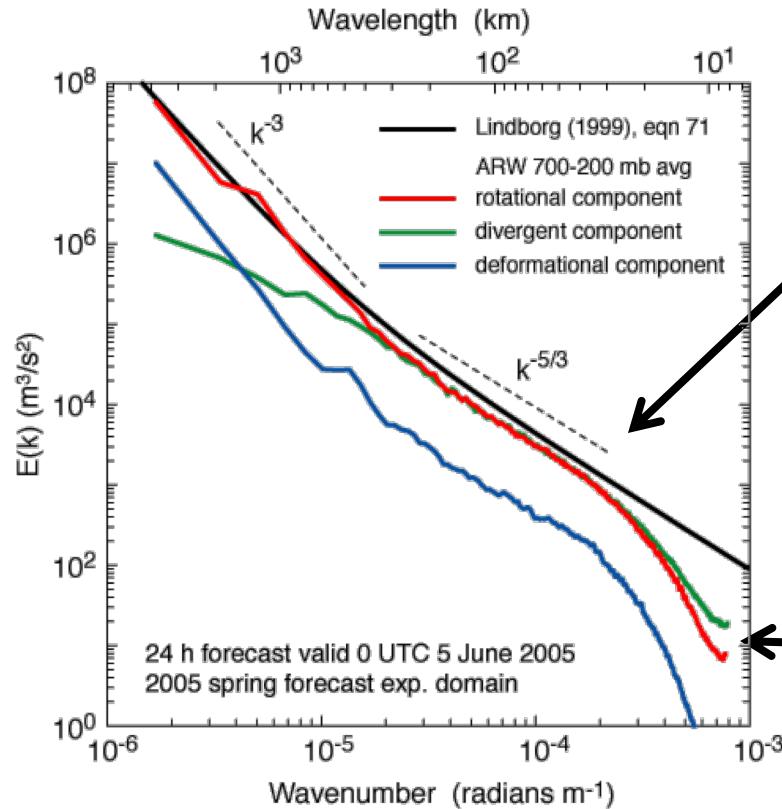
$$a_n = a_{n,0} \exp(-inut)$$

And so $q(x,t)$ is computed exactly!

$$q(x, t) = \sum_{n=1}^N a_n \psi_n = \sum_{n=1}^N a_{n,0} \exp(in(x - ut))$$

Advection at speed u

Energy Spectrum



Decay of energy with wavenumber

Upward tick of energy spectrum implies weak accumulation of energy at smallest scales

Wavenumber is proportional to the inverse wavelength. Hence, larger wavenumbers = shorter waves.

Source: WRF Decomposed Spectra Spring Experiment 2005 Forecast. Courtesy of Bill Skamarock.

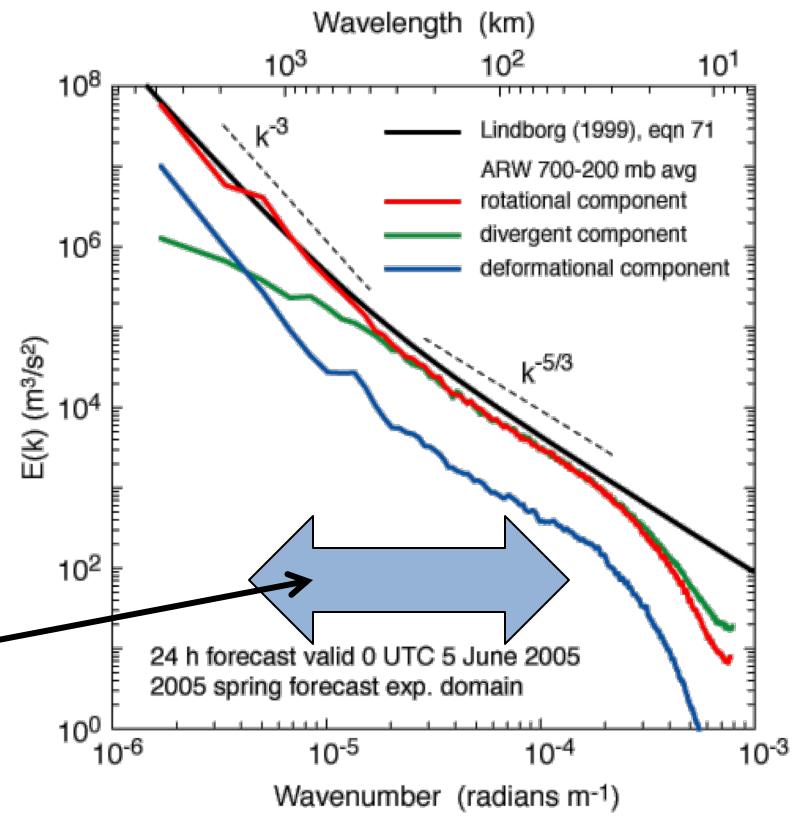
Non-Linear Equations

Non-linear differential equations, such as the ones that govern atmospheric motions include products of state variables with themselves:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \mathbf{g}$$

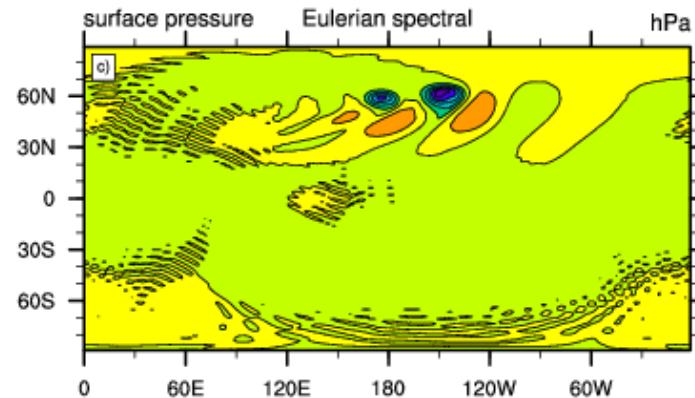
Non-linearity!

... causes mixing
between wavenumbers!



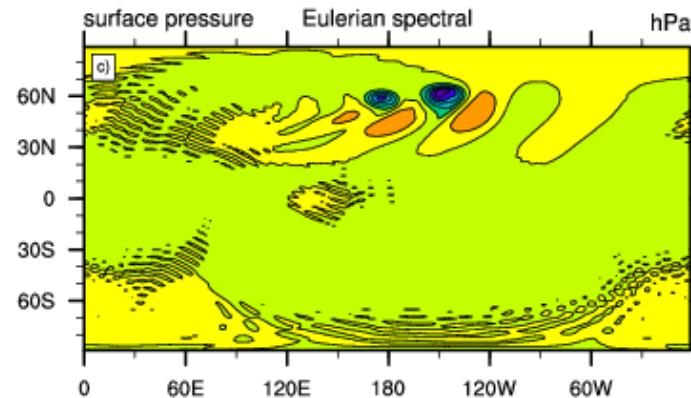
Spectral Methods

- The spatial component of the spectral transform method is “perfect” for linear differential equations. Errors are only introduced by the temporal discretization.
- In practice, the spectral transform method is not used for tracer advection since it is difficult to maintain monotonicity and positivity.
- Errors typically emerge as “spectral ringing.”



Spectral Methods

- Non-linear mixing can cause an accumulation of energy at the smallest grid scales, so additional diffusion is typically needed to remove energy here.
- The spectral transform method requires global communication to accurately handle non-linear terms. This tends to hurt the parallel performance of this method.

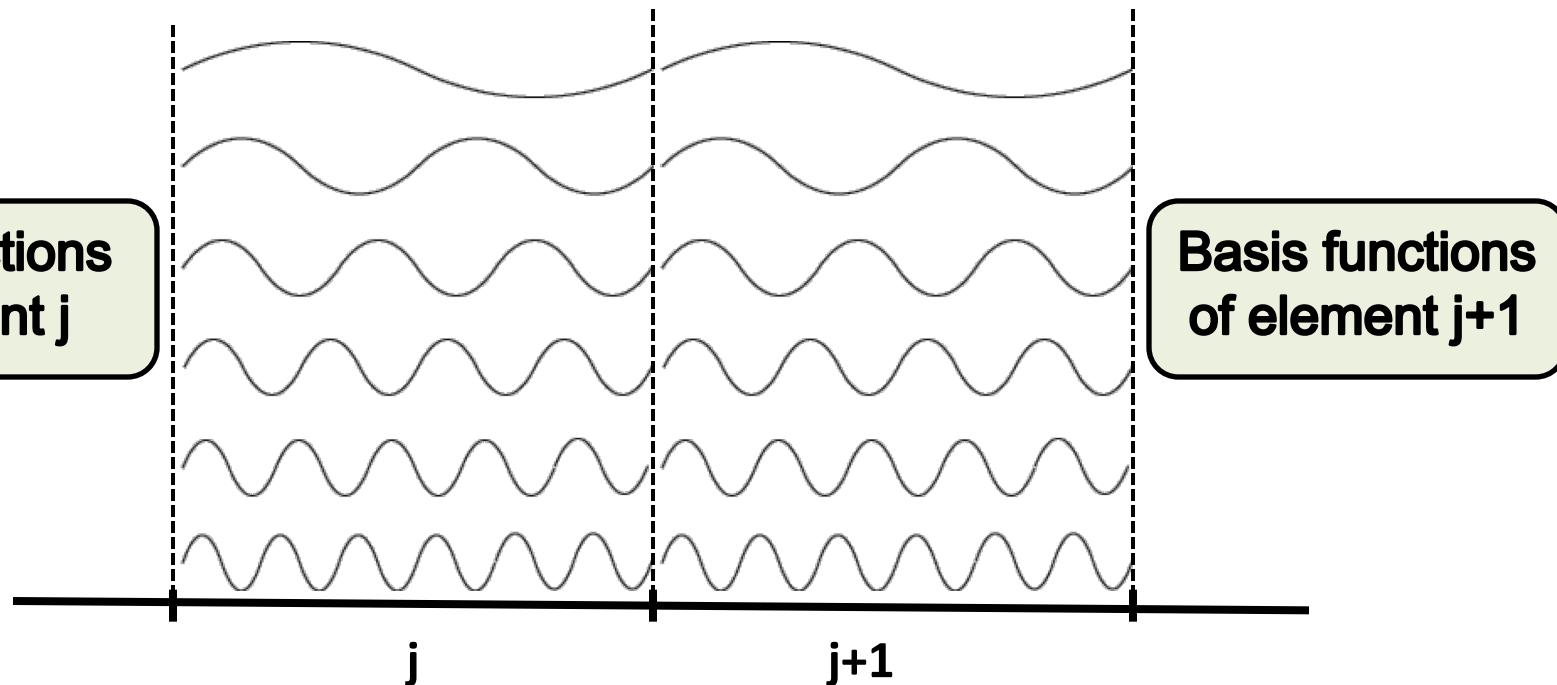


Finite Element Methods

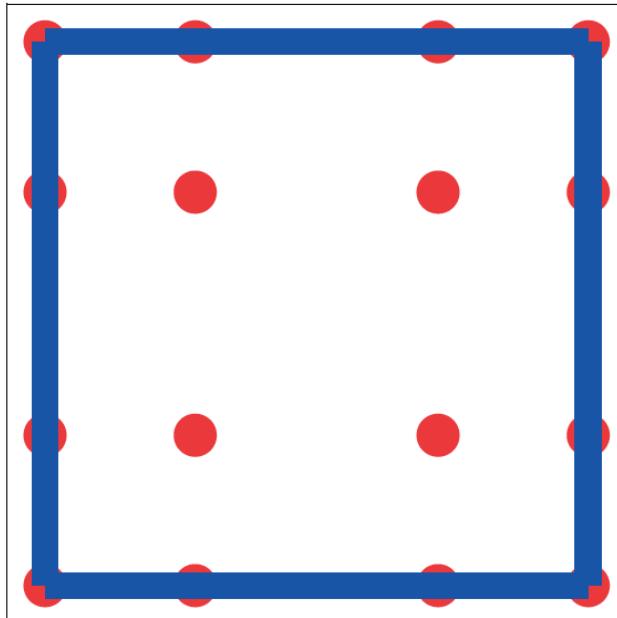
CAM-SE
NUMA

Finite Element Methods

- Finite element methods take the benefits of the spectral transform method with the locality principal of finite-volume methods.
- Can be thought of as spectral transform “in an element”



Spectral Element Method



Fourth order GLL nodes

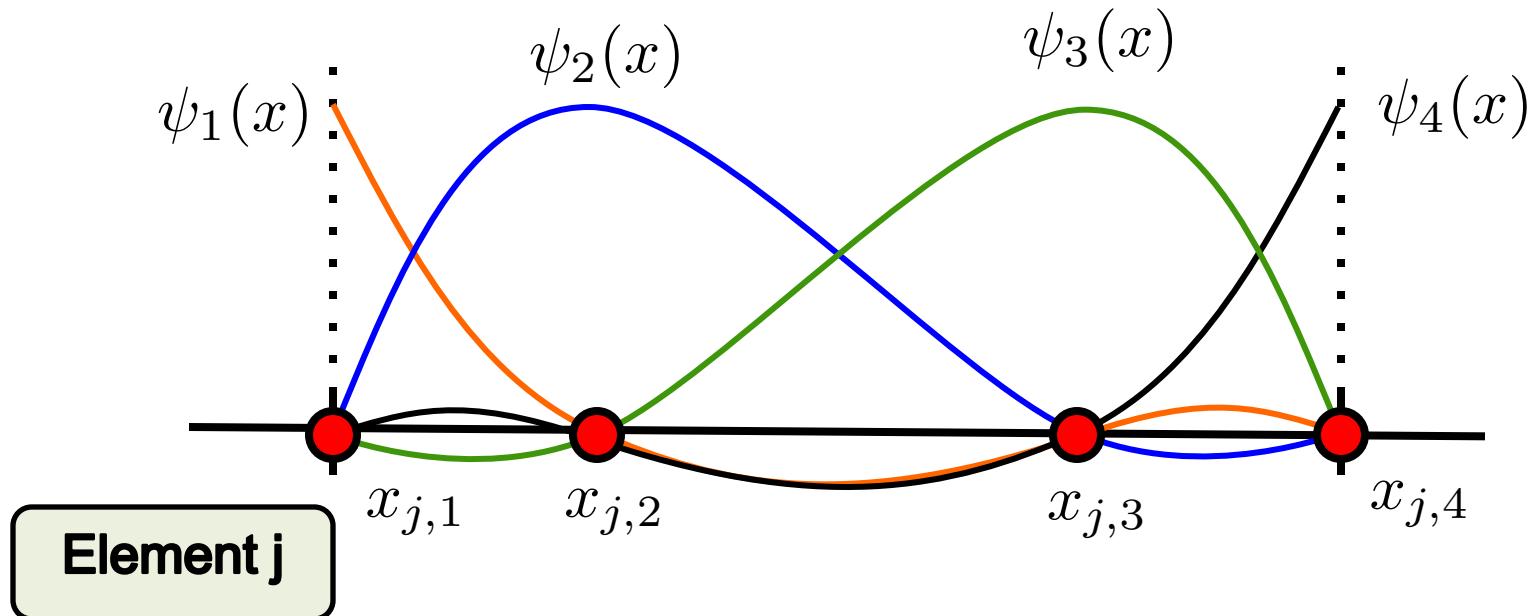
- A n th order finite element method requires n^d basis functions within each element (dimension d).
- To construct basis functions, use GLL nodes within a 2D element.
- Fit polynomials so that each basis function is 1 at one node and 0 at all other nodes.

Image: <http://trac.mcs.anl.gov/projects/parvis/wiki/Discretizations>

Finite Element Method

Expand q in terms of basis functions within an element:

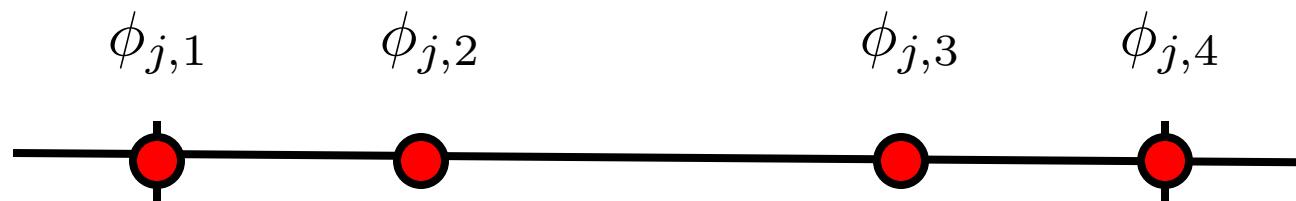
$$q(x, t) = \sum_{n=1}^N a_n(t) \psi_n(x)$$



Finite Element Methods

Note that the use of GLL nodes means that there is an implicit discrete integration rule:

$$\int_{\mathcal{S}_j} \phi(x, t) dx \approx w_1 \phi_{j,1} + w_2 \phi_{j,2} + w_3 \phi_{j,3} + w_4 \phi_{j,4}$$



Finite Element Methods

Expand q in terms of basis functions within an element:

$$q(x, t) = \sum_{n=1}^N a_n(t) \psi_n(x)$$

1D Conservation Eq'n

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} F(q) = 0$$

Substitute into the 1D conservation equation:

$$\sum_{n=1}^N \frac{da_n}{dt} \psi_n = - \frac{\partial}{\partial x} F \left(\sum_{n=1}^N a_n \psi_n \right)$$

Multiply by $\bar{\psi}_k$ and integrate over an element:

$$\sum_{n=1}^N \frac{da_n}{dt} \int_{\mathcal{S}_j} \psi_n \bar{\psi}_k dx = - \int_{\mathcal{S}_j} \frac{\partial F}{\partial x} \bar{\psi}_k dx$$

Finite Element Methods

Apply integration by parts:

1D Conservation Eq'n

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} F(q) = 0$$

$$\sum_{n=1}^N \frac{da_n}{dt} M_{n,k} = -F(x) \bar{\psi}_k \Big|_{\partial \mathcal{S}_j} + \int_{\mathcal{S}_j} F(x) \frac{d\bar{\psi}_k}{dx} dx$$

Time evolution
of coefficients

Flux through
edges

Internal
exchange

With mass matrix: $M_{n,k} = \int_{\mathcal{S}_j} \psi_n \bar{\psi}_k dx$

Finite Element Methods

$$\sum_{n=1}^N \frac{da_n}{dt} M_{n,k} = -F(x) \bar{\psi}_k \Big|_{\partial \mathcal{S}_j} + \int_{\mathcal{S}_j} F(x) \frac{d\bar{\psi}_k}{dx} dx$$

To evaluate internal exchange term,
use integration property on interior:

Internal
exchange

$$\int_{\mathcal{S}_j} \phi(x, t) dx \approx w_1 \phi_{j,1} + w_2 \phi_{j,2} + w_3 \phi_{j,3} + w_4 \phi_{j,4}$$

1D Conservation Eq'n

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} F(q) = 0$$

Finite Element Methods

$$\sum_{n=1}^N \frac{da_n}{dt} M_{n,k} = -F(x) \bar{\psi}_k \Big|_{\partial \mathcal{S}_j} + \int_{\mathcal{S}_j} F(x) \frac{d\bar{\psi}_k}{dx} dx$$

**Flux through
edges**

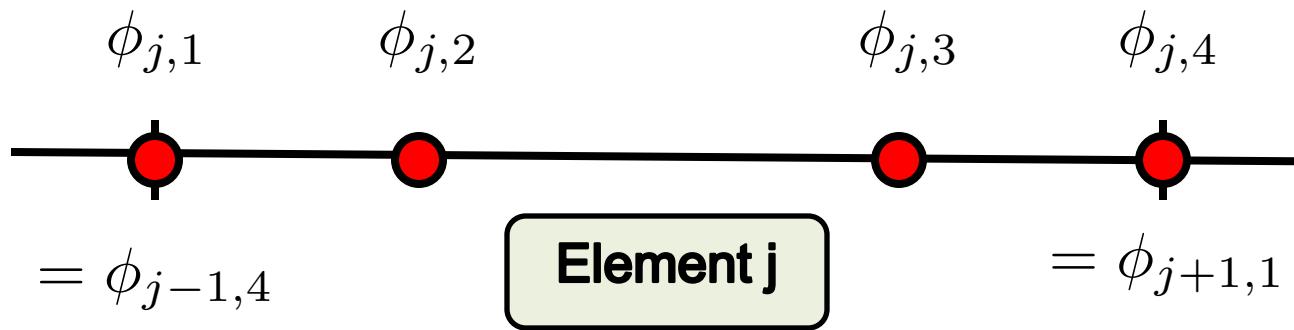
- Spectral Element method: Enforce continuity at element boundaries. Flux function is simple function evaluation.
- Discontinuous Galerkin method: Discontinuous at element edges. A Riemann solver must be applied to evaluate flux here.

Finite Element Methods

Q: How does Spectral Element method enforce continuity?

A: Easy! Evolve nodal values in both elements. Then take average:

$$\phi_{j,1}^{n+1} = \phi_{j-1,4}^{n+1} = \frac{\phi_{j,1}^* + \phi_{j-1,4}^*}{2}$$



Equivalence with Finite Difference

The spectral element method can be interpreted as a finite difference scheme.

1D Advection Equation

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

“Spectral” Derivative

$$\left(\frac{\partial q}{\partial x} \right)_{x=x_{j,3}} = \sum_{n=1}^N a_n \frac{d\psi}{dx}(x_{j,3})$$

