Numerical Methods I: (Horizontal) Spatial Discretizations

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Dynamical Core Model Intercomparison Project (DCMIP) 2012 Summer School

Outline

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

Part 1

Introduction

- Continuous versus discrete
- Gridding the sphere
- Numerical Methods: Issues

Continuous vs. Discrete

Atmospheric Modeling – Question One

- How do we best represent continuous data when only a (very) limited amount of information can be stored?

- How do we best represent continuous data discretely?

The Regular Latitude-Longitude Grid

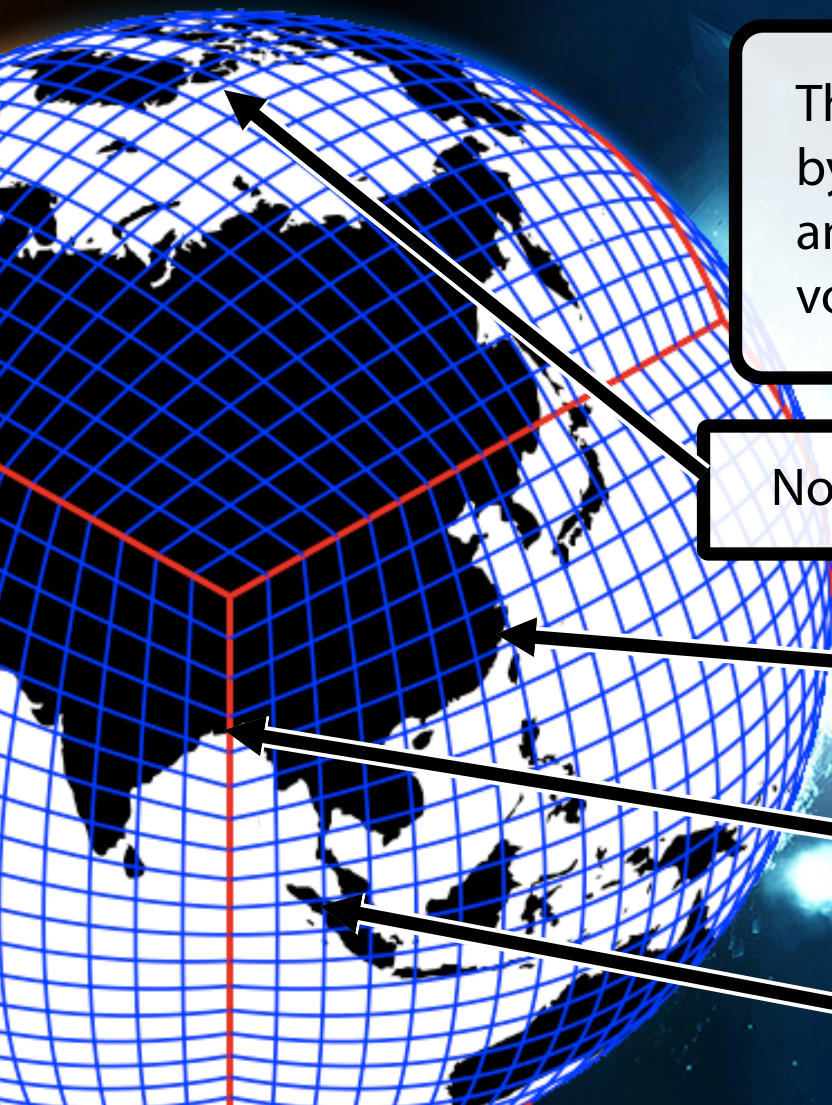
Grid lines are represented by lines of constant latitude and longitude.

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

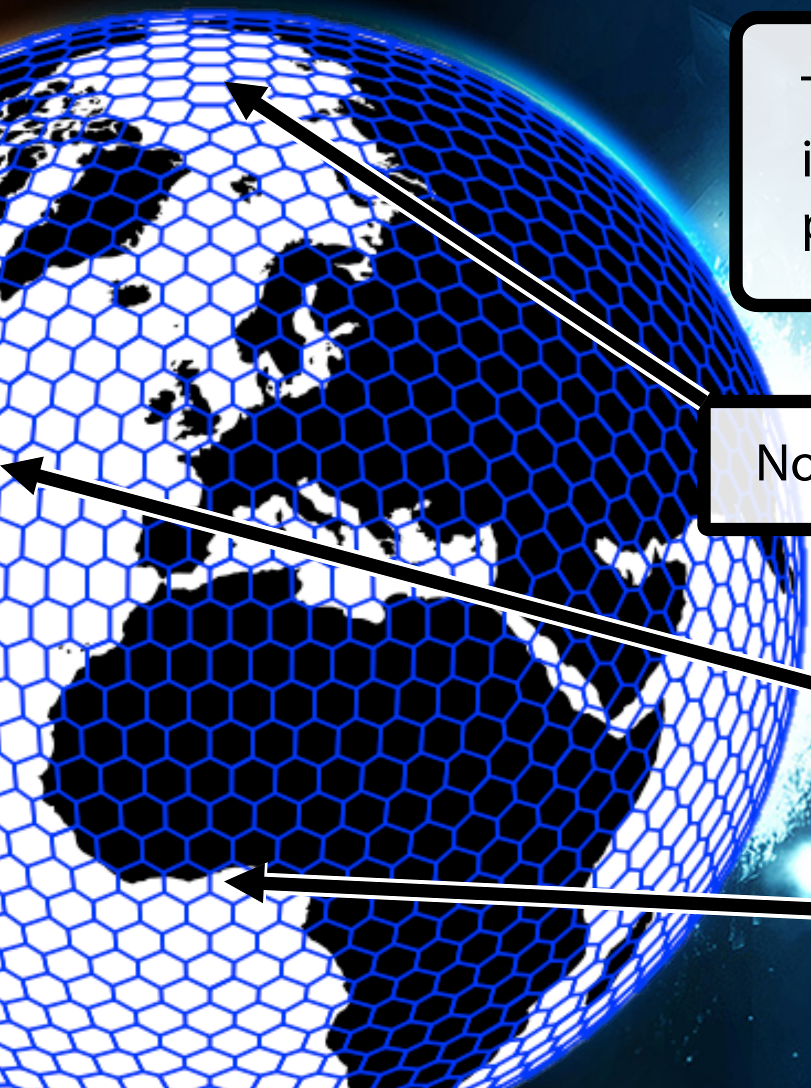
Grid faces individually regular

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.

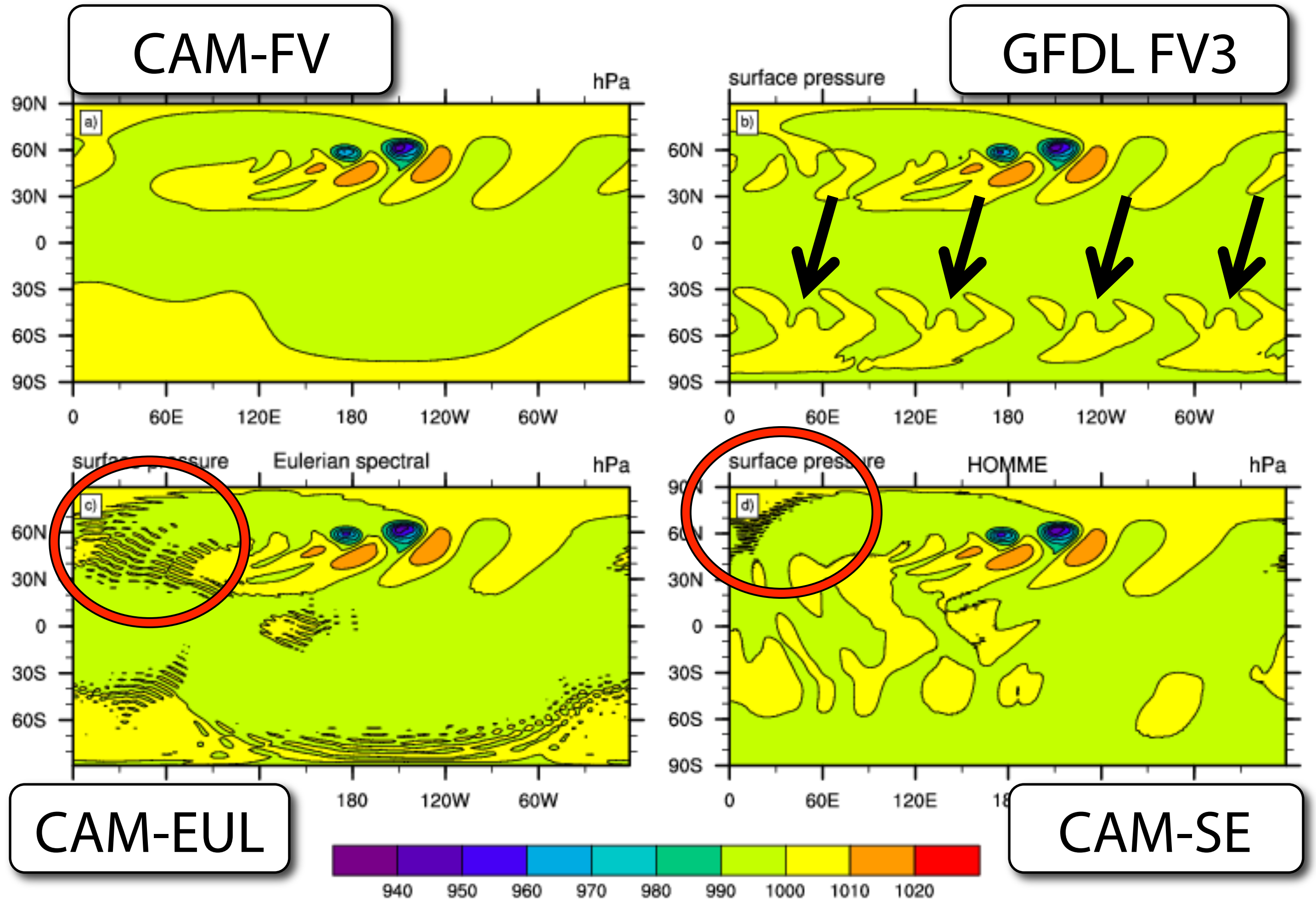


No polar singularities

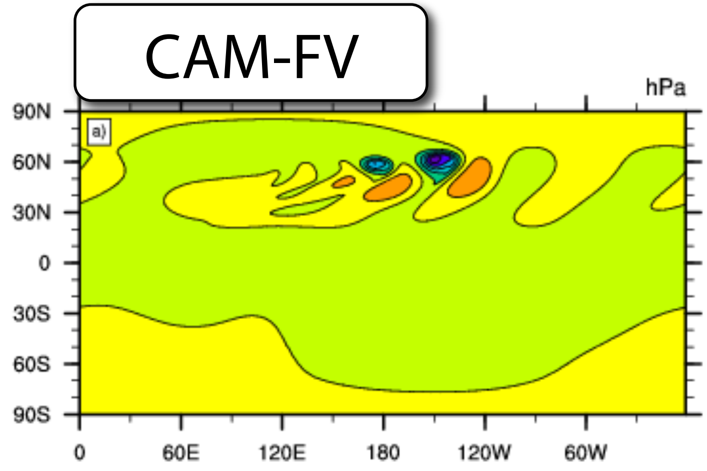
Grid largely unstructured

Most uniform element spacing

Numerical Methods: Issues



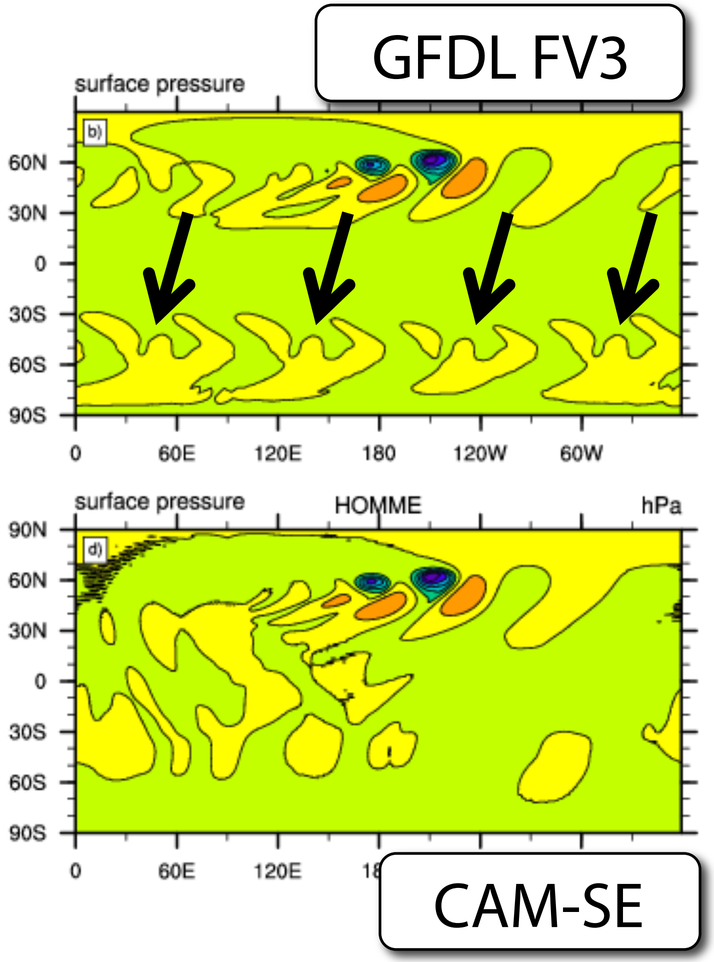
Numerical Methods: Issues

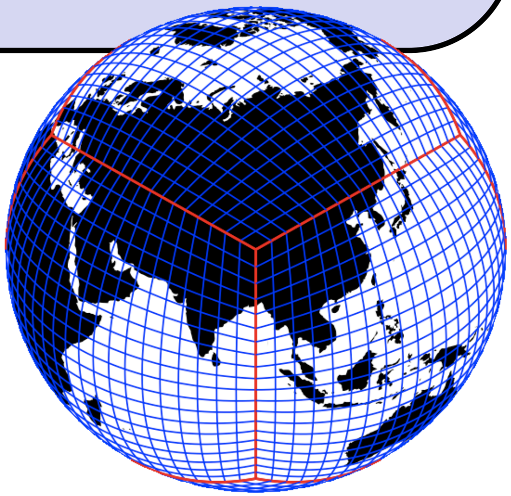


Although it is a standard in climate modeling, the CAM-FV model is known to possess a strong diffusive signature. Diffusion is enhanced as one approaches the poles in order to maintain stability.

Numerical Methods: Issues

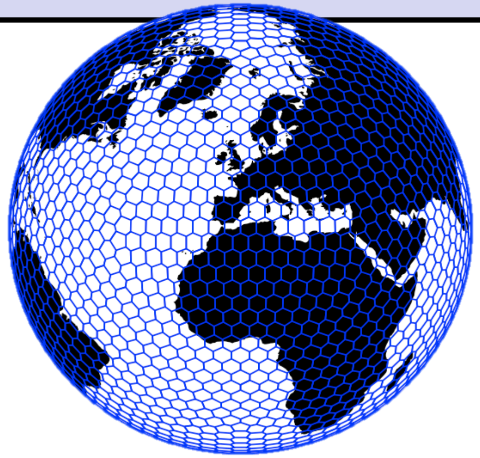
Both the GFDL FV3 (FVcubed) model and CAM-SE (spectral element) model are built on the cubed-sphere. This leads to an enhancement of the k=4 wave mode. The use of high-order numerics in CAM-SE is more effective at repressing this mode.



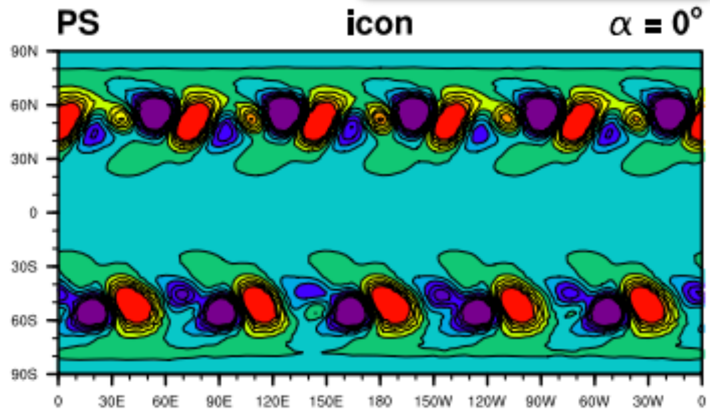


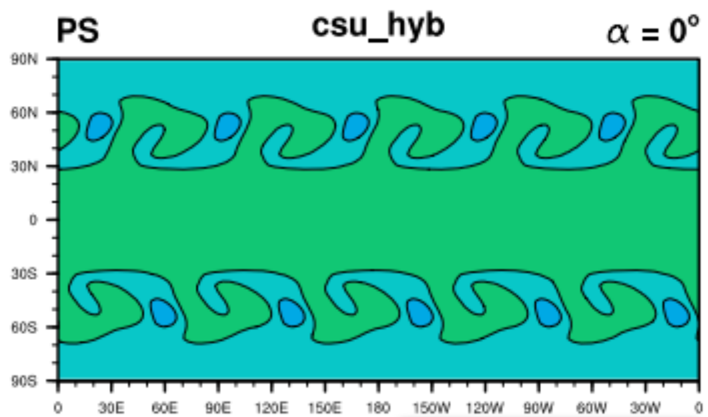
Numerical Methods: Issues

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.



ICON

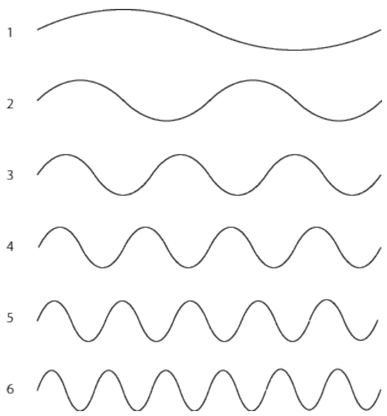


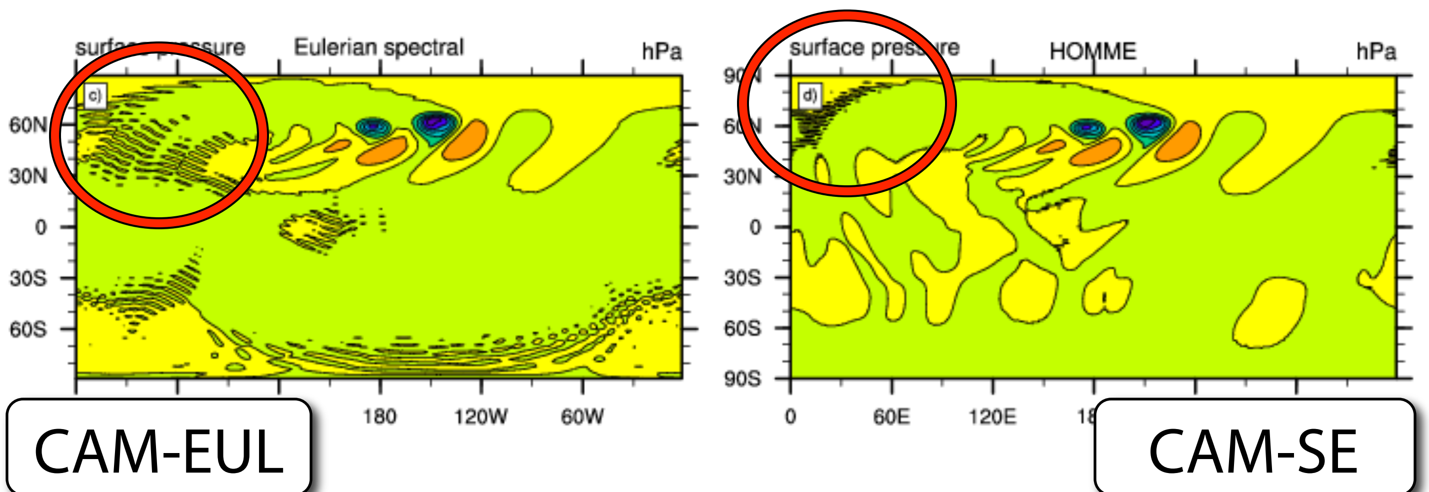


CSU

Numerical Methods: Issues

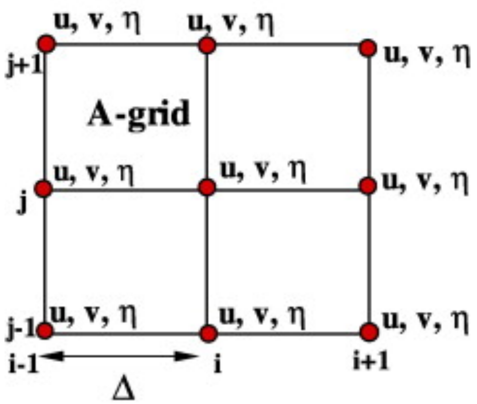
CAM-EUL (Eulerian) and CAM-SE (spectral element) use spectral methods, which are known to be prone to spectral ringing. This ringing is characterized by rapid oscillations due to enhancement of the high-frequency mode.





Numerical Methods: Grid 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.

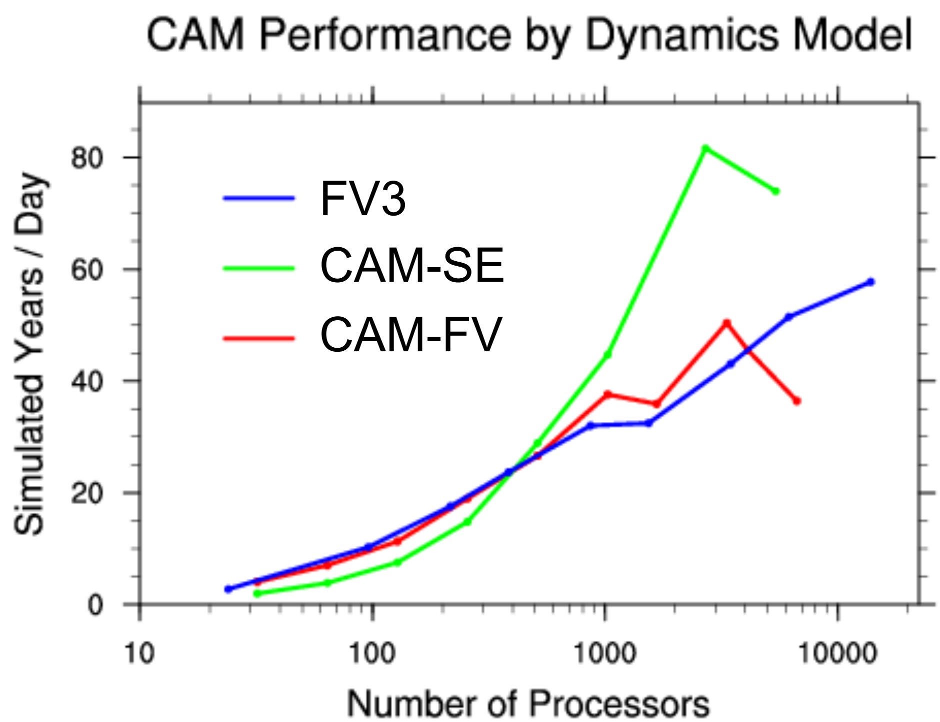


Summary: When it comes to designing numerical methods, there's no free lunch!

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.

Spectral Element
Discontinuous Galerkin
Spectral Volume



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)

Part 2

Finite Difference Methods

Advection of a Tracer

We are interested in solving the advection equation:

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

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

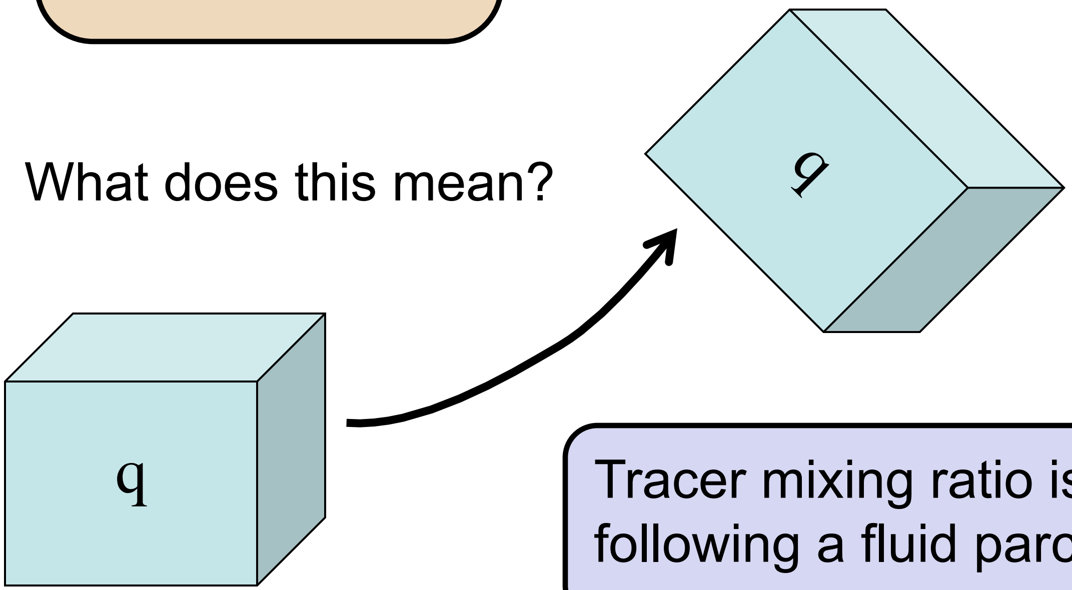
Lagrangian Frame

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

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

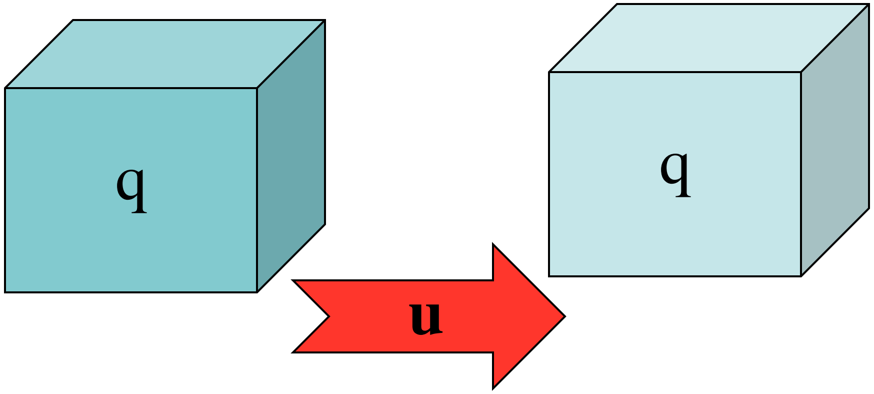
Lagrangian Frame

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

Eulerian Frame

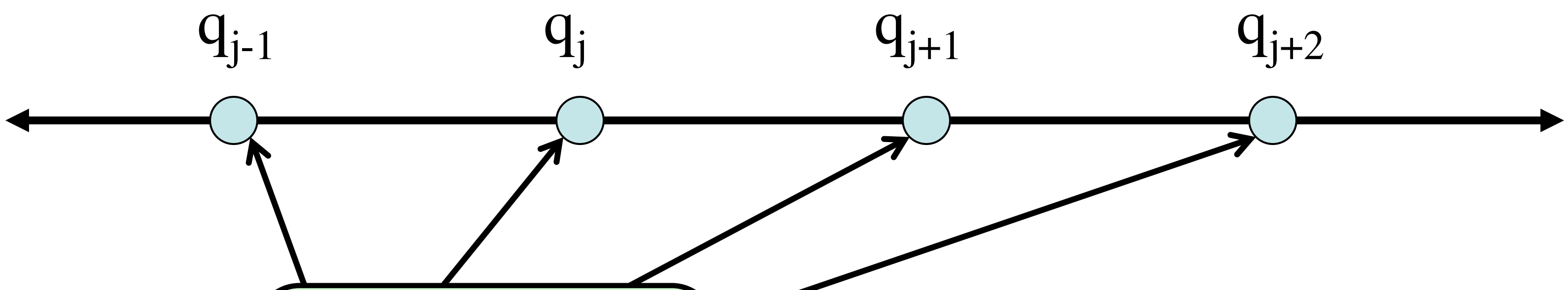
$$\frac{\partial q}{\partial t} + \mathbf{u} \cdot \nabla q = 0$$

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



Data is known pointwise (*DISCRETE*)

How do we understand the *CONTINUOUS* behavior of q?

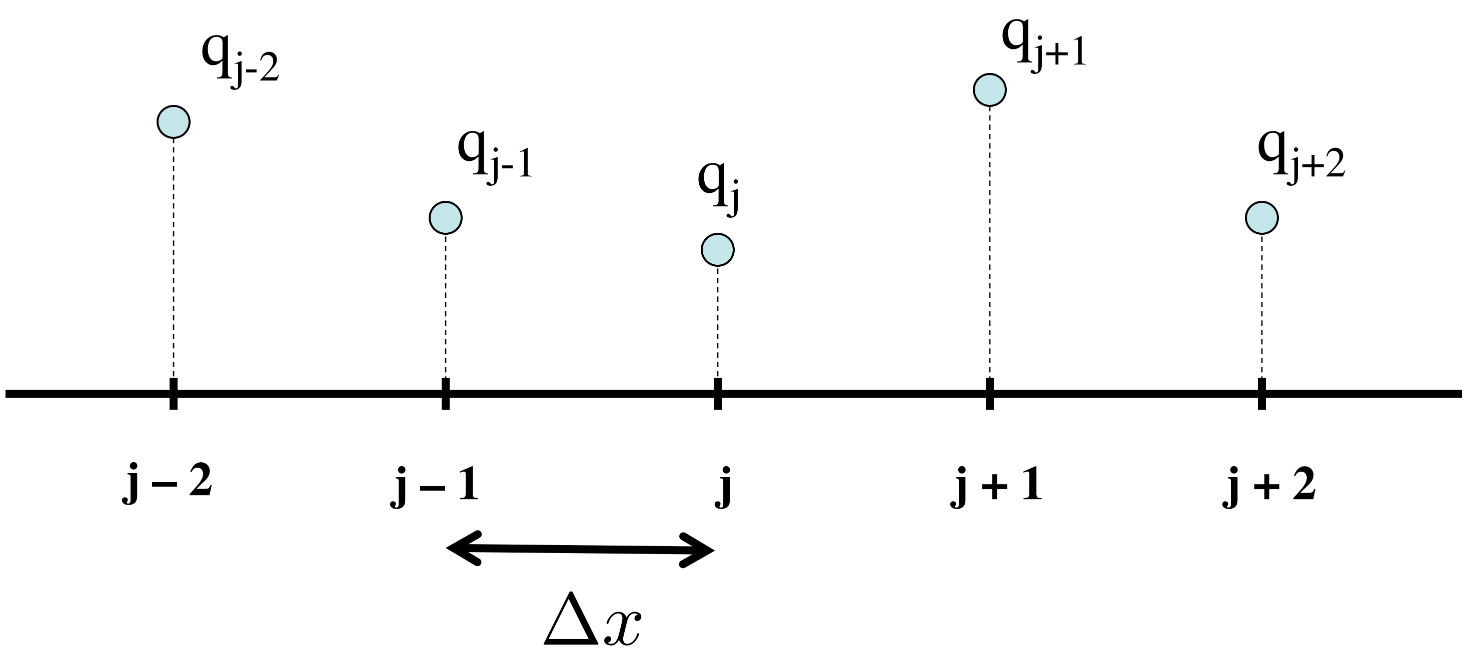
1D Advection Equation

Eulerian Frame

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

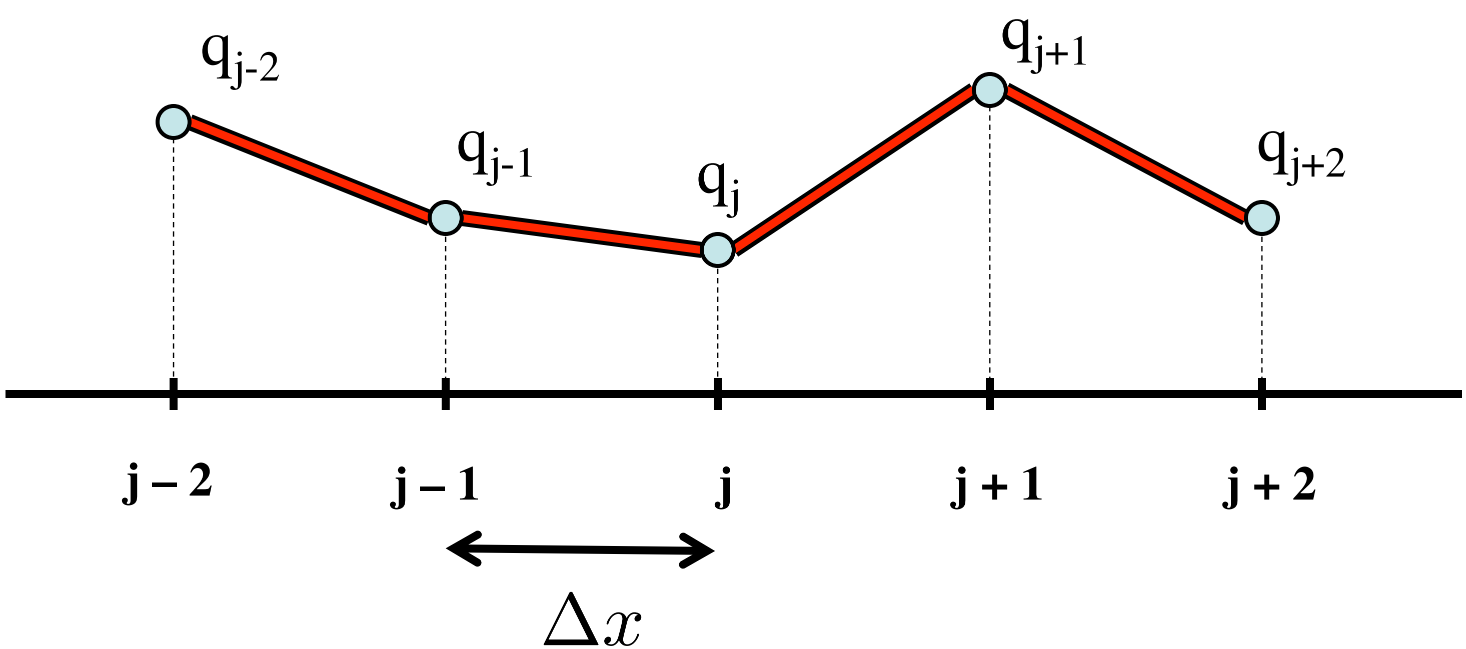
Basic Finite-Differences

- 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.



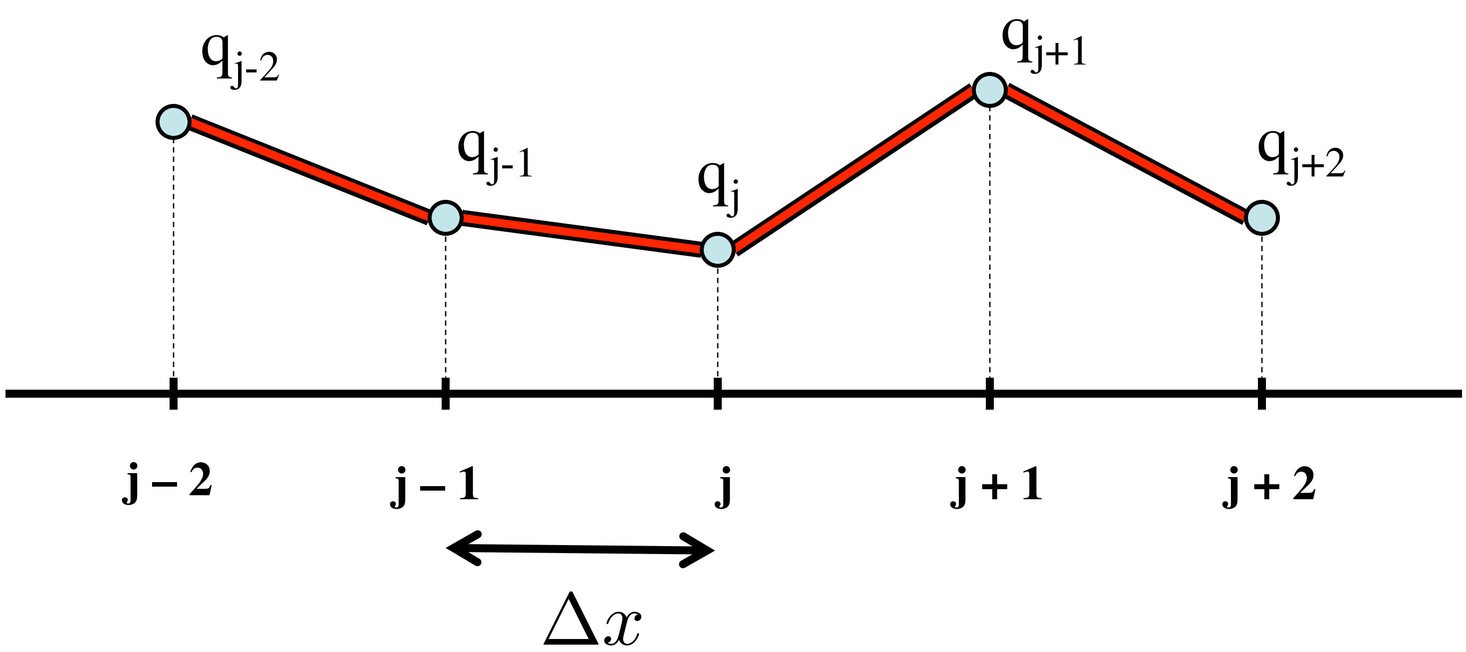
Basic Finite-Differences

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

1D Advection Equation

Eulerian Frame

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



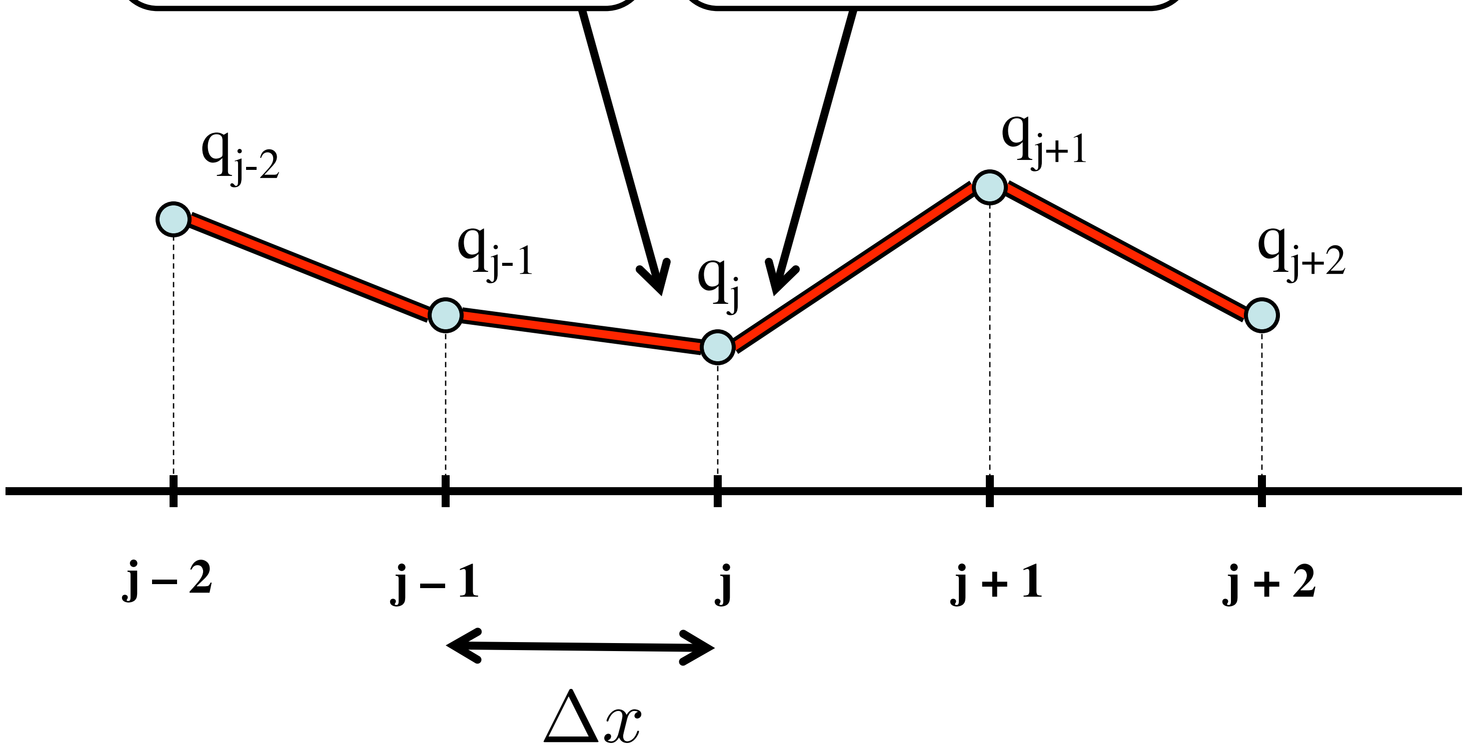
Basic Finite-Differences

"Left" Derivative

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

"Right" Derivative

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



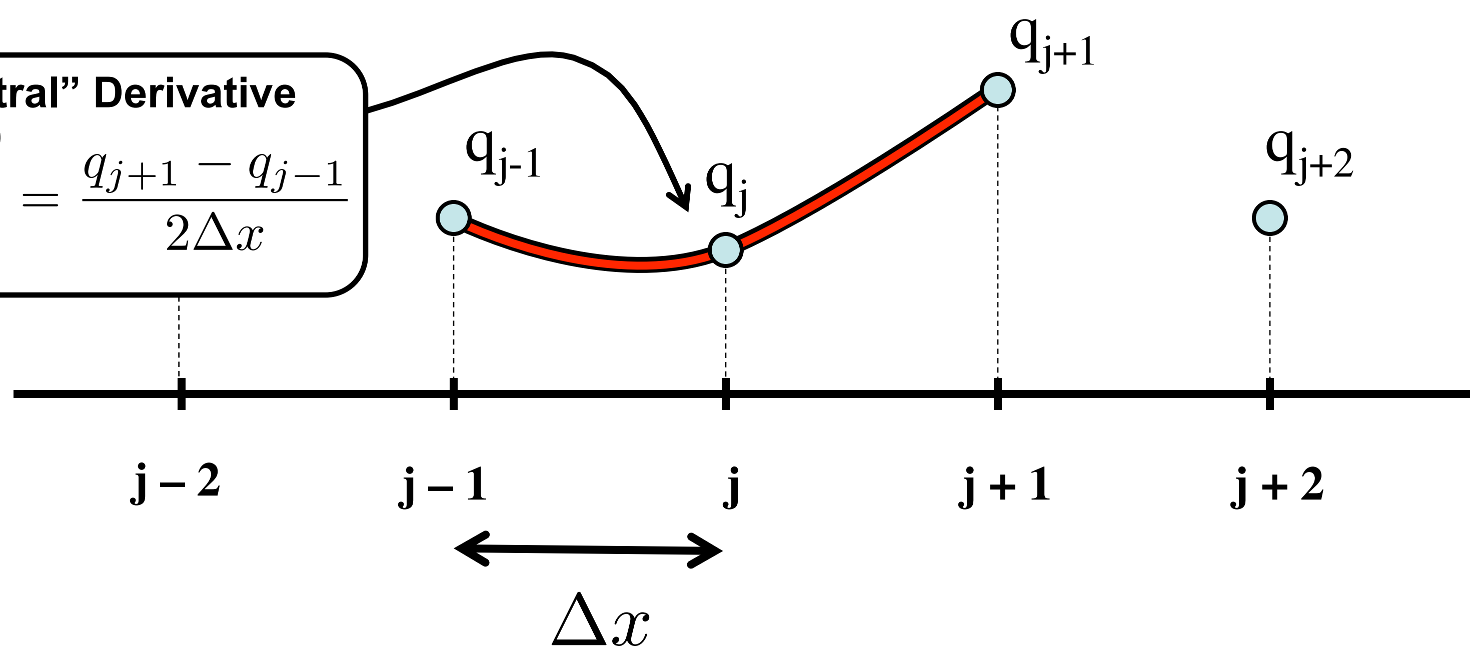
Basic Finite-Differences

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

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

“Central” Derivative

$$\left(\frac{\partial q}{\partial x}\right)^0_j = \frac{q_{j+1} - q_{j-1}}{2\Delta x}$$



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

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

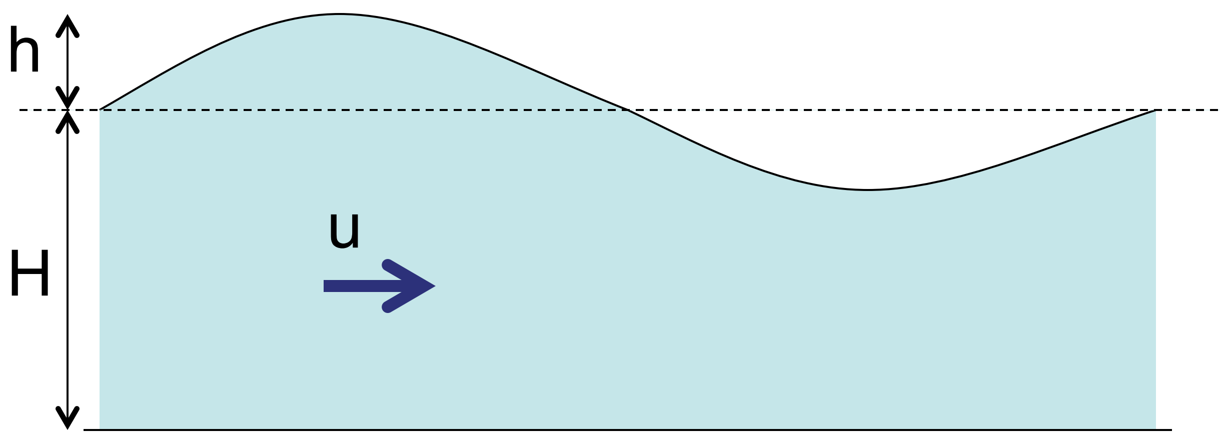
Central Scheme

1D Wave Equation

A bit more complicated (two coupled equations):

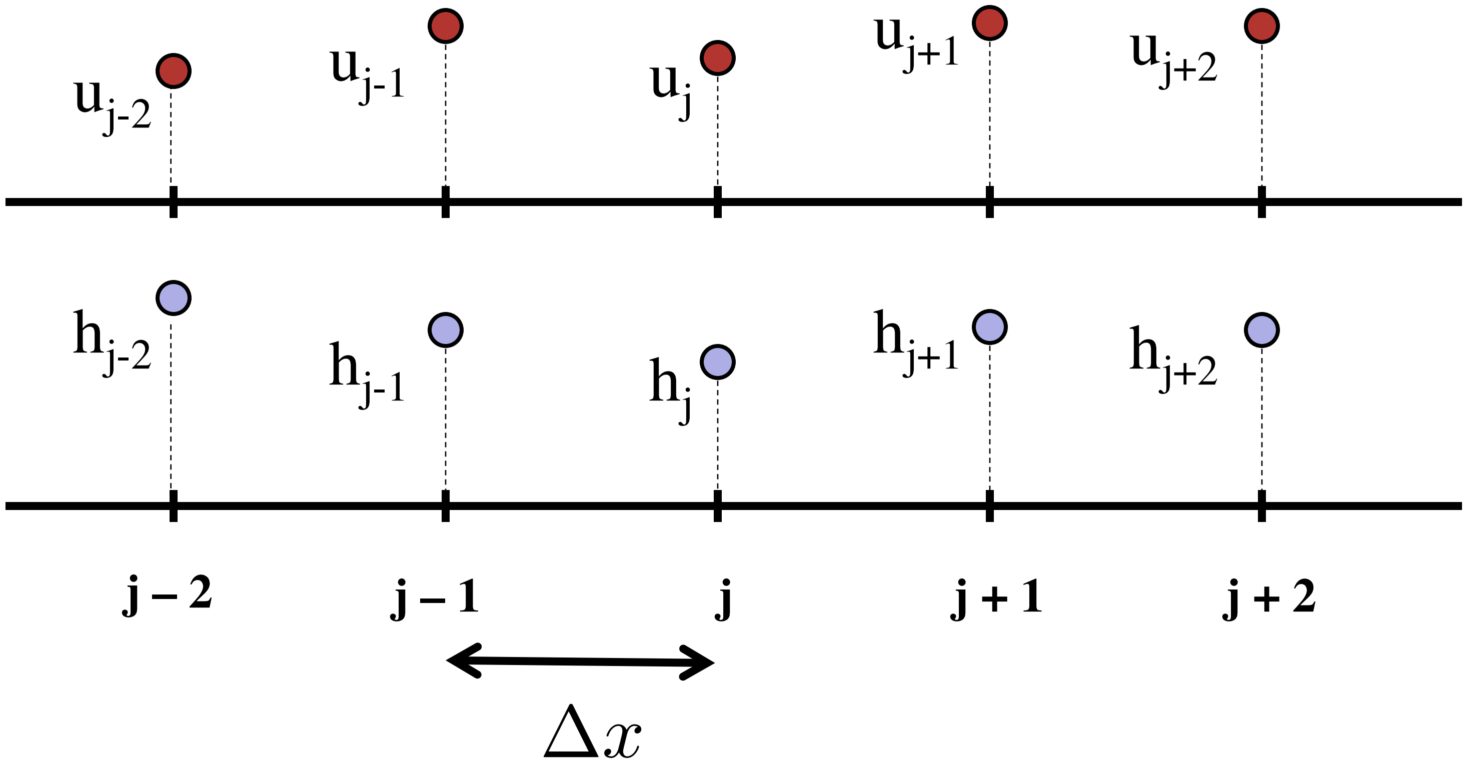
$$\frac{\partial h}{\partial t} + H \frac{\partial u}{\partial x} = 0 \qquad \frac{\partial u}{\partial t} + g \frac{\partial h}{\partial x} = 0$$

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



1D Wave Equation

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



1D Wave Equation

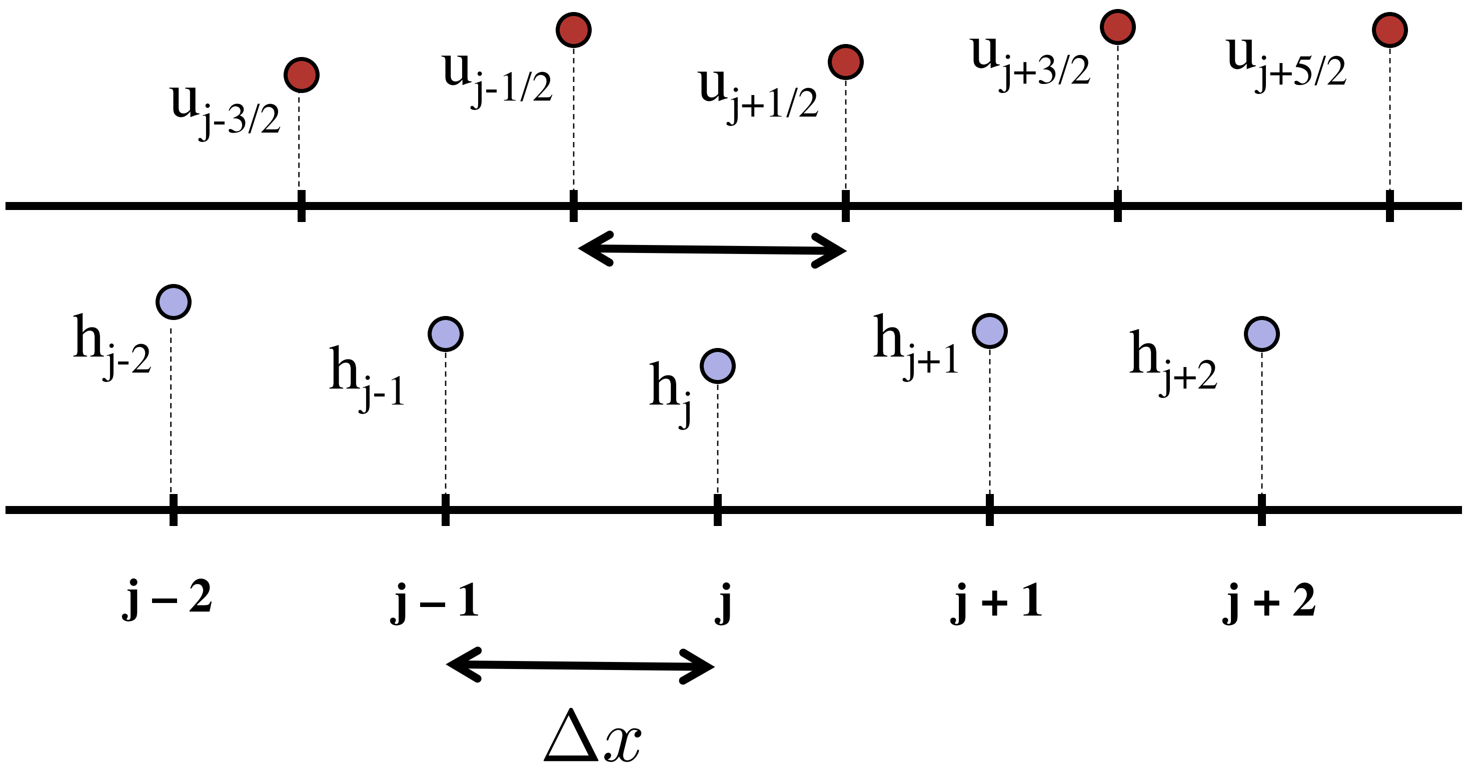
- Again using the central difference approximation we derived earlier, the wave equation takes the following discrete form:

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

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

1D Wave Equation

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



1D Wave Equation

- With staggered velocities, we can tighten the discretization:

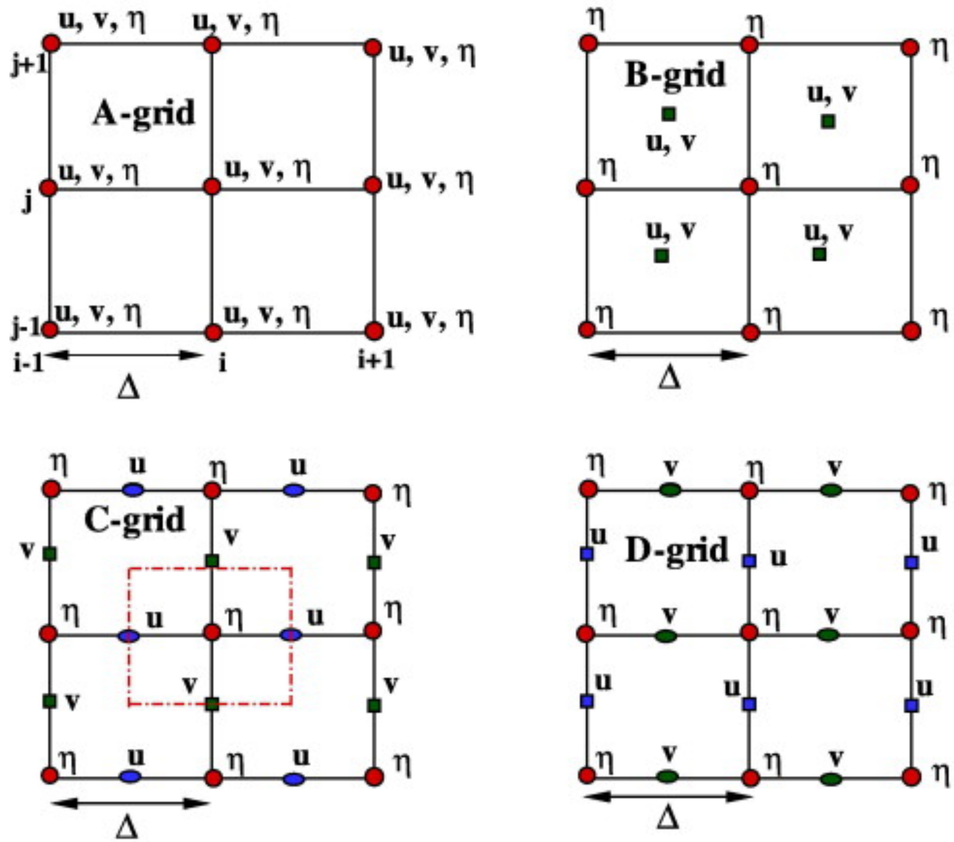
$$\frac{\partial h_j}{\partial t} + H \frac{u_{j+1/2} - u_{j-1/2}}{\Delta x} = 0$$

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

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

Arakawa Grid Types (2D)

CAM-SE MCore



WRF MPAS

CAM-FV

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

Finite-Difference Methods: Properties

- 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.

Part 3

Finite Volume Methods

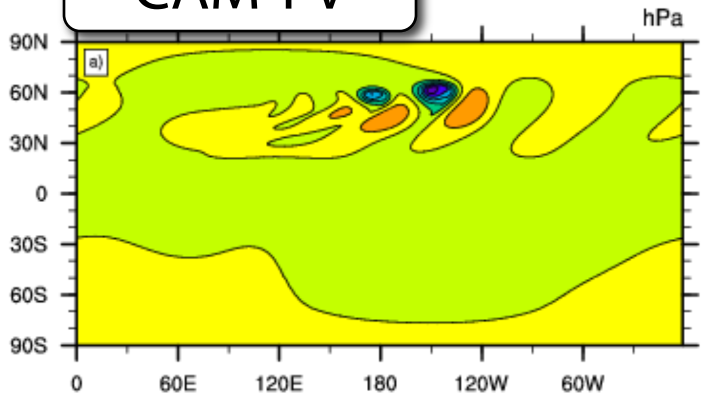
CAM-FV
GFDL FV3
MCore
MPAS

Finite-Volume Methods

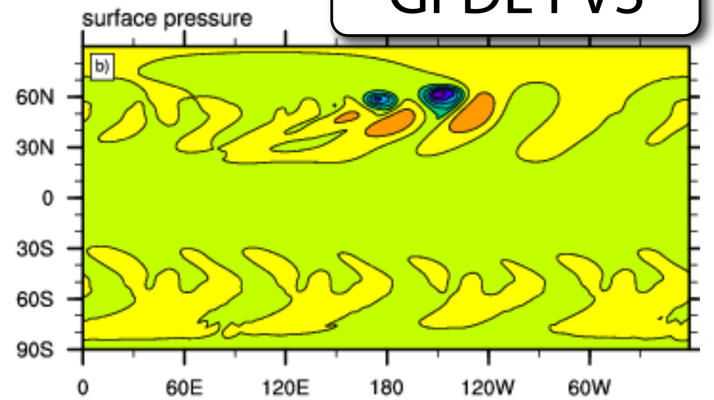
- Scalar variables (density, energy, tracers) are stored as element-averaged values (conservation)

- Velocities can be stored as pointwise values or as element-averaged momentum.

CAM-FV



GFDL FV3



Conservative Shallow-Water Eqn's

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

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

h	*Fluid height*
$\boldsymbol{u}$	*Fluid velocity vector*
p	*Fluid pressure*
$\boldsymbol{S}$	*Source terms (geometry, Coriolis, topography)*

The Finite-Volume Method

Given conservation law

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

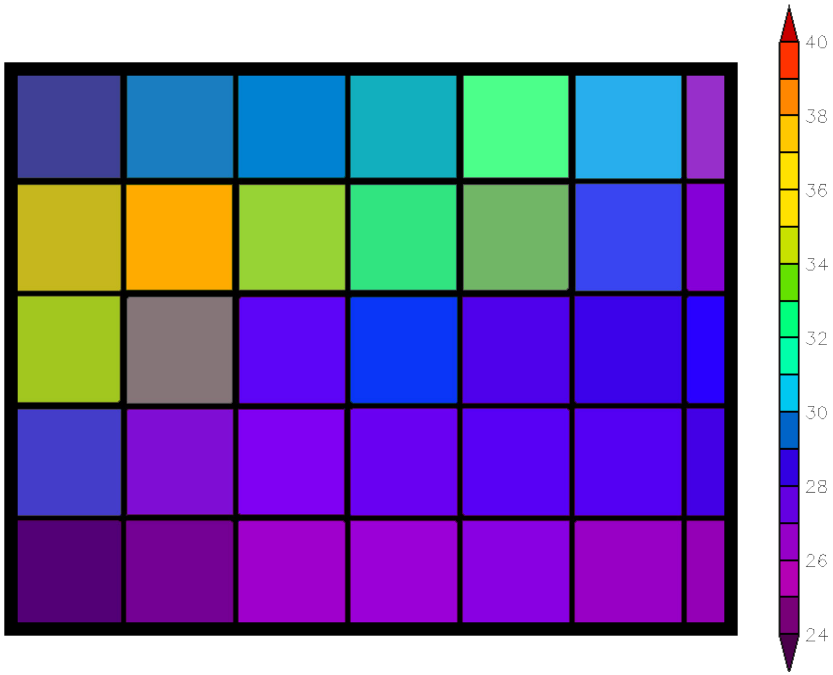
Integrate over an element $\mathcal{Z}$ with boundary $\partial\mathcal{Z}$ and apply Gauss' divergence theorem. This gives

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

Sub-Grid Scale Reconstruction

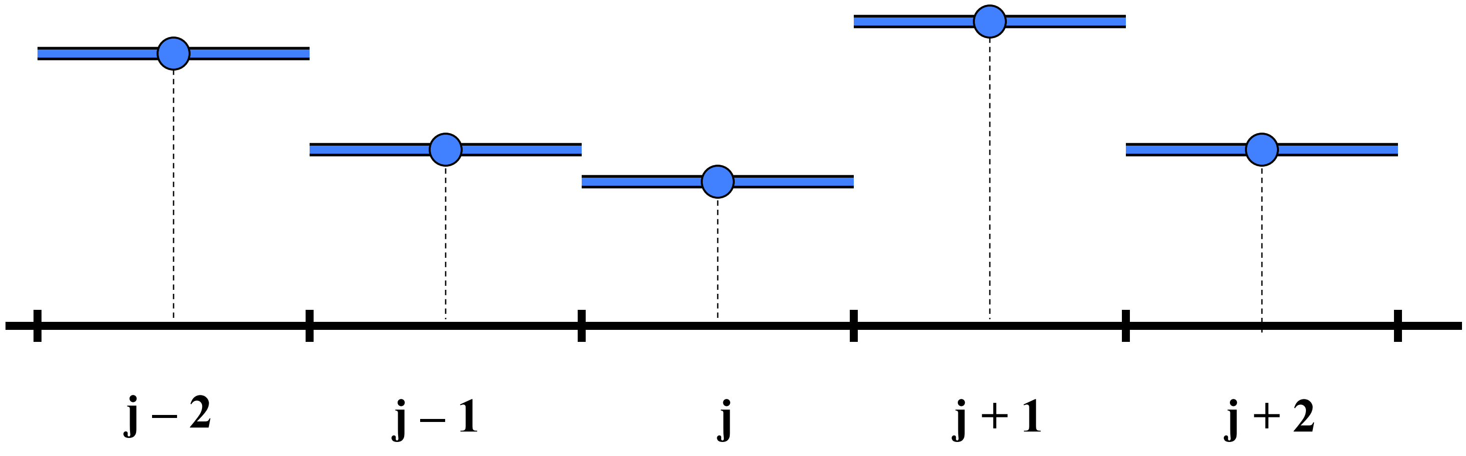
- Scalar variables (density, energy, tracers) are stored as element-averaged values.
- Neighboring values are needed to build a sub-grid-scale reconstruction.

Example: Surface temperature data



Sub-Grid Scale Reconstruction

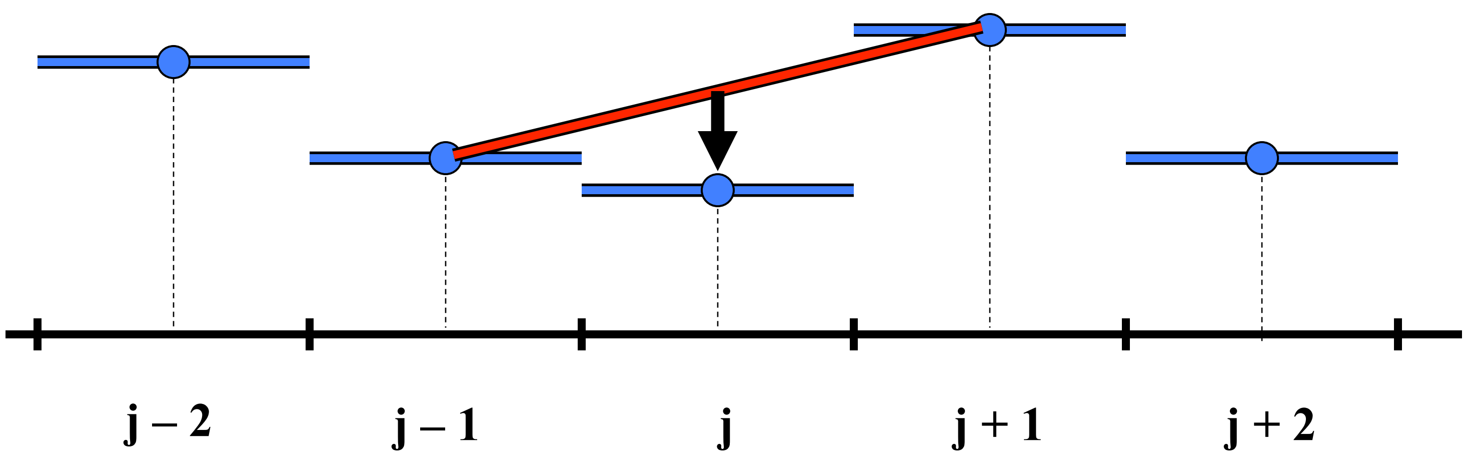
- State variables (density, energy, tracers) are stored as element-averaged values.
- Neighboring values are needed to build a sub-grid-scale reconstruction.



Sub-Grid Scale Reconstruction

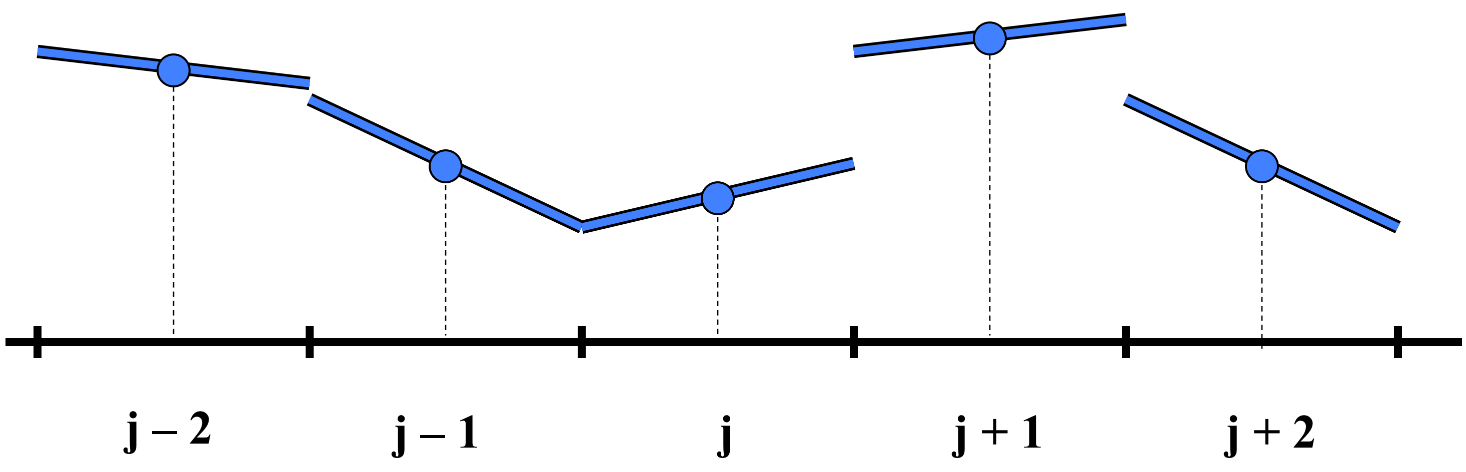
- A linear profile: $$\phi_j(x) = \overline{\phi}_j + \left(\frac{\partial \phi}{\partial x}\right)_j (x - x_j)$$

- An approximation to the slope in element **j** can be obtained by differencing neighboring elements.

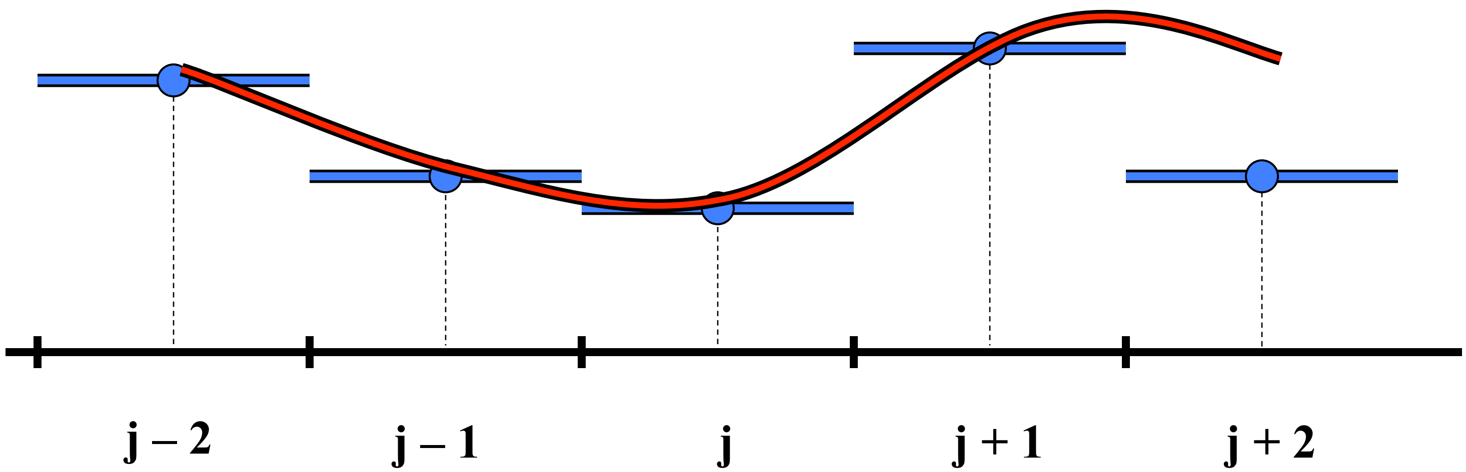


Sub-Grid Scale Reconstruction

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



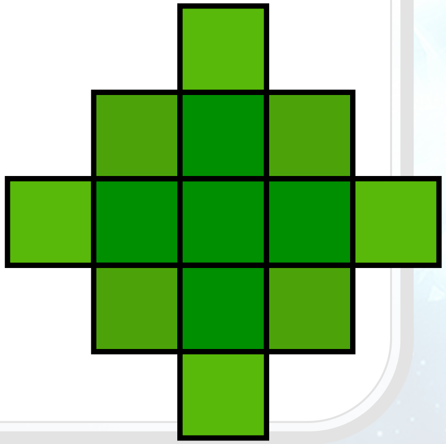
Sub-Grid Scale Reconstruction



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

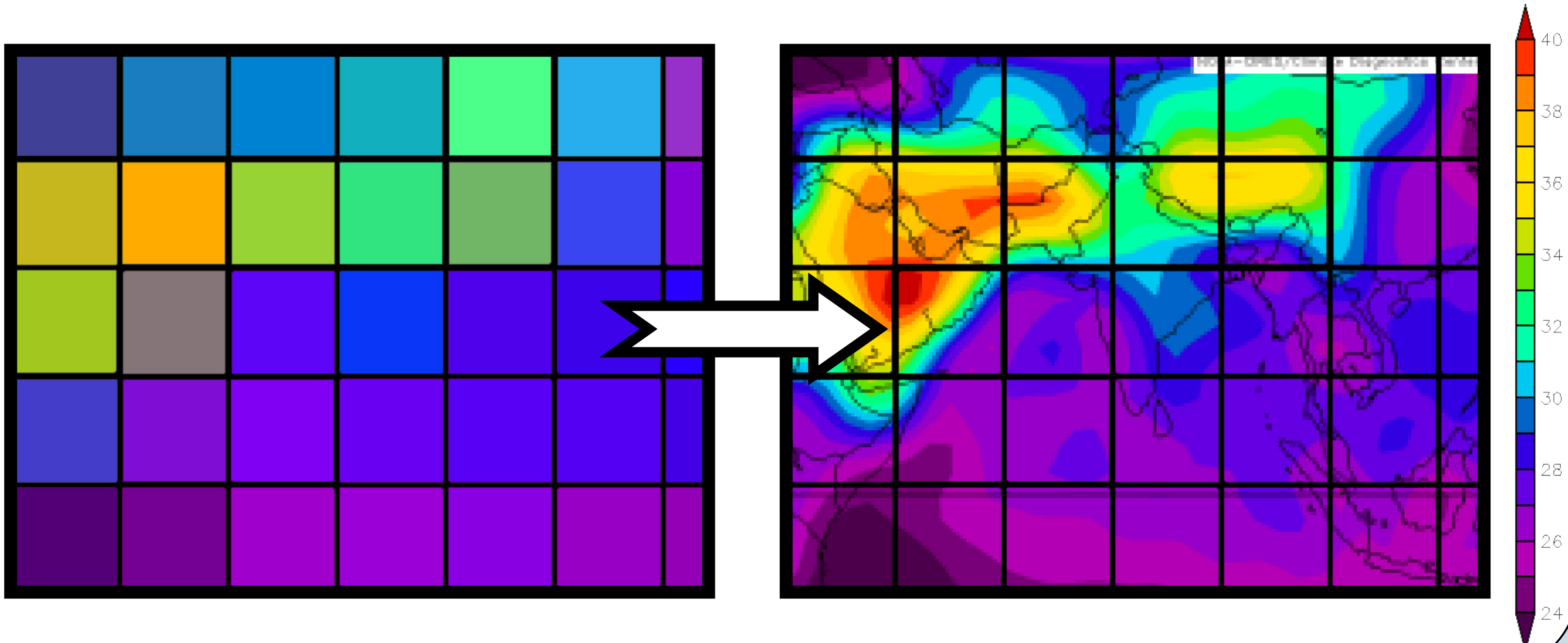
2D Stencil

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



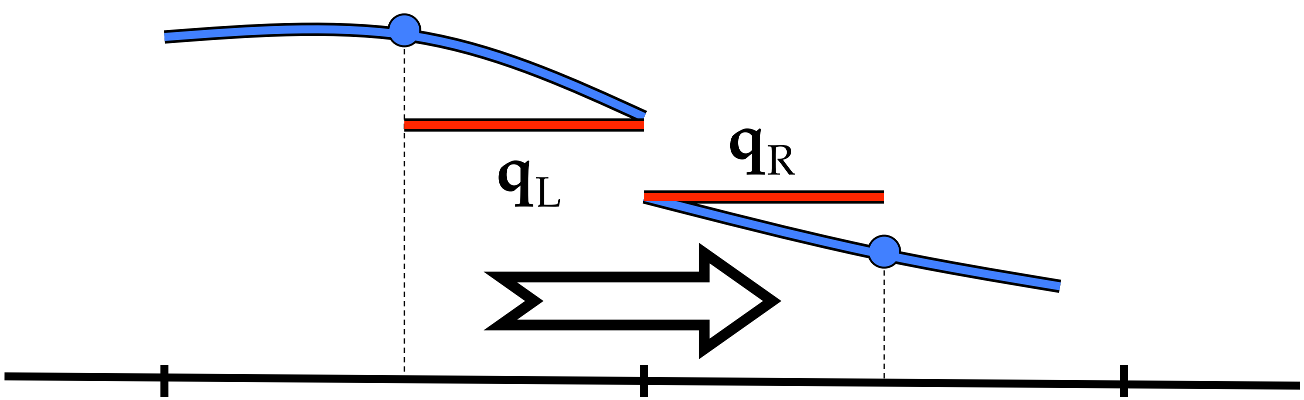
Sub-Grid Scale Reconstruction

- 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 $\mathbf{q}_\mathrm{L}$ and right value $\mathbf{q}_\mathrm{R}$), 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: Properties

- Finite-volume methods do not 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.

Part 4

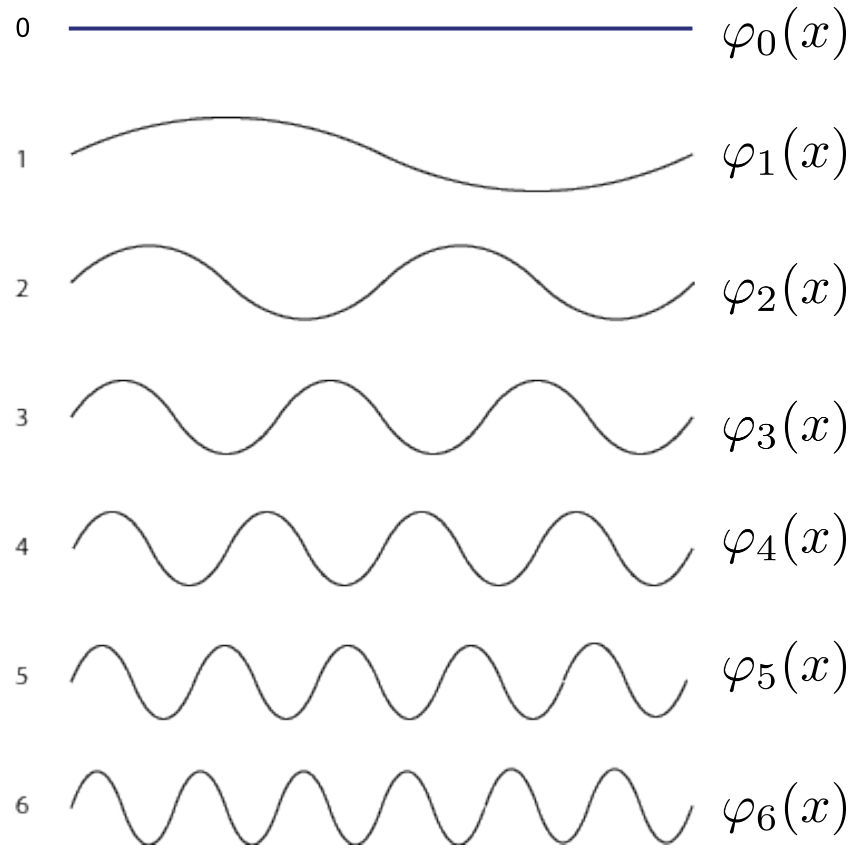
Spectral Methods

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:

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



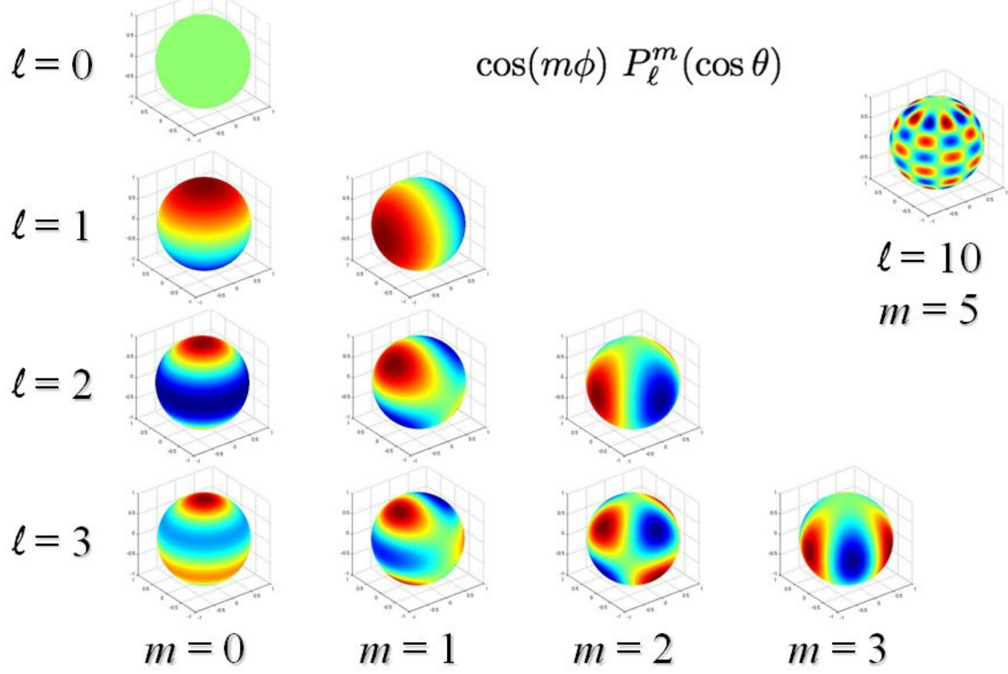
Linear Harmonics: Orthogonality

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

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

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 Transform: Advection

1D Advection Equation

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

Expand q in terms of basis functions:

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

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 $\overline{\psi}_k$ and integrate over domain :

$$\sum_{n=1}^{N} \frac{da_n}{dt} \int_S \psi_n \overline{\psi}_k dx = -u\sum_{n=1}^{N} a_n \int_S \frac{\partial \psi_n}{\partial x}\overline{\psi}_k dx$$

Spectral Transform: 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:

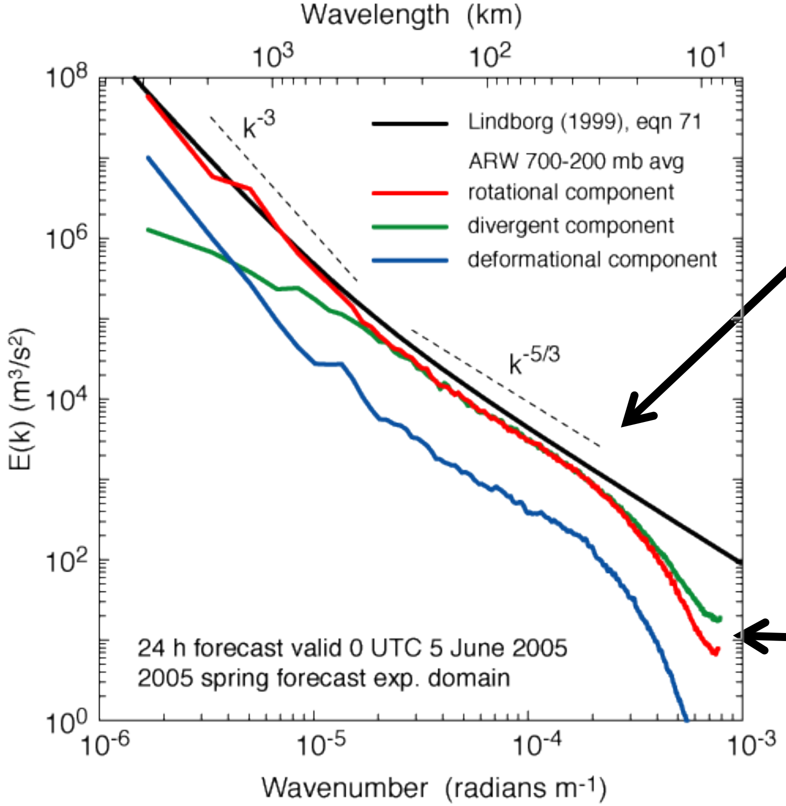
$$a_n = a_{n,0} \exp(-inut)$$

Advection at speed u

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

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

Phase Space / 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.

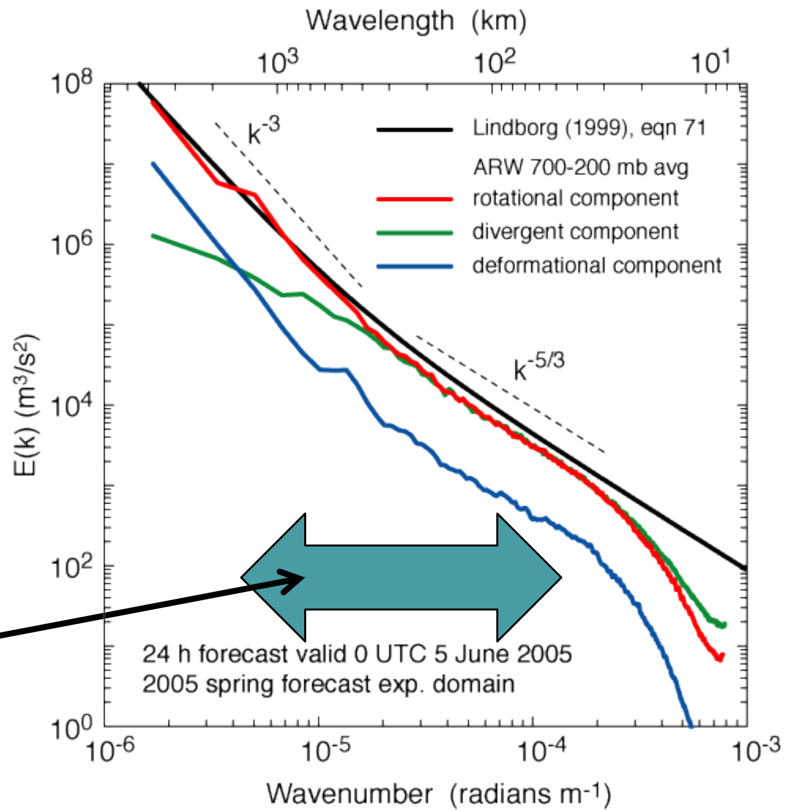
Non-Linear Equations

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!

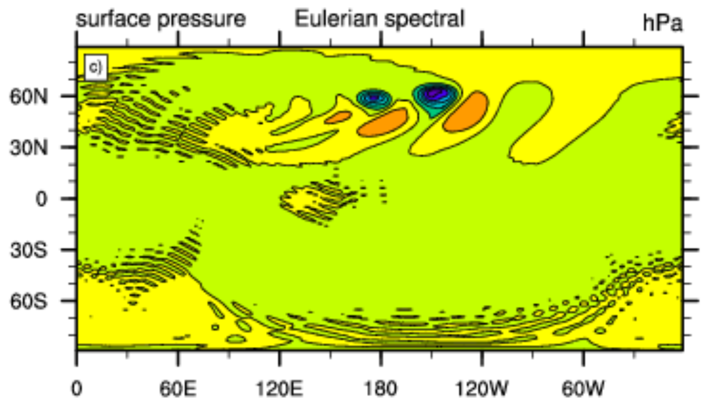


Spectral Transform: Properties

- 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.

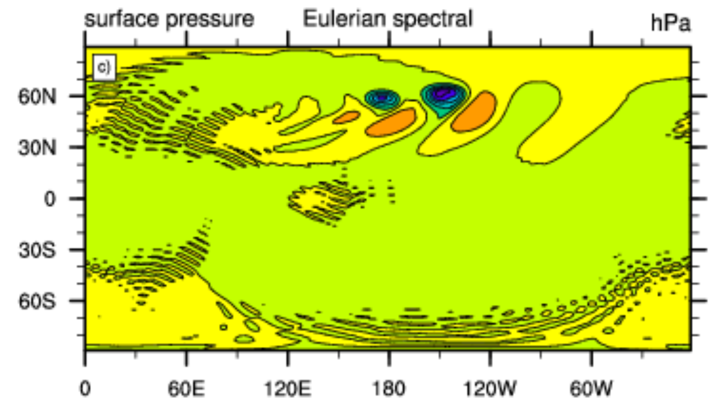
- Errors typically emerge as "spectral ringing."



Spectral Transform: Properties

- 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.



Part 5

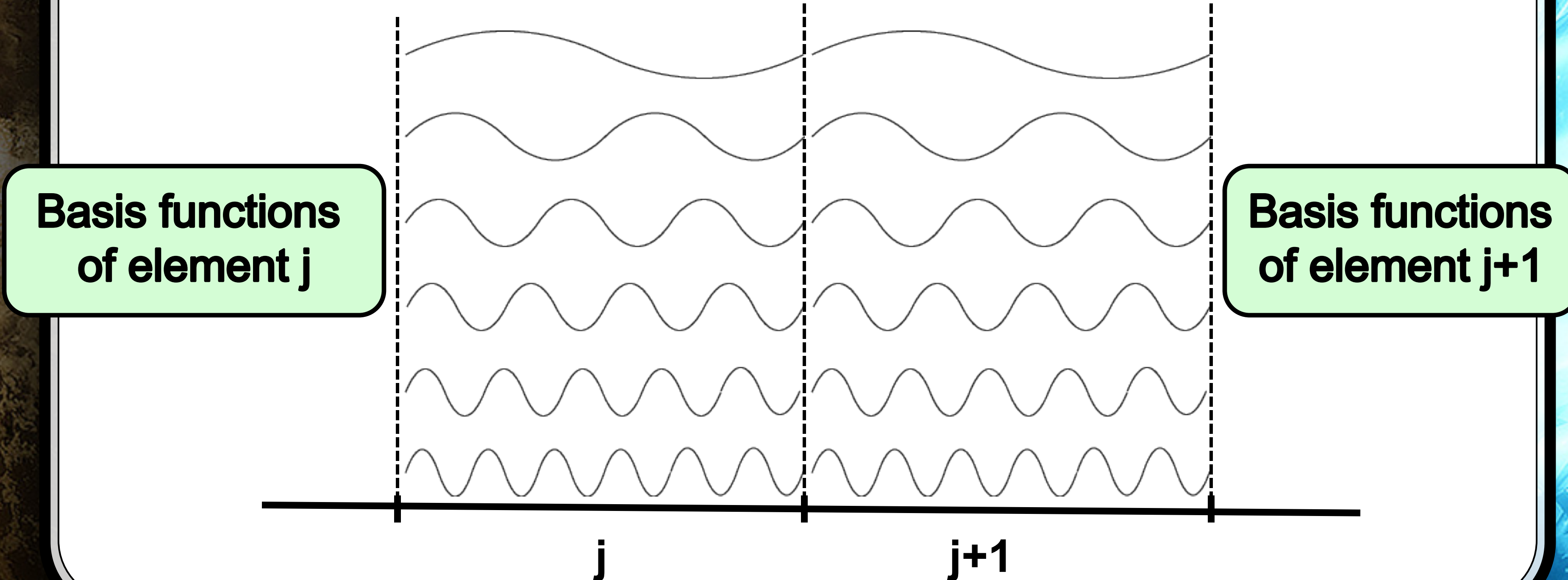
Finite Element Methods

CAM-SE
NUMA

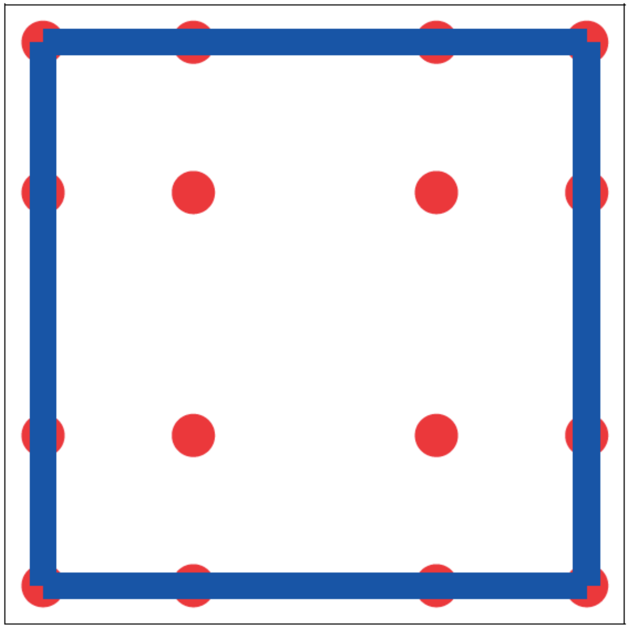
- *Spectral Element Method*
- *Discontinuous Galerkin Method*

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

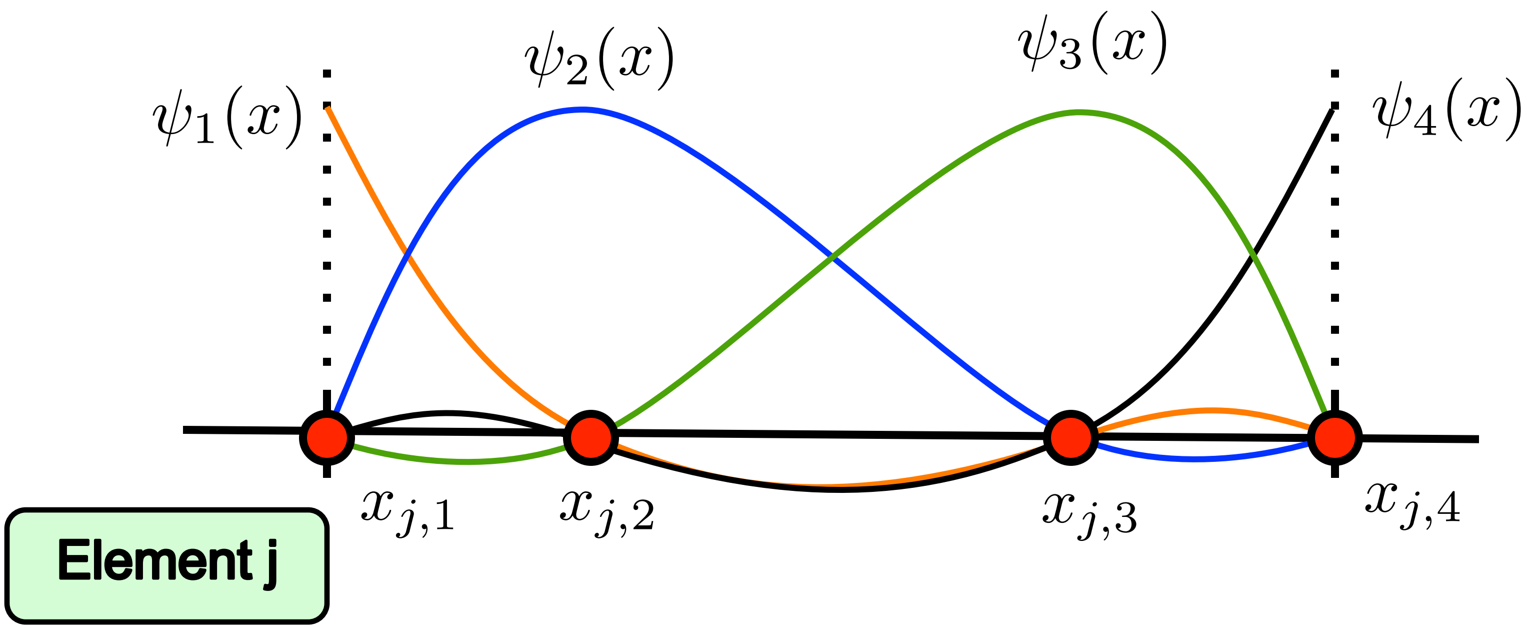
- A nth order finite element method requires n^d basis functions within each element (dimension d).
- To construct basis functions, use GLL nodes within a 2D element.
- Fit polynomials so that each basis function is 1 at one node and 0 at all other nodes.

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

Finite Element Method

Expand q in terms of basis functions within an element:

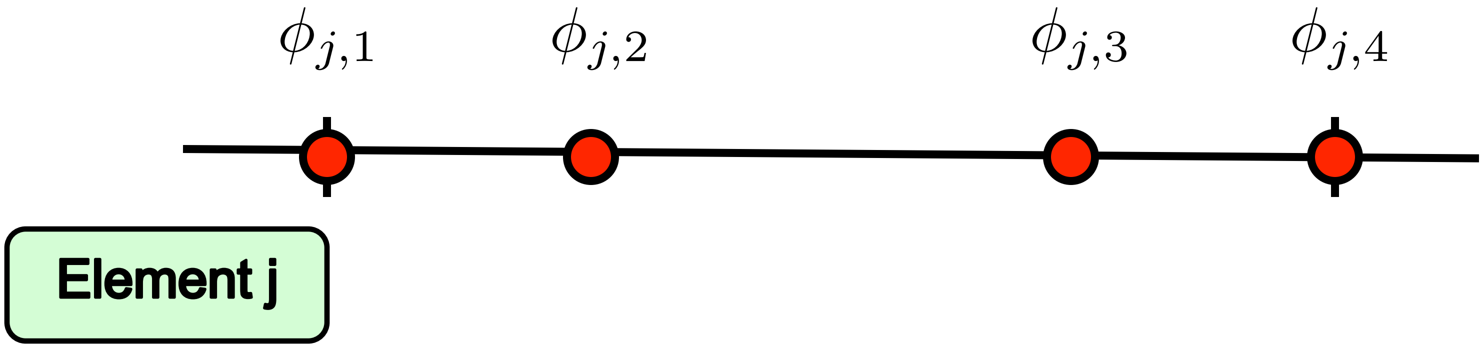
$$q(x,t) = \sum_{n=1}^{N} a_n(t)\psi_n(x)$$



Finite Element Method

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 Method

1D Conservation Eq'n

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

Expand q in terms of basis functions within an element:

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

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 $\overline{\psi}_k$ and integrate over an element:

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

Finite Element Method

1D Conservation Eq'n

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

Apply integration by parts:

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

Time evolution of coefficients

Flux through edges

Internal exchange

With mass matrix:

$$M_{n,k} = \int_{\mathcal{S}_j} \psi_n \overline{\psi}_k dx$$

Finite Element Method

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

Internal exchange

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

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

1D Conservation Eq'n

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

Finite Element Method

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

Flux through edges

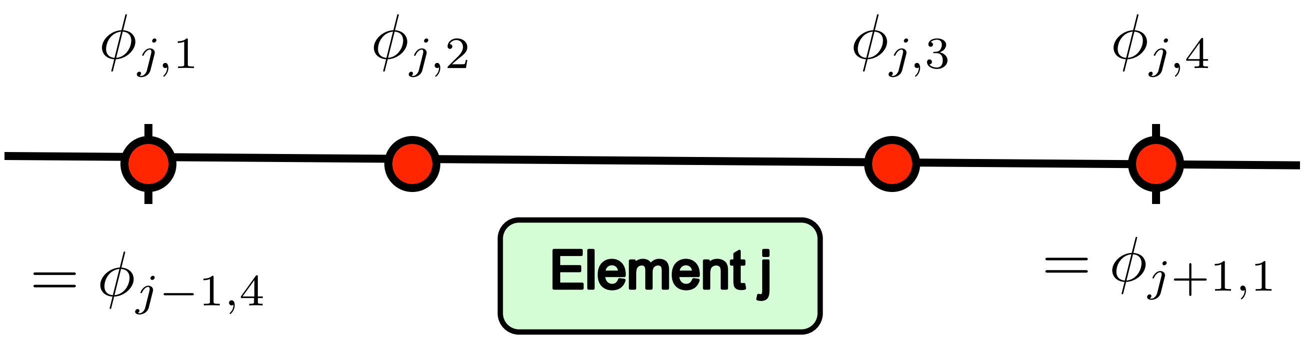
- **Spectral Element method**: Enforce continuity at element boundaries. Flux function is simple function evaluation.
- **Discontinuous Galerkin method**: Discontinuous at element edges. A Riemann solver must be applied to evaluate flux here.

Finite Element Method

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

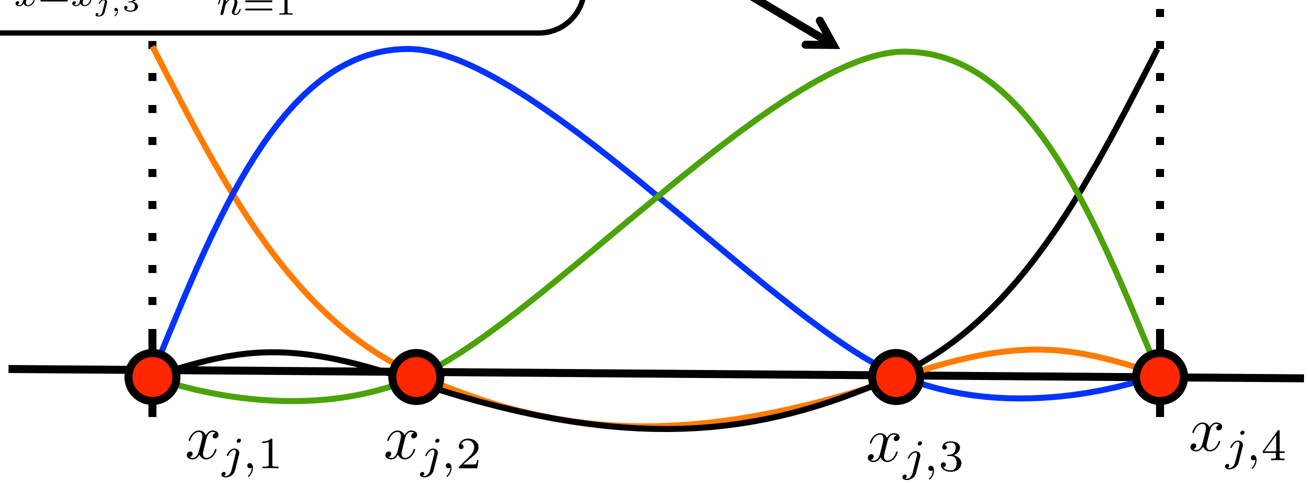
The spectral element method can be interpreted as a finite difference scheme.

1D Advection Equation

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

"Spectral" Derivative

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



Part 6

Future Directions

- *Multi-resolution modeling*

Multi-Resolution Modeling

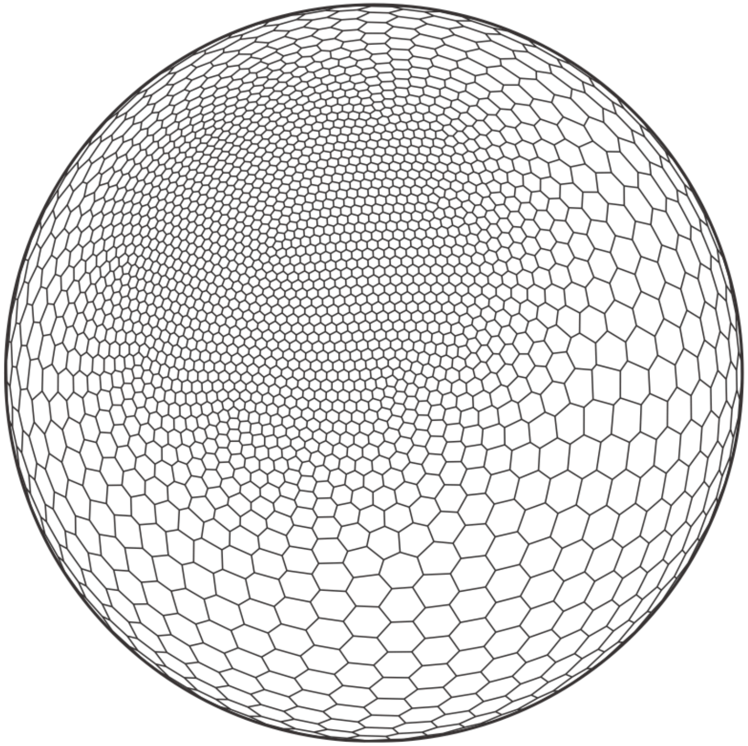
- Better understanding of the effects of global climate change on regional climate and weather extremes (enhanced resolution in regions of interest).
- Better resolution of the Intertropical Convergence Zone (ITCZ) and tropics, to correctly resolve tropical cyclone seeding regions.
- Adaptive mesh refinement used for tracking tropical cyclones in the midlatitudes; possibly used to improve forecasts of hurricane intensity.

Ongoing Work on Multi-Res Models

Several projects are now underway tackling the development of multi-resolution models.

- The spectral-element dynamical core (CAM-SE), to be the default in the next version of the Community Earth System Model (CESM) will soon support variable mesh resolutions.
- The Model for Prediction Across Scales (MPAS, NCAR) uses stretched grids to enhance regions of interest (static refinement only).
- FVcubed model (GFDL) – options under development for both stretched and embedded refinement.
- Non-hydrostatic Unified Model of the Atmosphere (NUMA, NPS)

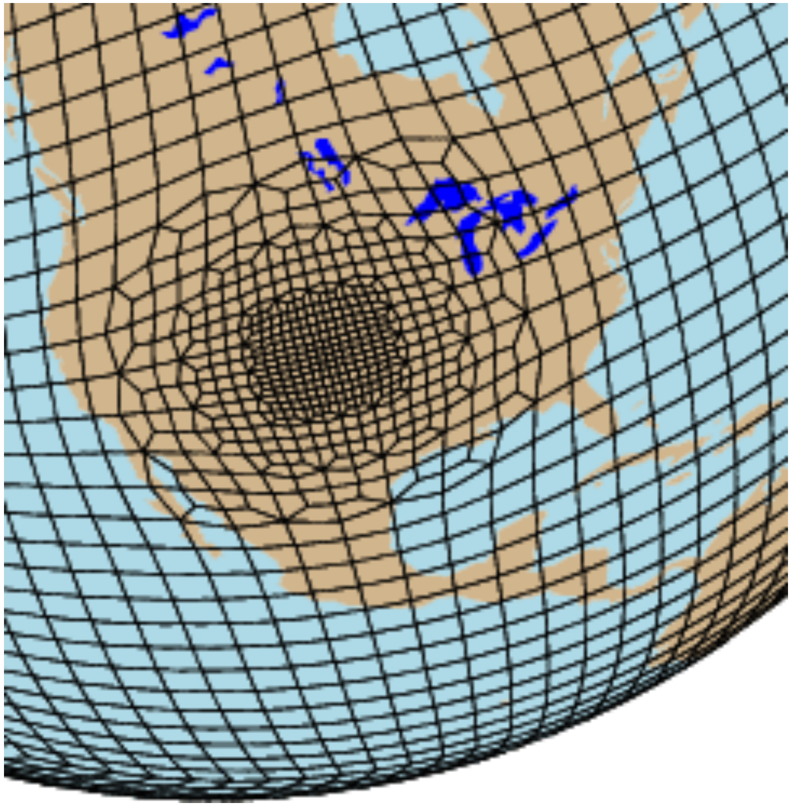
Designing a Multi-Resolution Model



Model for Prediction Across Scales (MPAS) Stretched Grid

MCore / Chombo Non-conformal Grid

CAM-SE Grid Refinement



Source: Michael Levy, Sandia National Labs.

Thank You