# Transport and a Goldilocks Search

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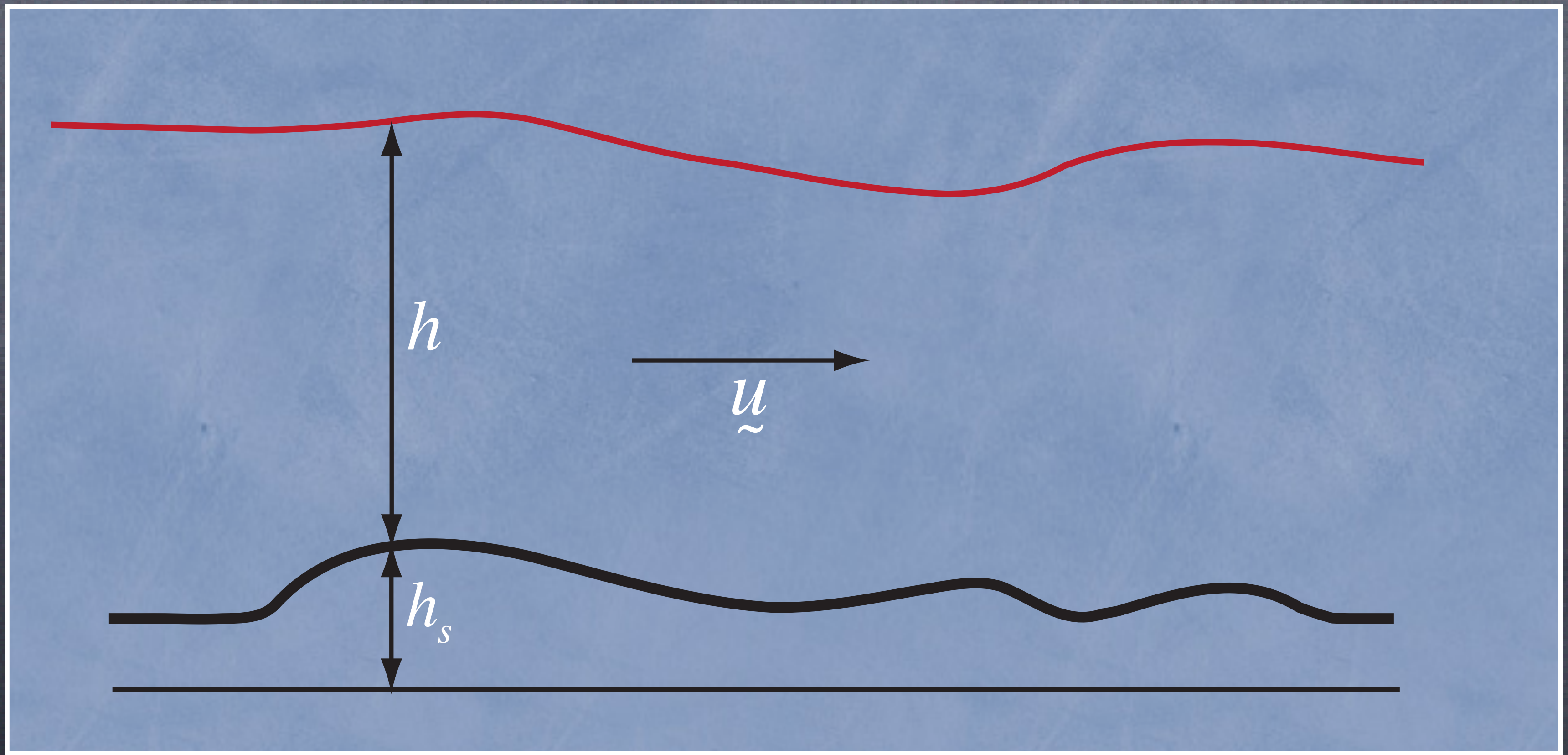
# First, let's define our equations.

$$\frac{\partial h}{\partial t} + \nabla \cdot (h \underset{\sim}{u}) = 0$$ thickness plays the role of pressure (uniform density).

$$\frac{\partial \underset{\sim}{u}}{\partial t} + (\omega + f)\underset{\sim}{k} \times \underset{\sim}{u} = -g\nabla(h + h_s) - \frac{1}{2}\nabla \|\underset{\sim}{u}\|^2$$ velocity is in the tangent plane.

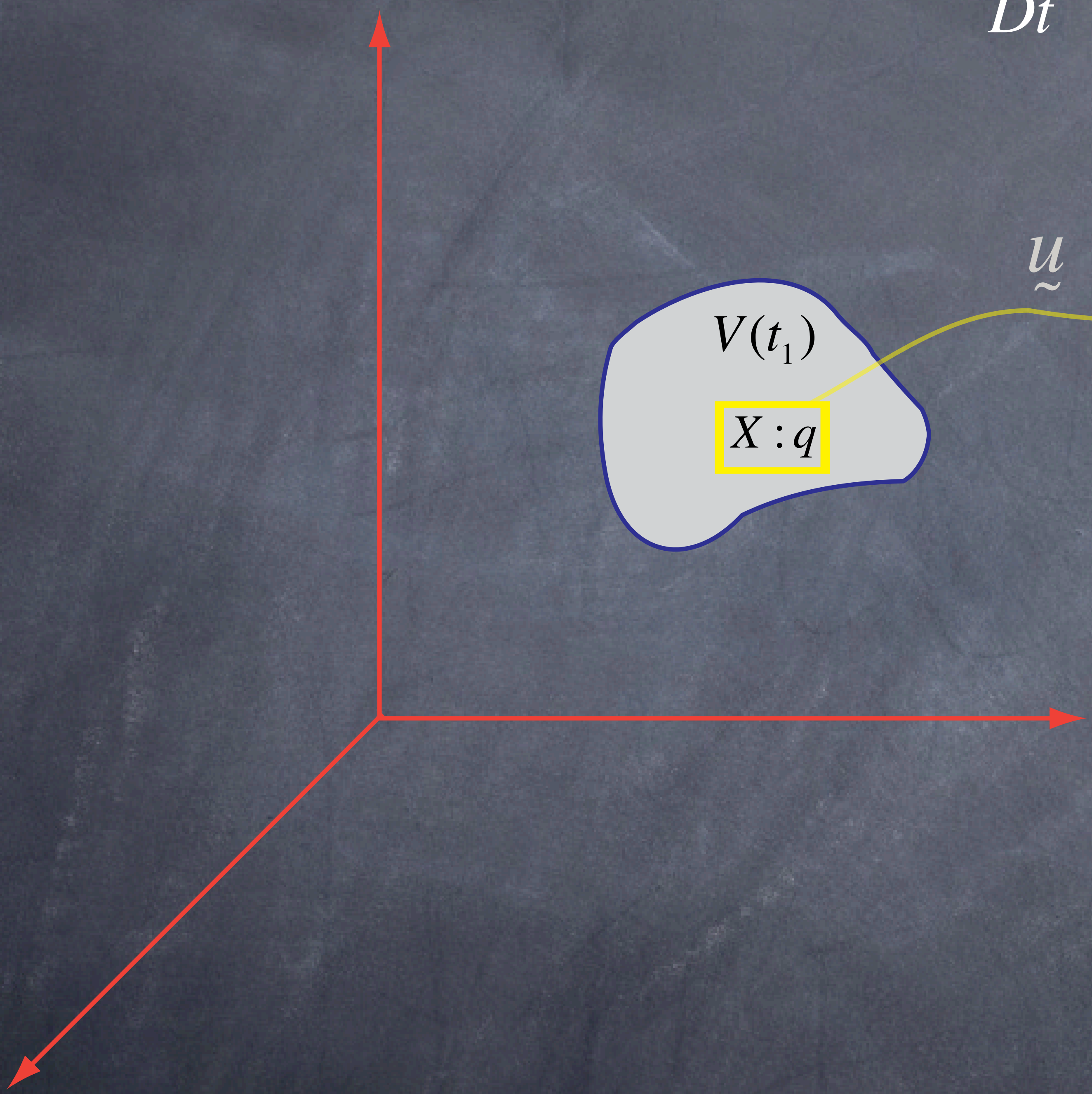
$$\omega = \underset{\sim}{k} \cdot (\nabla \times \underset{\sim}{u})$$ only keep track of the vertical component of vorticity.

$$\eta = \omega + f$$ definition of absolute vorticity.



# And add tracer transport ....

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




At some time, $t_1$, we tag all particles in the fluid with an additional label that represents the value of the tracer (q) field.

This label is "conserved" (i.e. does not change) as the particle moves through the fluid, thus (by definition): $Dq/Dt = 0$.

Note that q is a concentration, i.e. q has units of $kg_{something}/kg_{mass}$.

Unfortunately (as we will see later), we are not able to remain in the Lagrangian reference frame, so recall $\frac{Dq}{Dt} = \frac{\partial q}{\partial t} + \underset{\sim}{u} \cdot \nabla q$ .

**advective form** →

$$\frac{\partial q}{\partial t} + \underset{\sim}{u} \cdot \nabla q = 0 \qquad \frac{\partial h}{\partial t} + \nabla \cdot (h\underset{\sim}{u}) = 0$$

$$h\left[\frac{\partial q}{\partial t} + \underset{\sim}{u} \cdot \nabla q\right] = 0 \qquad q\left[\frac{\partial h}{\partial t} + \nabla \cdot (h\underset{\sim}{u})\right] = 0$$

$$h\frac{\partial q}{\partial t} + h\underset{\sim}{u} \cdot \nabla q = 0 \qquad q\frac{\partial h}{\partial t} + q\nabla \cdot (h\underset{\sim}{u}) = 0$$

**flux form** →

$$\frac{\partial (hq)}{\partial t} + \nabla \cdot (hq\underset{\sim}{u}) = 0$$

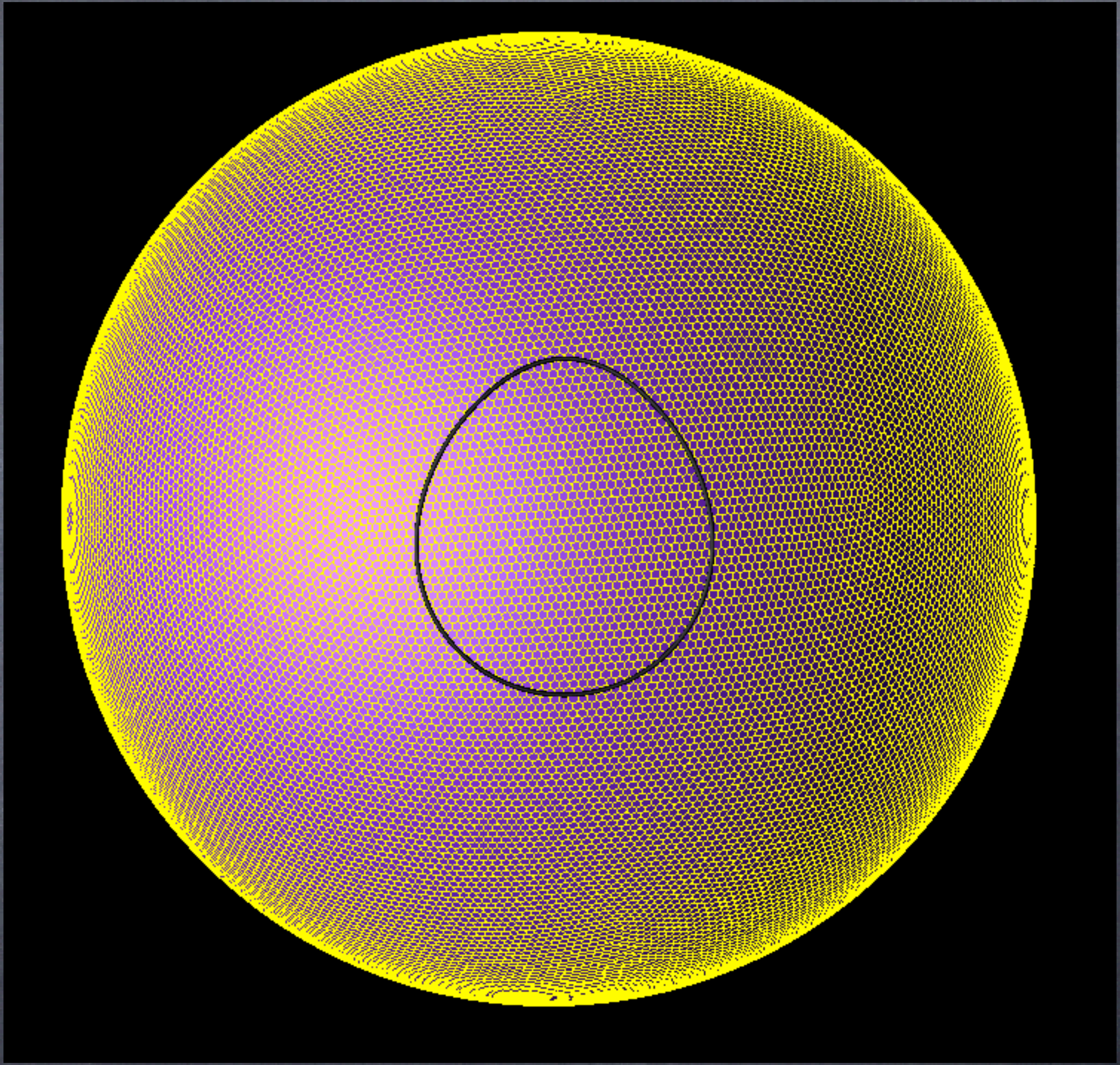
# Next, let's define our physical setting.

The SW equations are discretized on the sphere.

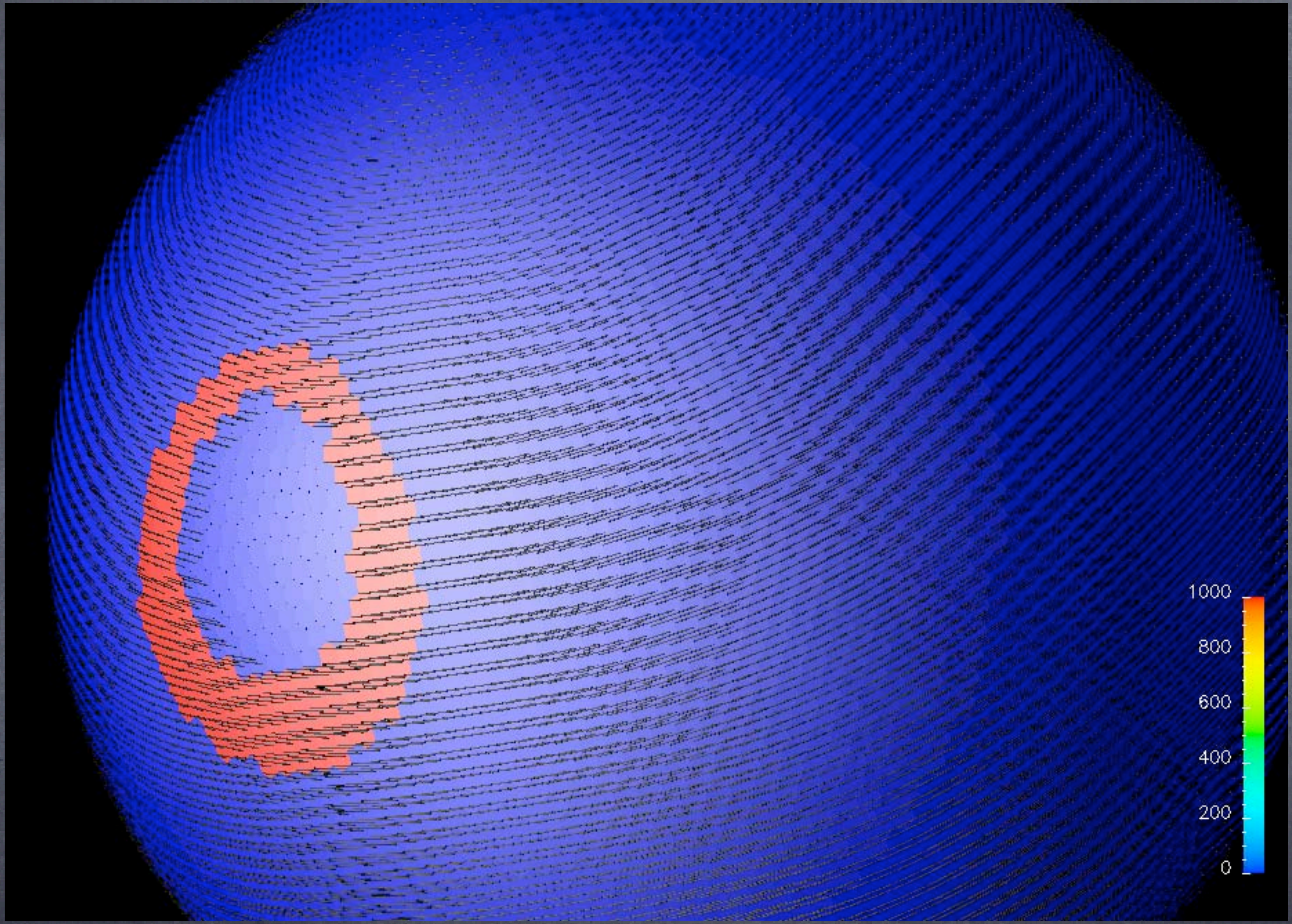
There is a mountain located at 30N. As we will see, this mountain protrudes through the fluid to create an island.

Before t=0 times, the flow is in geostrophic balance with a jet of 20 m/s at the equator, decaying to zero at the poles.

At t=0, the mountain appears instantaneously creating a large forcing to which the flow has to adjust.



# Some motivation .... simulation of $\frac{Dq}{Dt} = 0$




Recall that the particle tags should be invariant in time.
Also note that at t=0, there are only two types of labels: 0 and 1000.
By the end, there are very few locations with 1000 (the scheme is diffusive).

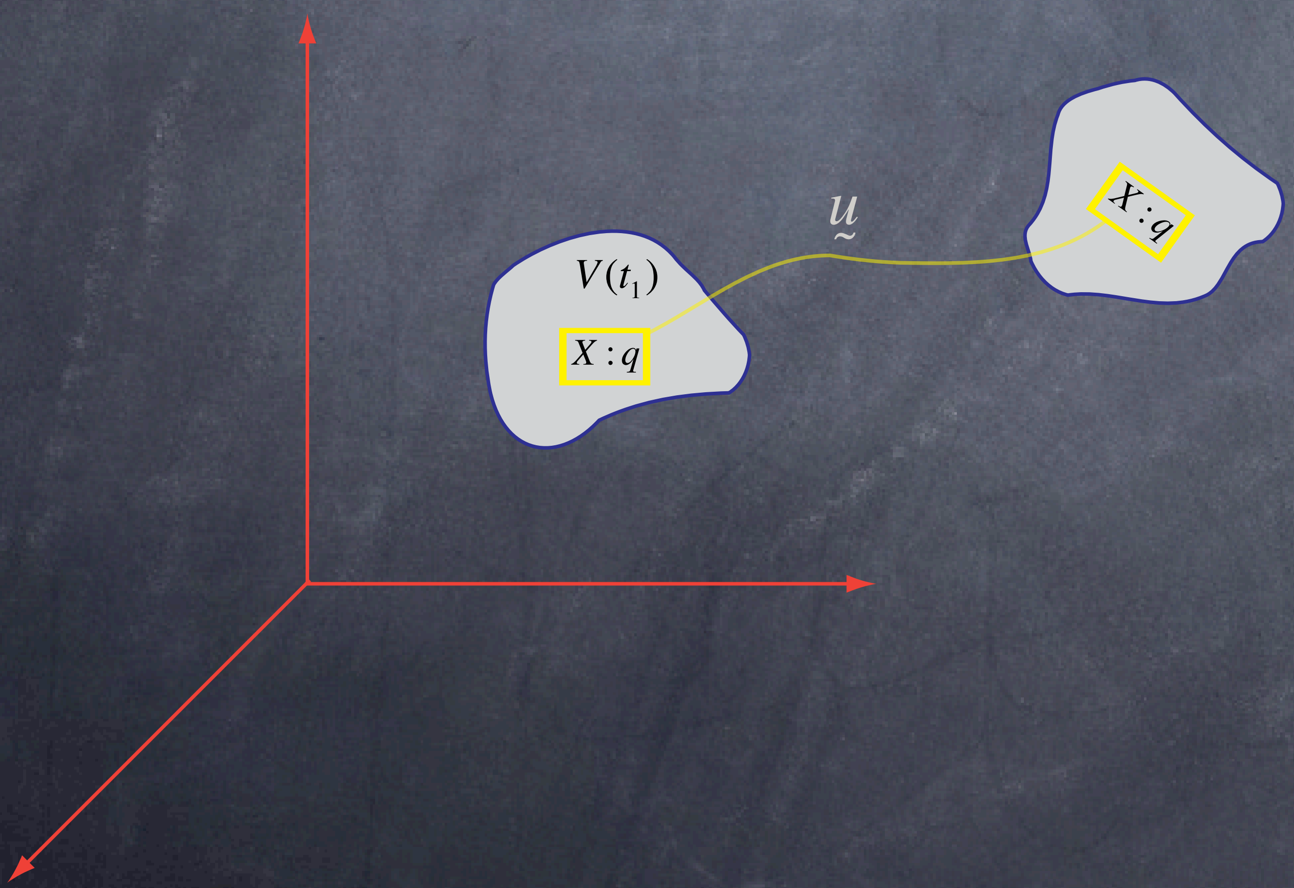
# Transport and Monotonicity

The particle perspective of $\frac{Dq}{Dt} = 0$ leads to the following conclusions:

$\min(q(t = t_0)) \leq q \leq \max(q(t = t_0) \quad \forall\, t > t_0$ ⟵ New extrema are not allowed.

$q_i^{n+1} = \sum_{j=1}^{N} \alpha_j q_j^n \quad \alpha_j \geq 0$ ⟵ **New values are an interpolation of old values.**

$0 \leq \alpha_j \leq 1, \quad \sum_{j=}^{N} \alpha_j = 1$ ⟵ required for consistency

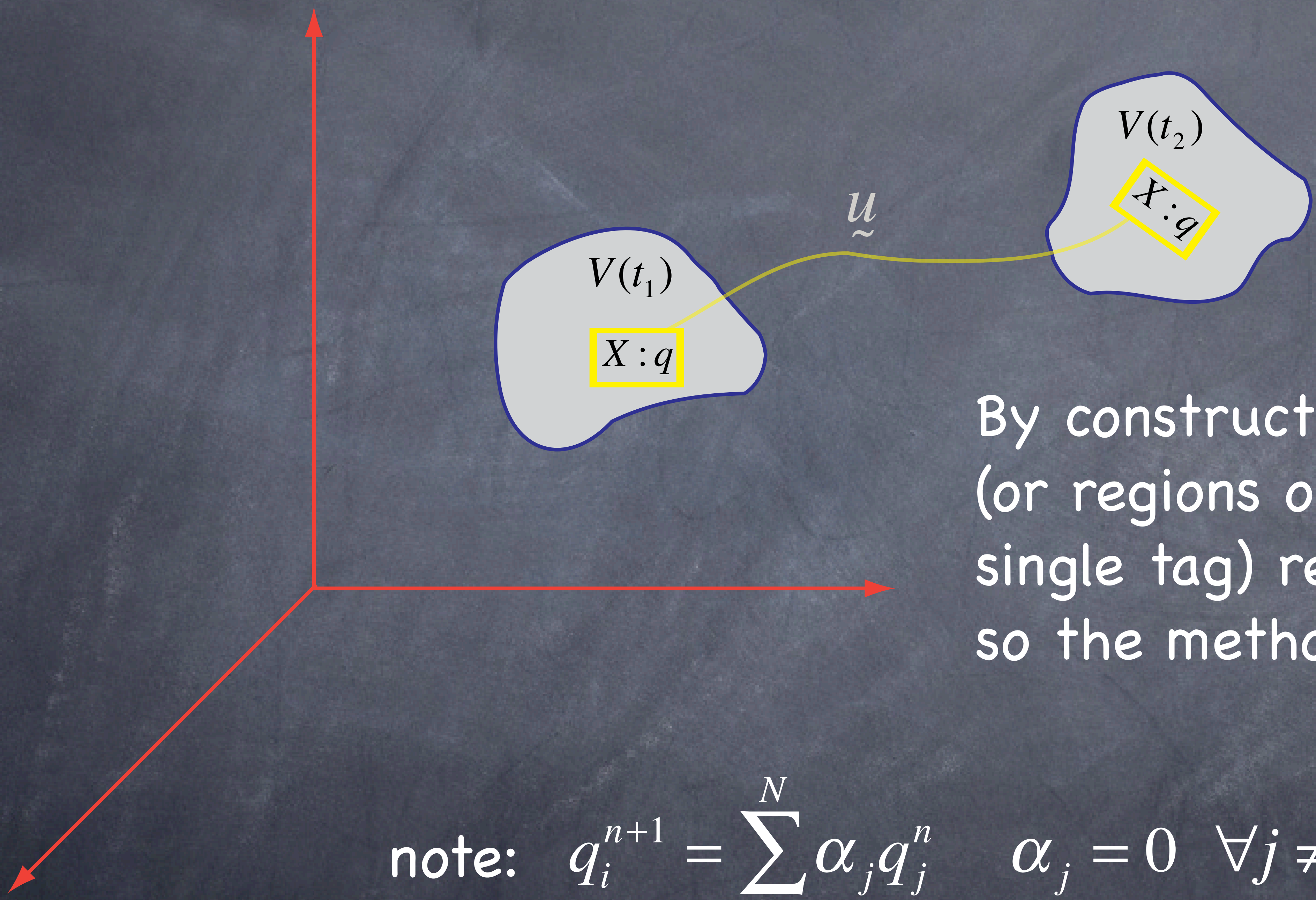



## The transport conundrum

1) Monotonicity is a property of the continuous operator.

2) Godunov (1959) proved that only 1st-order accurate interpolators have the properties to guarantee monotonicity.

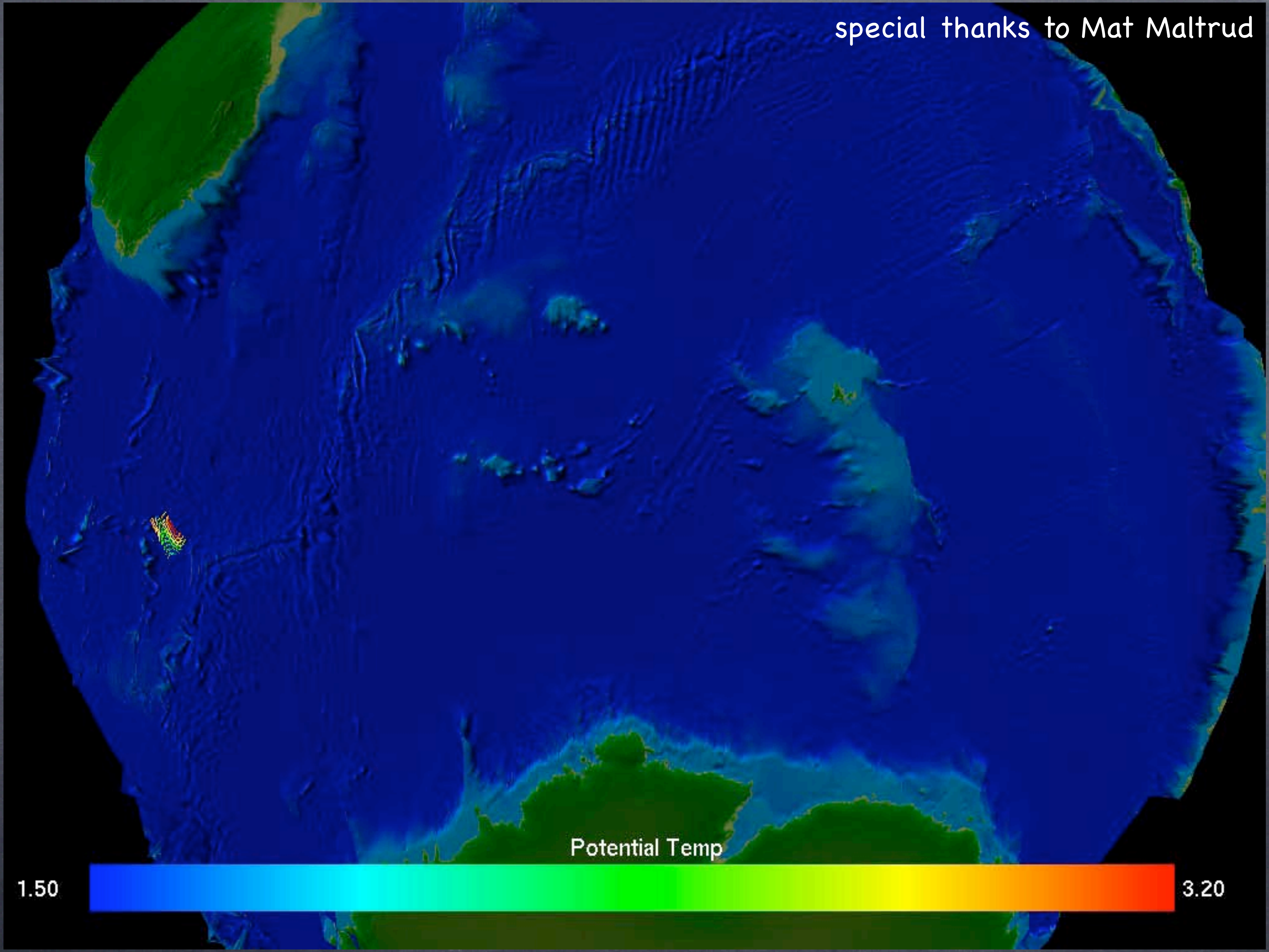
# Why not pose the problem in the reference frame moving with the fluid?




By construction, particle tags (or regions of fluid given a single tag) remain unchanged, so the method is non-diffusive.

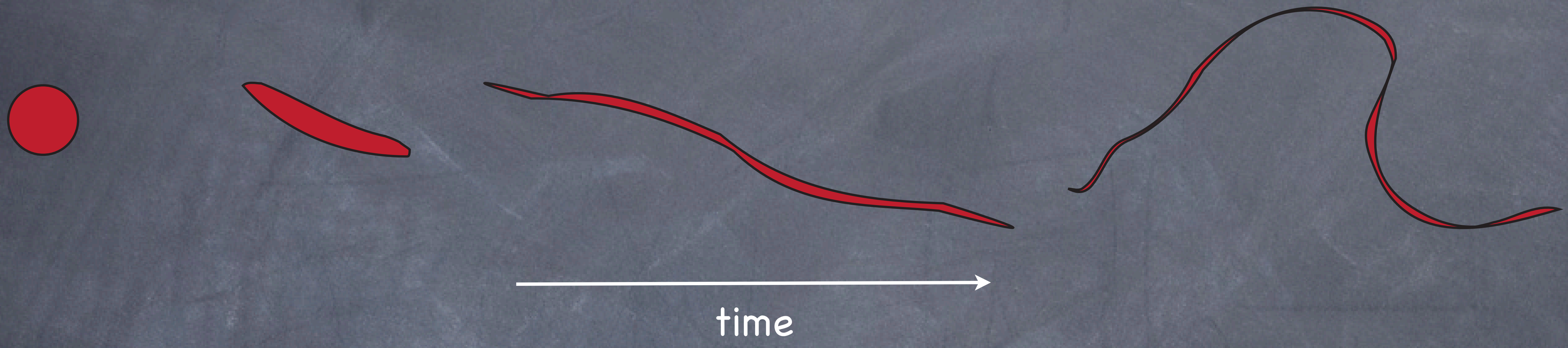
note: $q_i^{n+1} = \sum_{j=1}^{N} \alpha_j q_j^n \quad \alpha_j = 0 \;\; \forall j \neq i$

# The reason: Particles disperse rapidly, implying strong shearing/stretching/folding of a (once) compact fluid regions.

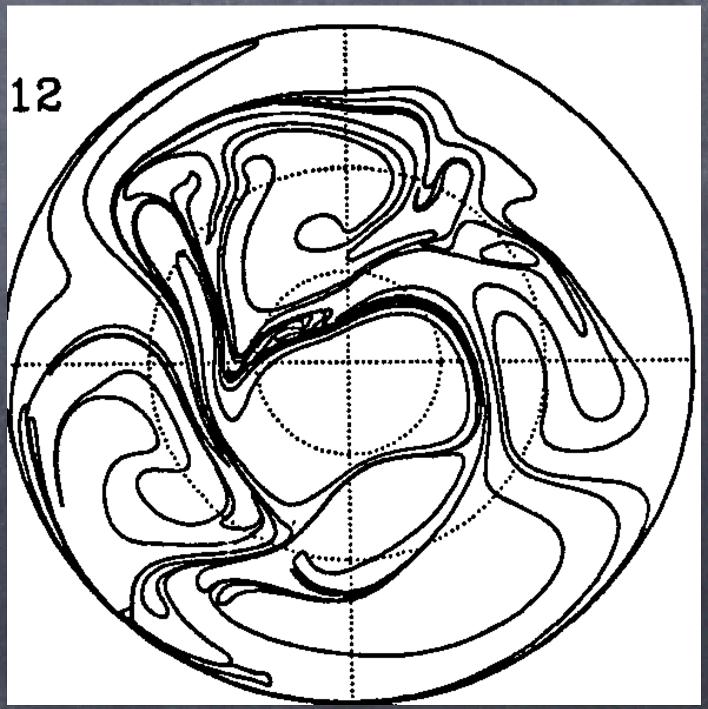



Global, eddy-resolving 1/10 deg ocean simulation (LANL POP model) with particle tracking.

# Tracking these rapidly deforming regions in time is a huge challenge.




contour surgery




Waugh (1993)

Contour surgery tracks the evolution of vortex lines, so it is a fully-Lagrangian method.

A significant amount of effort is required to clip filaments that get too thin.

So if we can't track a specific fluid region for long-times, we are compelled to make use of a fixed-grid in some manner.

So we basically have two choices for our tracer equation:

**advective form** $\longrightarrow$ $$\frac{\partial q}{\partial t} + \underset{\sim}{u} \cdot \nabla q = 0$$ $\longleftarrow$

- semi-Lagrangian methods
- global spectral methods
- spectral element methods
- mesh-free finite-difference methods

**flux form** $\longrightarrow$ $$\frac{\partial (hq)}{\partial t} + \nabla \cdot (hq\underset{\sim}{u}) = 0$$ $\longleftarrow$

- finite-volume methods
- discontinuous Galerkin methods
- spectral element methods

The chemistry models used in climate-mode essentially require a conservative form of tracer transport (i.e. the flux form).

That said, the advective form has been used with great success in weather prediction models using semi-Lagrangian transport.

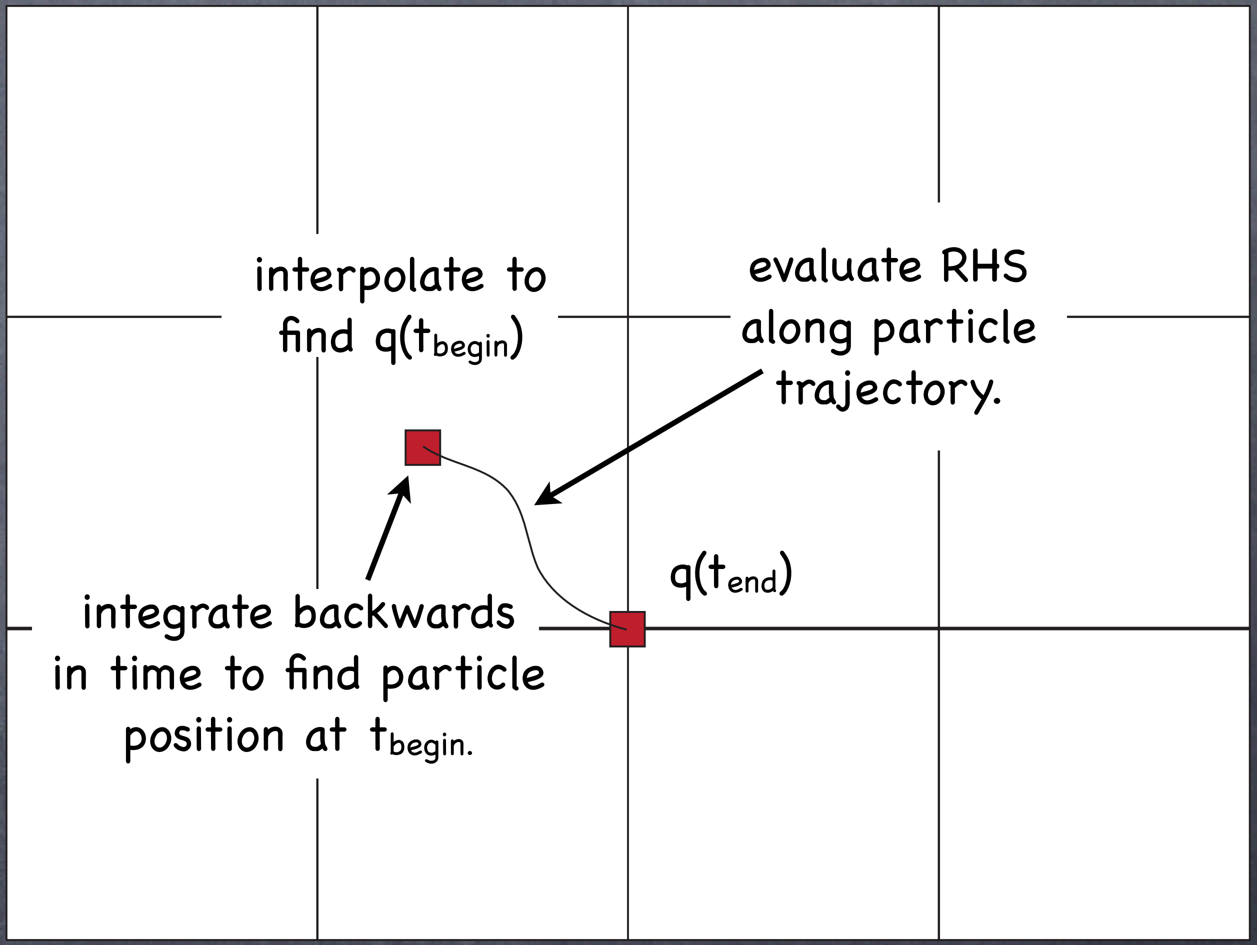
$$\frac{Dq}{Dt} = \frac{\partial q}{\partial t} + \underset{\sim}{u} \cdot \nabla q = 0$$

1) start with $\frac{Dq}{Dt} = 0$.

2) integrate along a particle backward in time from $t_{end}$ to $t_{begin}$, where we require the particle to "land" on the mesh at $t_{end}$.

3) using mesh values of q, interpolate to find the value of q at the location where the particle resided at $t_{begin}$.

4) set $q(t_{end}) = q(t_{begin})$




note: sources of q need to be evaluated along the particle trajectory.

For the remainder of the presentation we will focus on the flux-form of tracer transport.

The flux-form of tracer transport is useless without a mass equation, because while our prognostic variable is (hq), in the end we are interested in q.

The procedure in time:

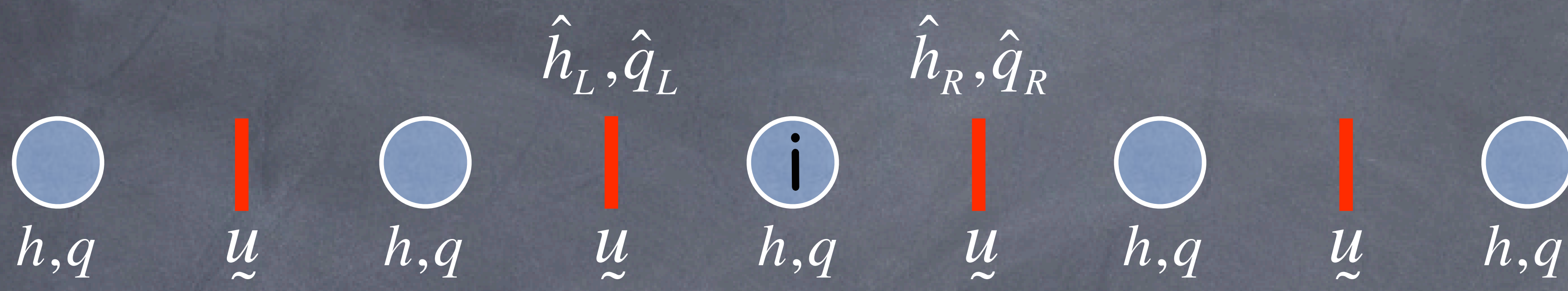
$$h^{n+1} = h^n - dt\left[\overline{\nabla\cdot(h\underset{\sim}{u})}\right]$$

← overbar denotes possible time-averaging

$$(hq)^{n+1} = (hq)^n - dt\left[\overline{\nabla\cdot(hq\underset{\sim}{u})}\right]$$

$$q^{n+1} = \frac{(hq)^{n+1}}{h^{n+1}}$$

## Spatial discretization: Start in 1D, assume $\underset{\sim}{u}$ is given.




$$h_i^{n+1} = h_i^n - dt\left[(\hat{h}_R \underset{\sim}{u}_R) - \hat{h}_L \underset{\sim}{u}_L)\right]/dl_i$$

$$(hq)_i^{n+1} = (hq)_i^n - dt\left[(\hat{q}_R \hat{h}_R \underset{\sim}{u}_R) - \hat{q}_L \hat{h}_L \underset{\sim}{u}_L)\right]/dl_i$$

If q is a constant, the tracer equation reduces to the mass equation. Is there a simple way to guarantee that this will be the case in our discrete system?

# Mass/tracer consistency.

$$h_i^{n+1} = h_i^n - dt\,\overline{\left[(\hat{h}_R \underset{\sim}{u}_R) - \hat{h}_L \underset{\sim}{u}_L)\right]}/dl_i$$

$$(hq)_i^{n+1} = (hq)_i^n - dt\,\overline{\left[(\hat{q}_R \hat{h}_R \underset{\sim}{u}_R) - \hat{q}_L \hat{h}_L \underset{\sim}{u}_L)\right]}/dl_i$$

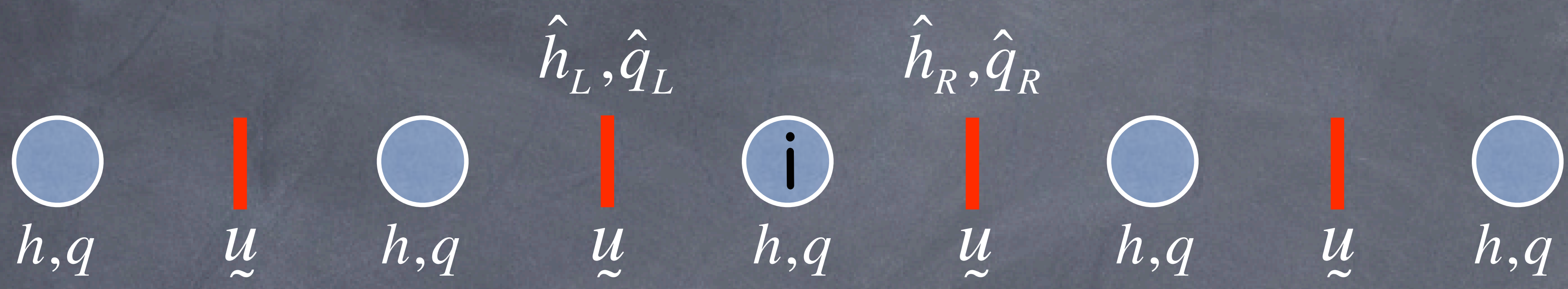
Let $M_R = \hat{h}_R \underset{\sim}{u}_R$ and $M_L = \hat{h}_L \underset{\sim}{u}_L$.

$$h_i^{n+1} = h_i^n - dt\,\overline{\left[(M_R) - M_L)\right]}/dl_i$$

$$(hq)_i^{n+1} = (hq)_i^n - dt\,\overline{\left[(M_R \hat{q}_R) - M_L \hat{q}_L)\right]}/dl_i$$

Expressing the tracer flux as the mass flux times some $\hat{q}$ AND guaranteeing that $\hat{q}$ is an interpolation of it neighbors (i.e. $\hat{q}$ is bounded by neighbor data) is sufficient to ensure that a constant $q$ remains constant and reduces to the mass equation.

# Spatial discretization: Start in 1D, assume $\underset{\sim}{u}$ is given.




$$h_i^{n+1} = h_i^n - dt\left[(\hat{h}_R \underset{\sim}{u}_R) - \hat{h}_L \underset{\sim}{u}_L)\right]/dl_i$$

$$(hq)_i^{n+1} = (hq)_i^n - dt\left[(\hat{q}_R \hat{h}_R \underset{\sim}{u}_R) - \hat{q}_L \hat{h}_L \underset{\sim}{u}_L)\right]/dl_i$$

No matter how fancy, intricate or complicated the transport scheme is, it can always be boiled down to two questions:

1) What is $\hat{h}$?

2) What is $\hat{q}$?

# Determining $\hat{q}$: High-order interpolation

We have our data defined at our nodes, our task is to determine $\hat{q}$ at the interfaces.

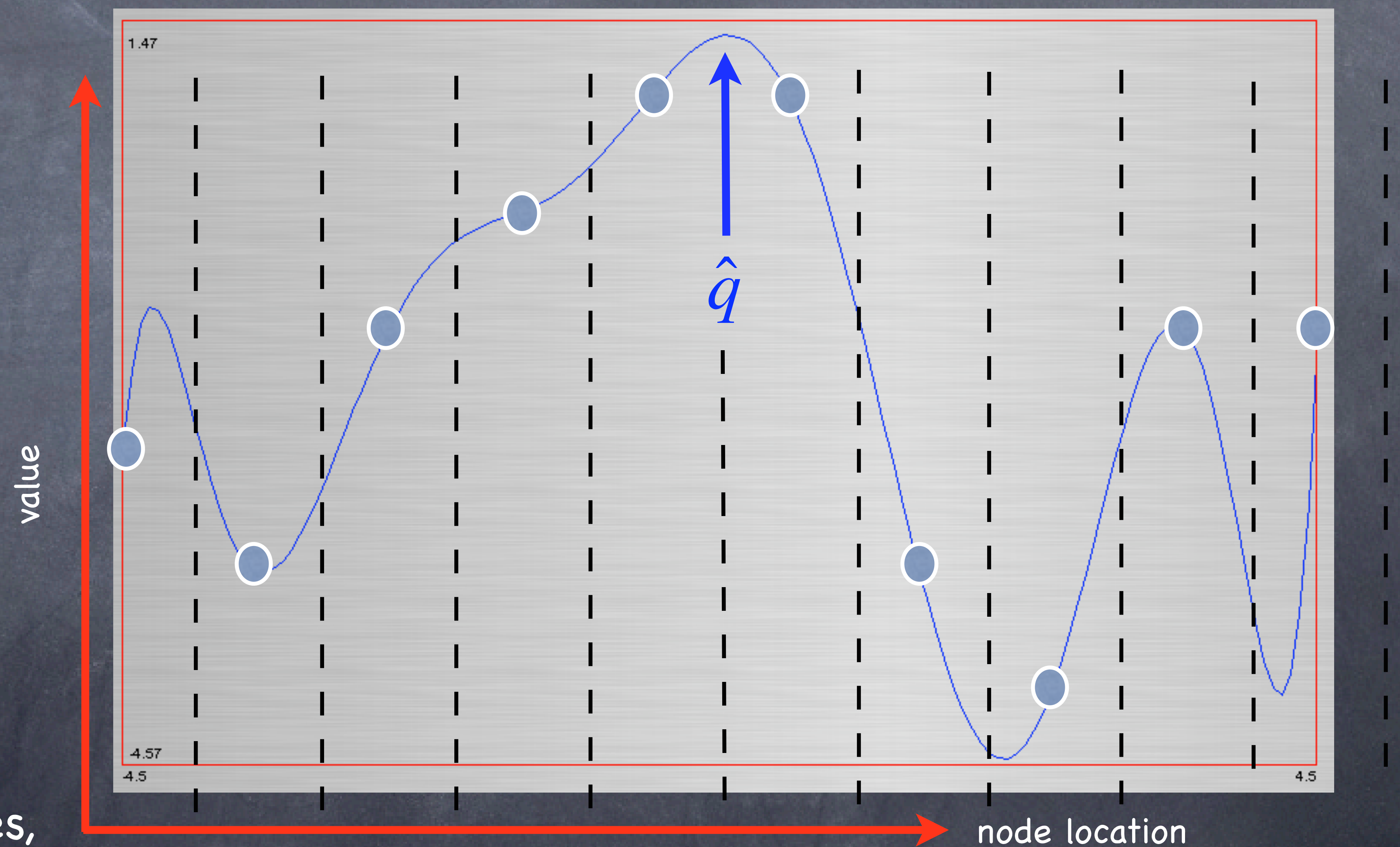
We can think of our node data as a sampling from the underlying continuous field, so fitting the data with a high order (and therefore formally accurate) polynomial makes sense.

<u>Assessment</u>

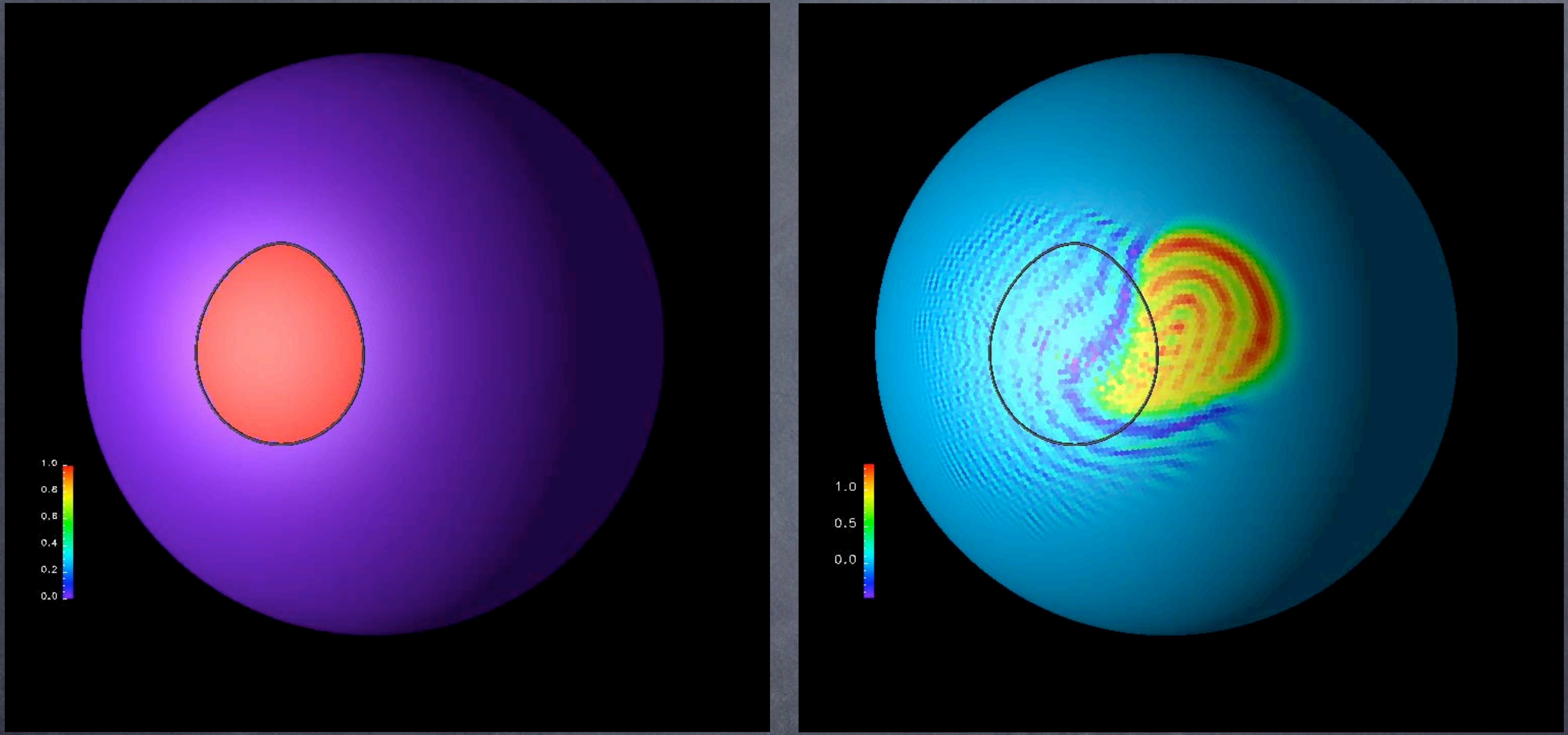
1) This is a very accurate reconstruction (9th order, in fact).

2) The reconstructed $\hat{q}$ is "out of bounds" in that it overshoots and undershoots all of the mesh data.

3) These over/under shoots can, in some cases, contaminate the simulation.

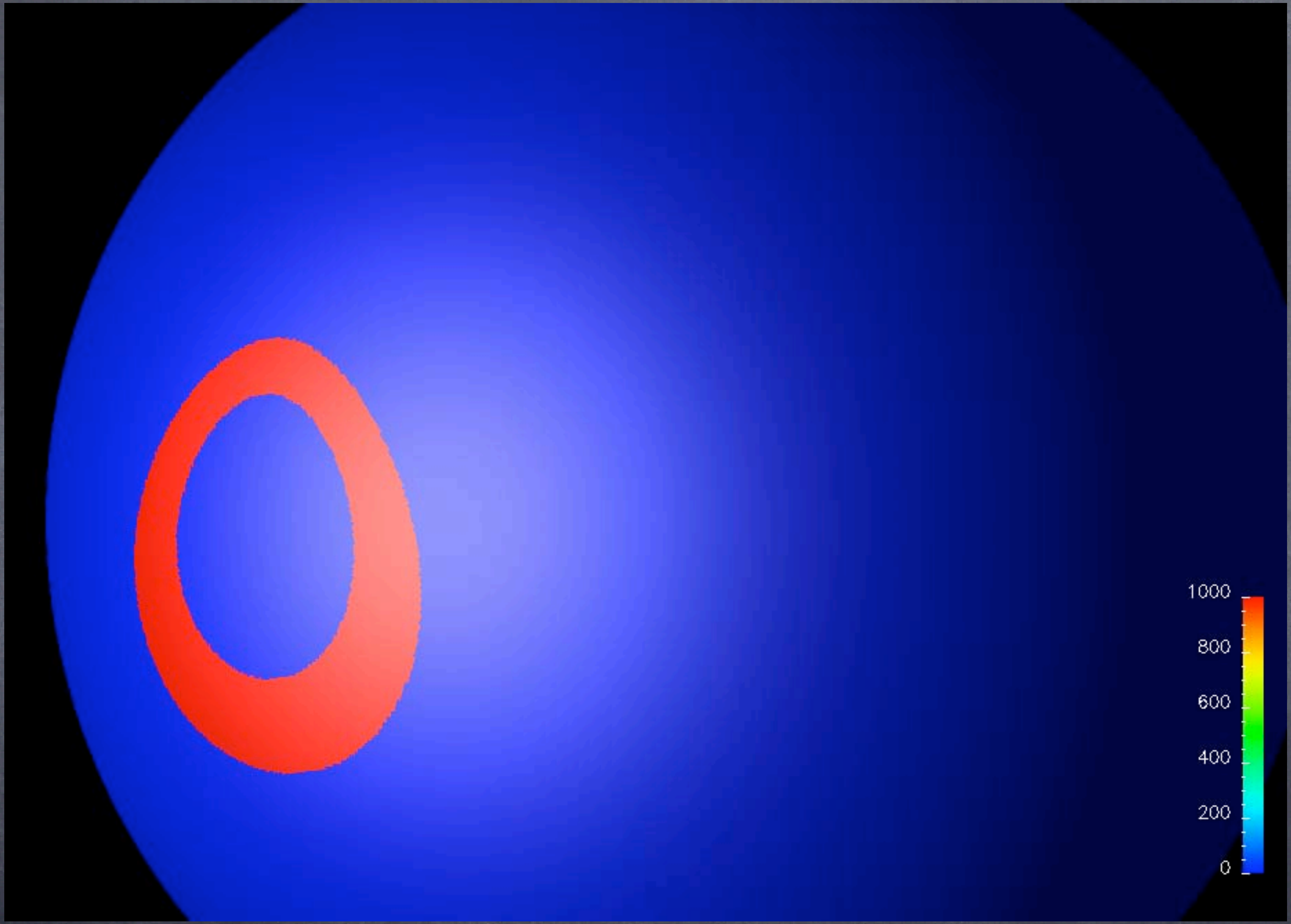


# An example of impact of under/over shoots.



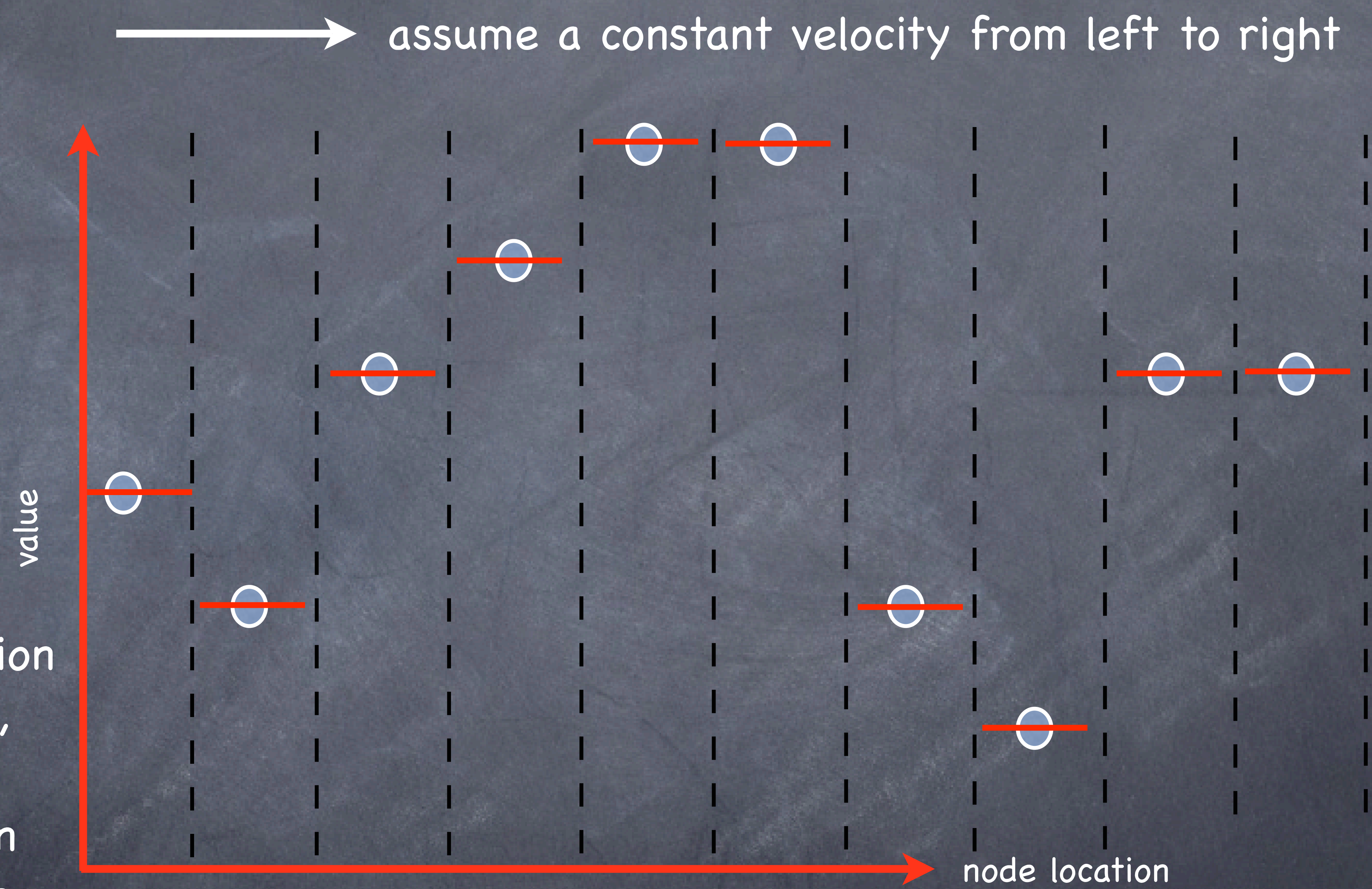
# Example of dispersion:

Note: overshoots are permitted (more on this below).




Whether or not over/under shoots are acceptable is problem dependent. For example, a slight overshoot on $CO_2$ concentration is likely to be benign, while an undershoot leading to negative specific humidity will cause havoc.

# Determining $\hat{q}$: Low-order interpolation




1) Assume a piece-wise constant reconstruction.

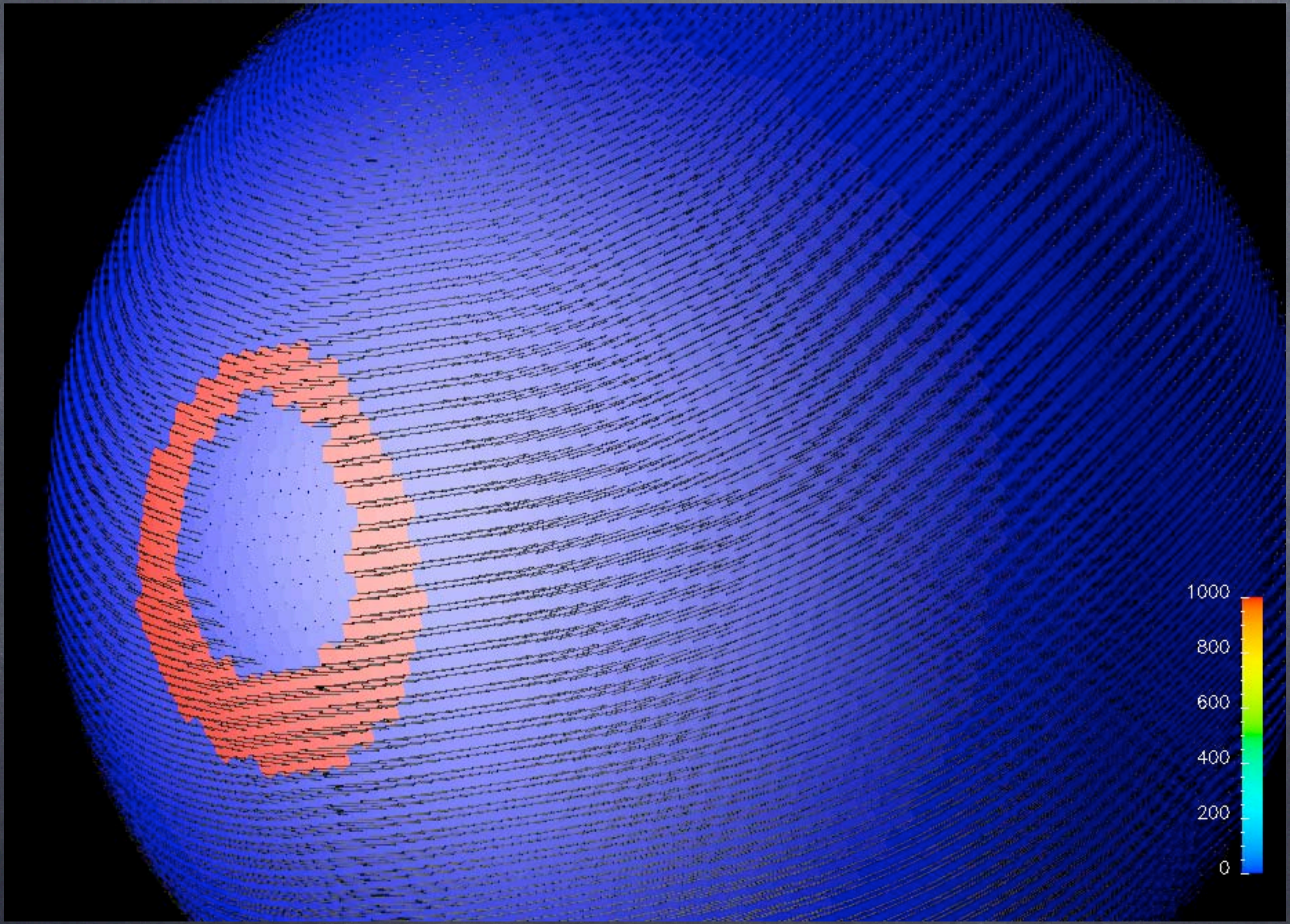
2) Recognize that the transport is from left to right and set $\hat{q}$ to its **upstream** neighbor.

3) Since the reconstruction is only 1st order accurate, the leading truncation error is $(\Delta x)^2$ resulting in a highly diffusive scheme.

$$q_i^{n+1} = q_i^n + u \cdot dt\,[q_{i-1}^n - q_i^n]$$

Satisfies Godunov's Theorem for $u \cdot dt \leq 1$

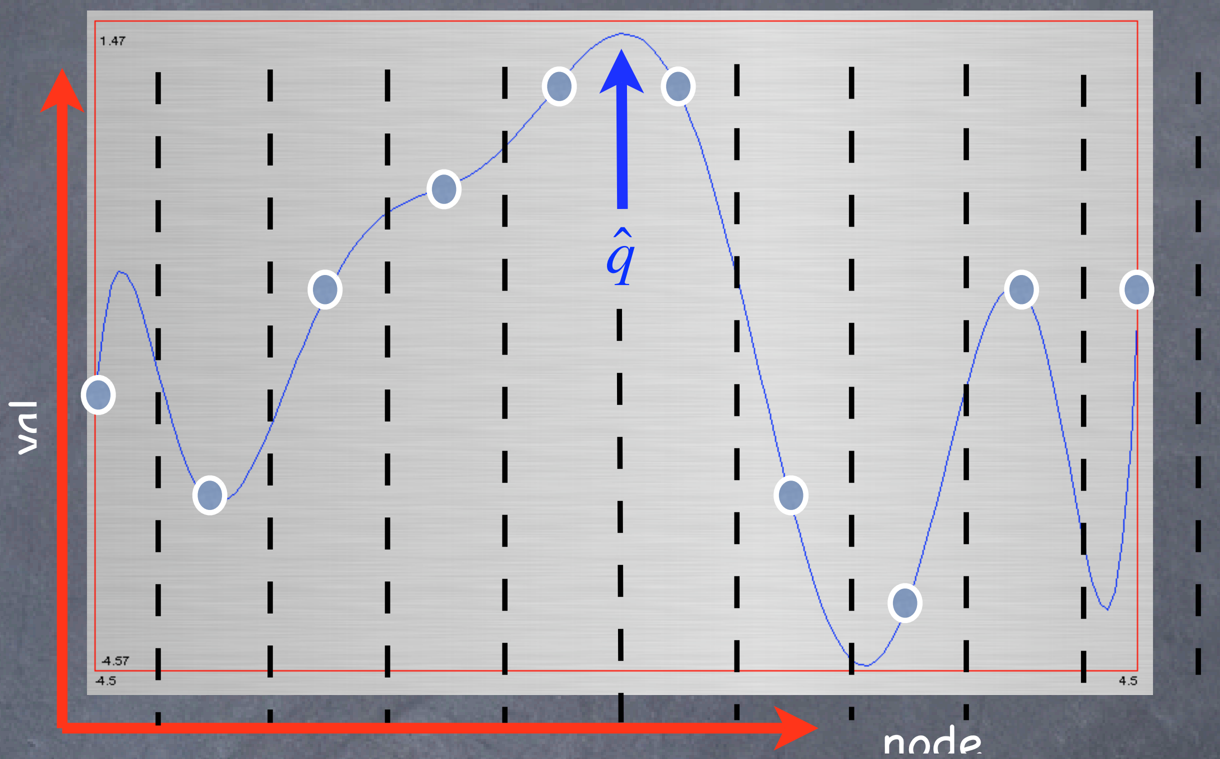
# Example of diffusion: transport is monotone.



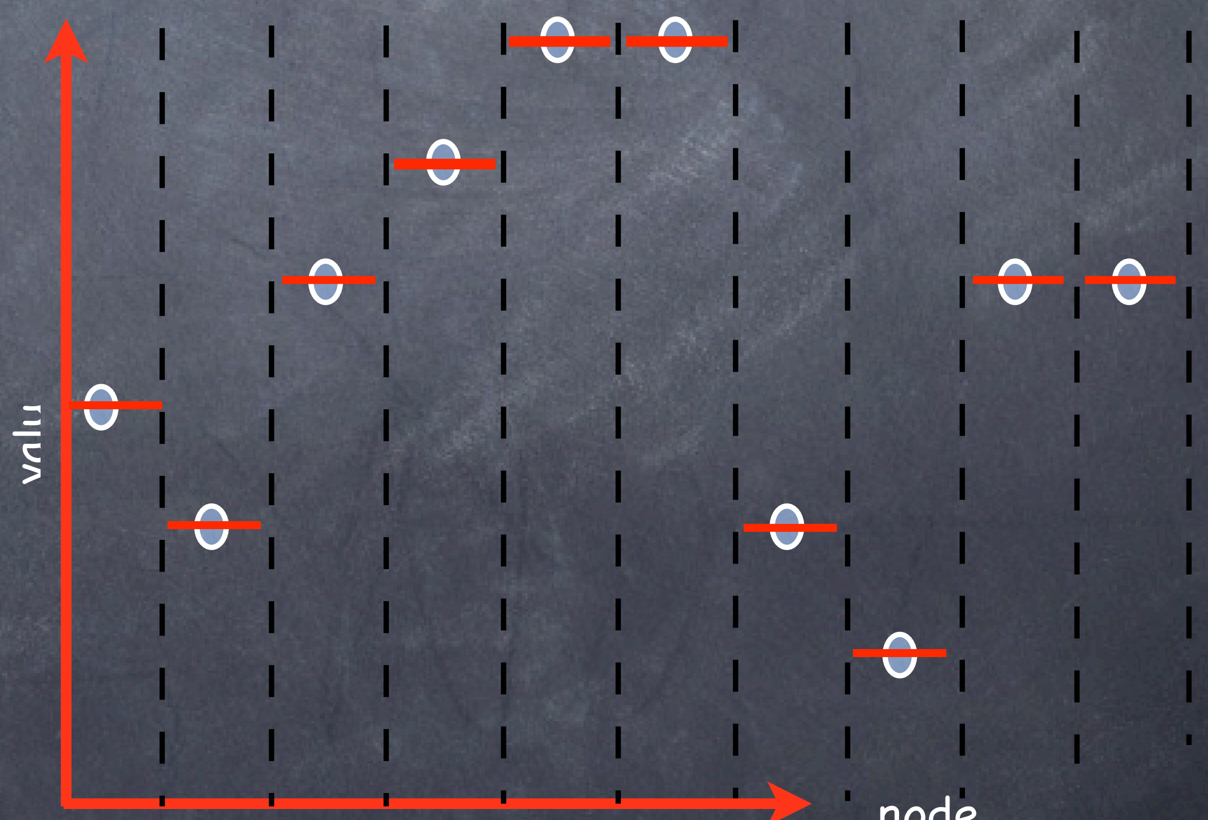

The excessive smoothing significantly degrades the quality of the simulation.

# So we are left with a Goldilocks search ....

This $\hat{q}$ is too hard.




This $\hat{q}$ is too soft.



# .... but (according to the literature) all of these $\hat{q}$ are just right ...

**Contents** [hide]



The point here is twofold:

1) The appropriate transport scheme is problem specific.
2) A tremendous amount of effort has been given to the topic of transport.

We can broadly think of schemes in one of two ways: the scheme either **limits the flux** or the scheme **limits the reconstruction**.

In either case, the attempt is to modify $\hat{q}$ in such a way as to minimize the diffusivity, maximize the formal accuracy and guarantee something about the bounds on the resulting tracer distribution.

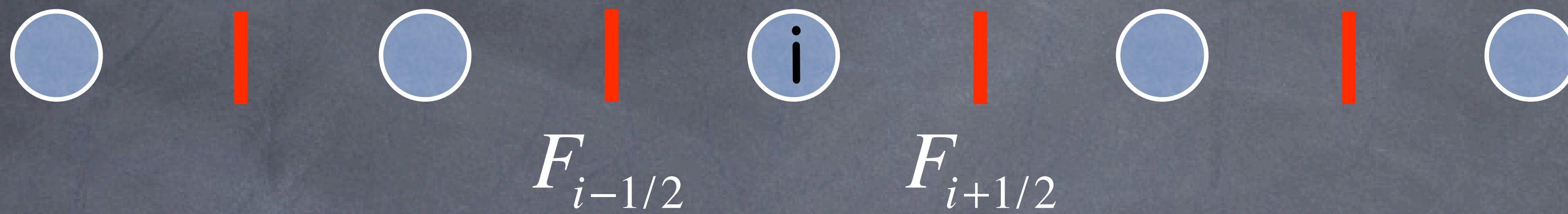
The "guarantees" generally all into one of three categories:

1) monotone (as defined above)

2) total variation diminishing (variance between adjacent nodes reduces in time).

3) positive definite (just keep it above zero!).

# Approach #1: Limiting the Flux




$L_{i+1/2} = M_{i+1/2}\hat{q}^{LOW}_{i+1/2}$ Low-order flux that guarantees, say, monotonicity.

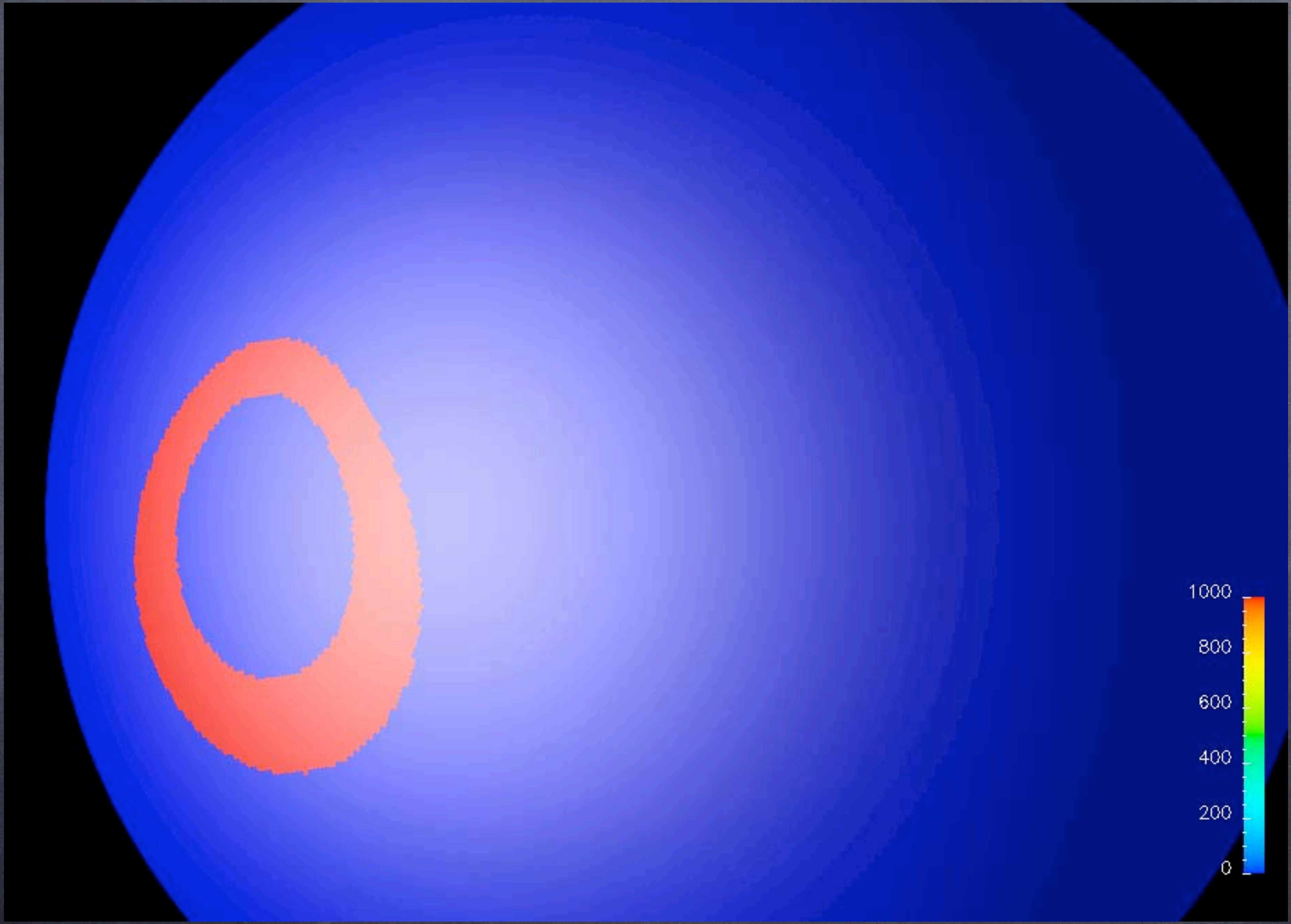
$H_{i+1/2} = M_{i+1/2}\hat{q}^{HIGH}_{i+1/2}$ High-order flux that we would like to use.

$$F_{i+1/2} = L_{i+1/2} + \phi_{i+1/2} \cdot \left(H_{i+1/2} - L_{i+1/2}\right)$$
$$F_{i-1/2} = L_{i-1/2} + \phi_{i-1/2} \cdot \left(H_{i-1/2} - L_{i-1/2}\right)$$
$$0 \le \phi \le 1$$

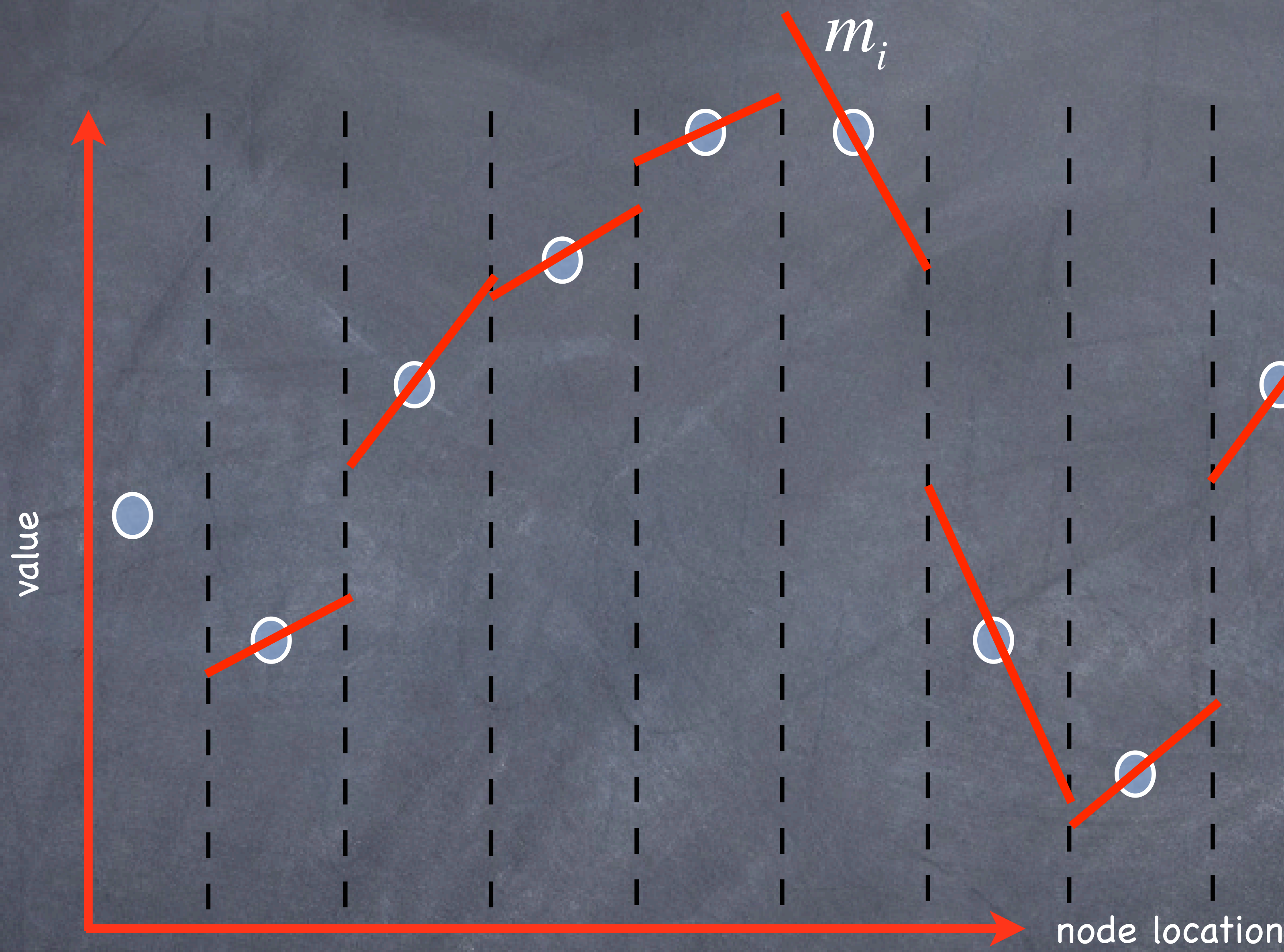
The name of the game is to maximize $\phi$ while still maintaining some constraint on the tracer field (e.g. monotonicity). This can be an iterative procedure (i.e. guess $\phi$ , find new q, guess new $\phi$ , ....) or it can be a deterministic where a suboptimal value of $\phi$ results.

Note: $\hat{q}^{final}_{i+1/2} = F_{i+1/2} / M_{i+1/2}$ $\quad \min(\hat{q}^{LOW}_{i+1/2}, \hat{q}^{HIGH}_{i+1/2}) \le \hat{q}^{final}_{i+1/2} \le \max(\hat{q}^{LOW}_{i+1/2}, \hat{q}^{HIGH}_{i+1/2})$

# Limiting the Flux:
# Limiting to maintain q as positive definite.



# Approach #2: Limiting the Reconstruction




$$q_i(x) = q_{mean} + m_i(x - \overline{x})$$

$$m_i = (q_{i+1} - q_{i-1}) / (x_{i+1} - x_{i-1})$$

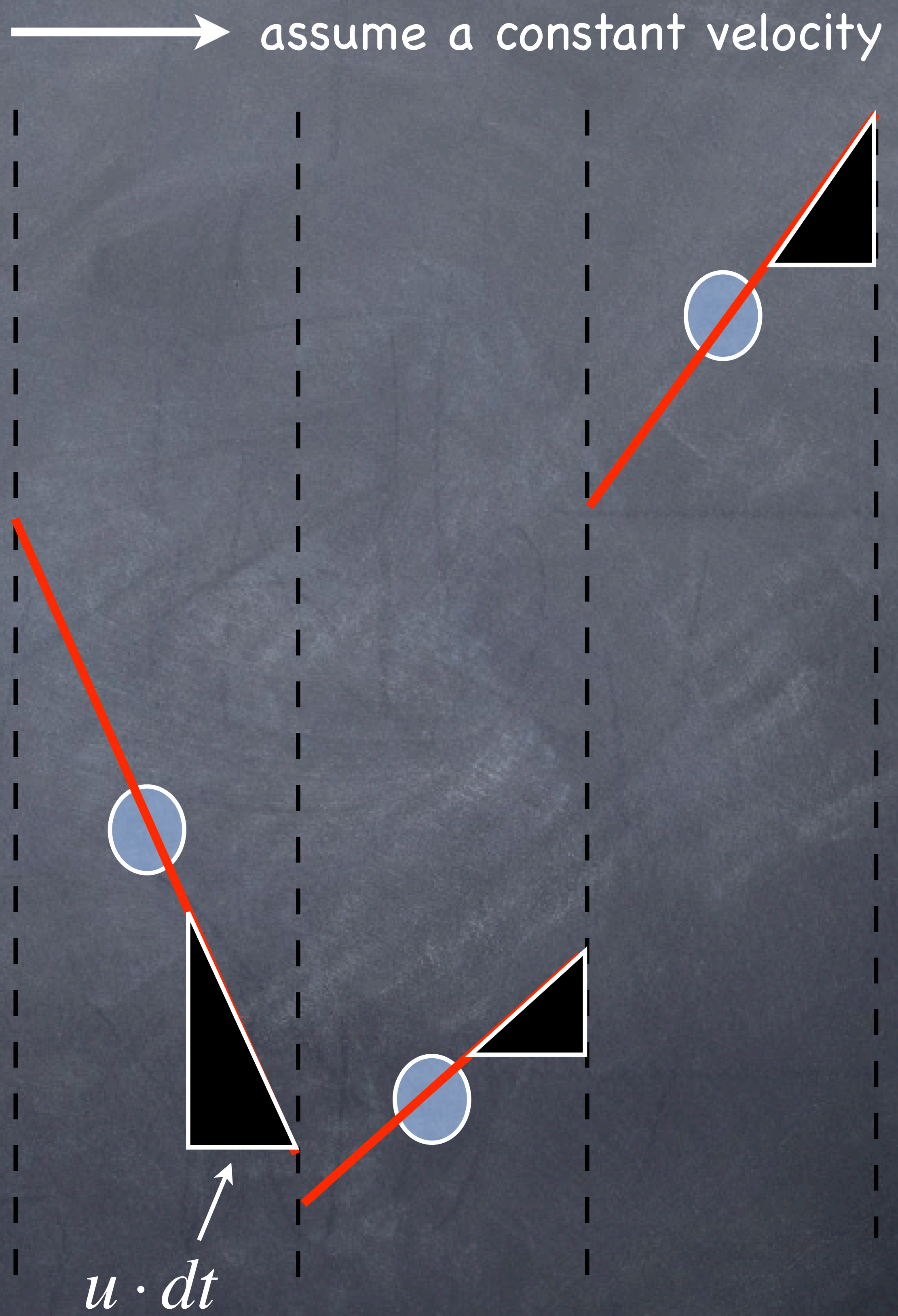
# Using the reconstruction w/o modification

The flux is the "area under the curve."

$$F_{i+1/2} = \int_{\hat{x}}^{\hat{x}-u\cdot dt} q_i(\lambda)d\lambda$$

If we use the linear reconstruction without modification, we will have a 2nd-order accurate transport scheme that will, in general, create new extrema (i.e. have significant dispersive error).

The question is how can we limit the reconstruction in order to maintain, say, a monotone transport scheme?



# Using the reconstruction with limiting

First we generalize our reconstruction with a limiting parameter:

$$q_i(x) = q_{mean} + \alpha_i m_i (x - \bar{x}) \qquad 0 \le \alpha_i \le 1$$

$$q_{\min} = \min\left[q_{i+1}, q_i, q_{i-1}\right]$$

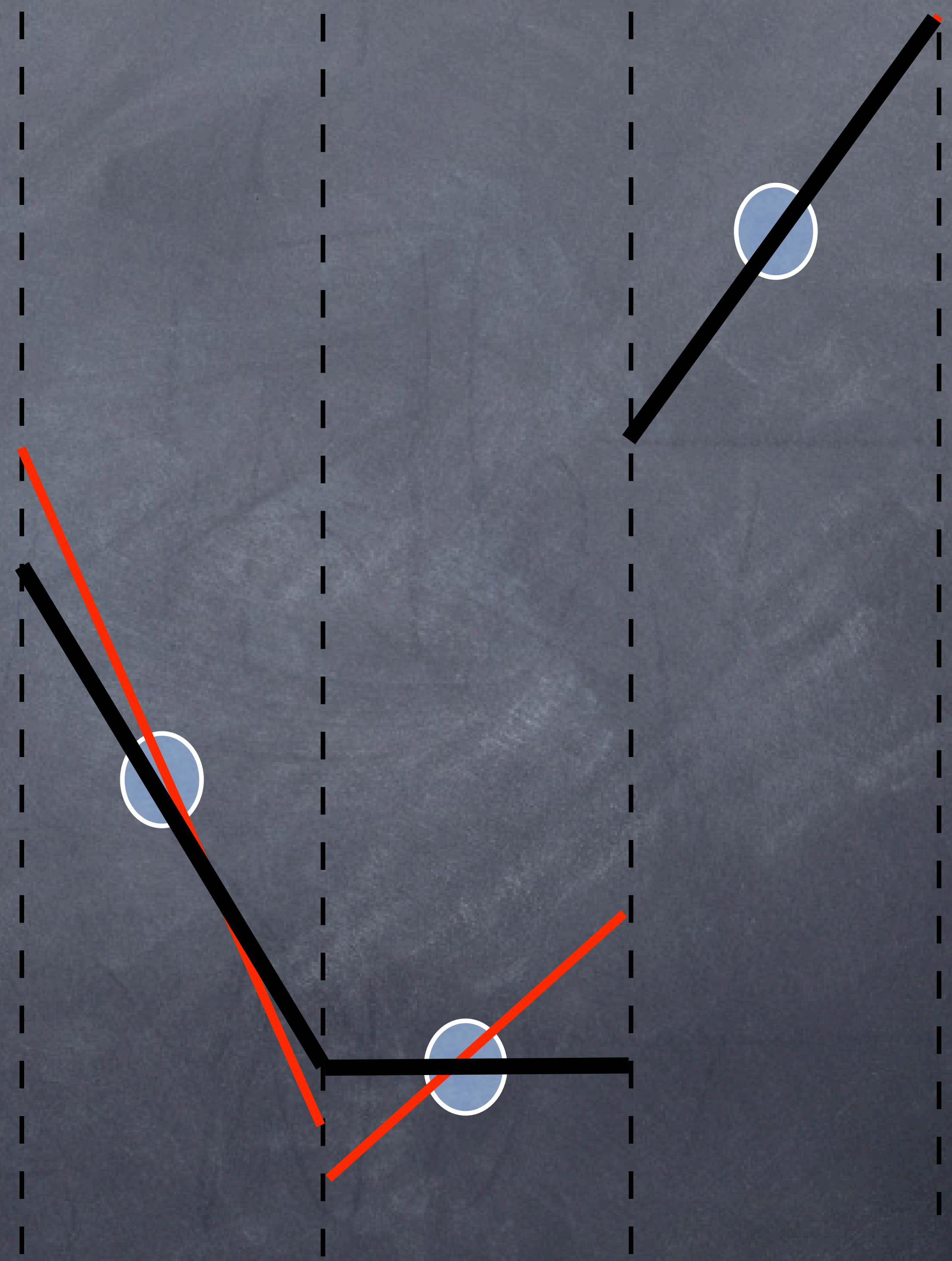
$$q_{\max} = \max\left[q_{i+1}, q_i, q_{i-1}\right]$$

$$\alpha_{\min} = \max\left[0, \left(\frac{q_{\min} - q_{mean}}{\min\left[q_i(x)\right] - q_{mean}}\right)\right]$$

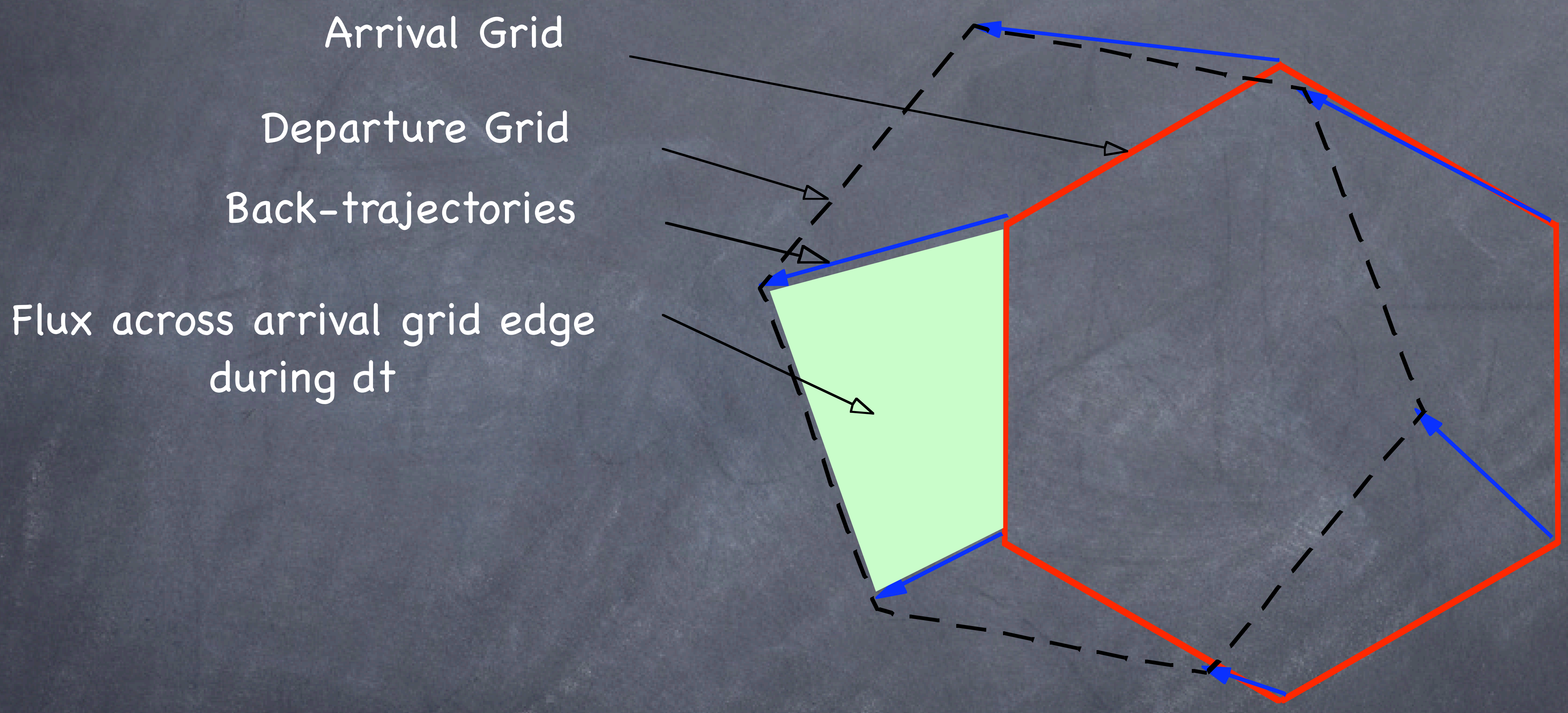
$$\alpha_{\max} = \max\left[0, \left(\frac{q_{\max} - q_{mean}}{\max\left[q_i(x)\right] - q_{mean}}\right)\right]$$

$$\alpha_i = \min\left[1, \alpha_{\min}, \alpha_{\max}\right]$$

→ assume a constant velocity

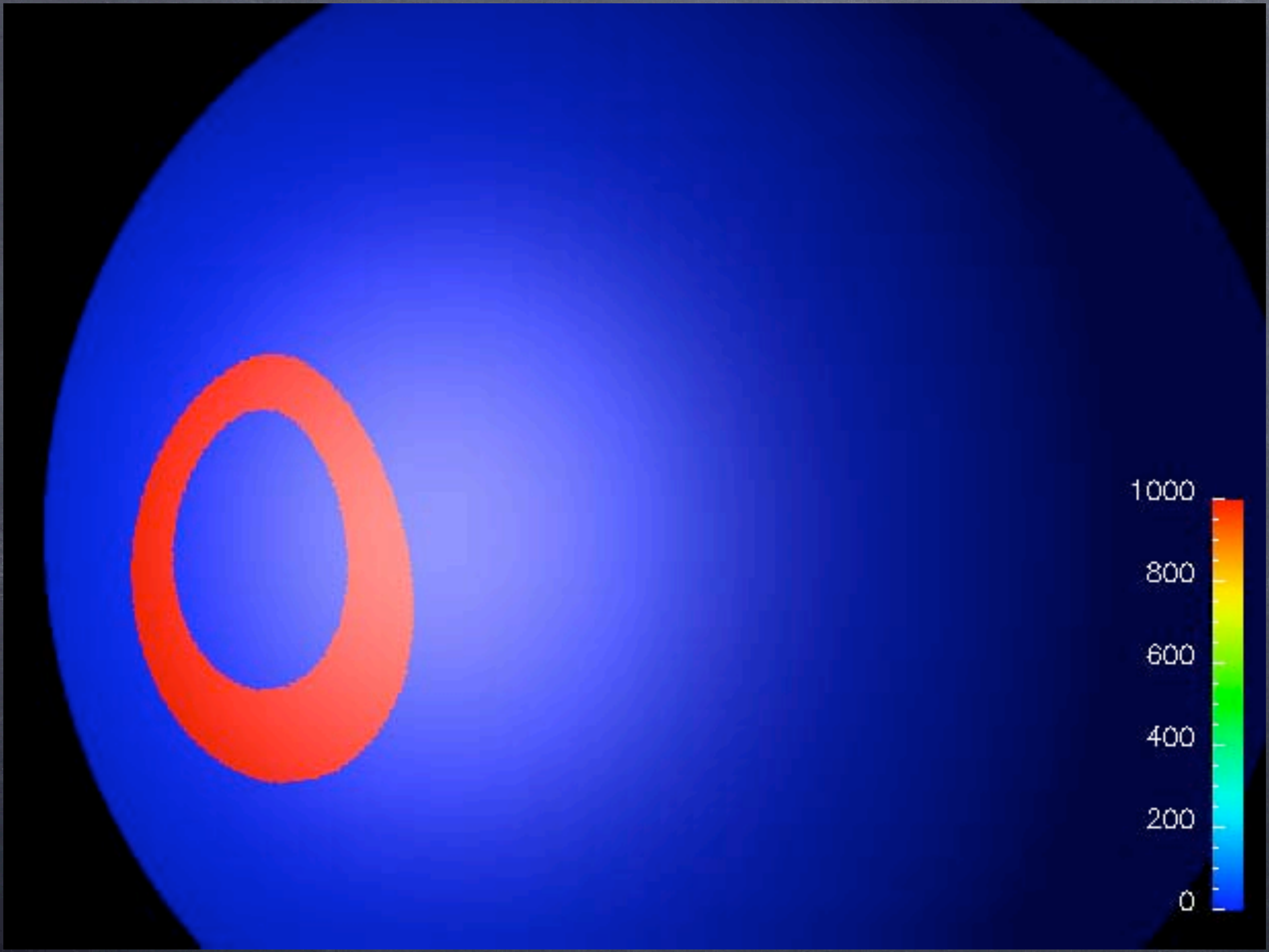


# Putting it all together: Transport with 2D limiting.



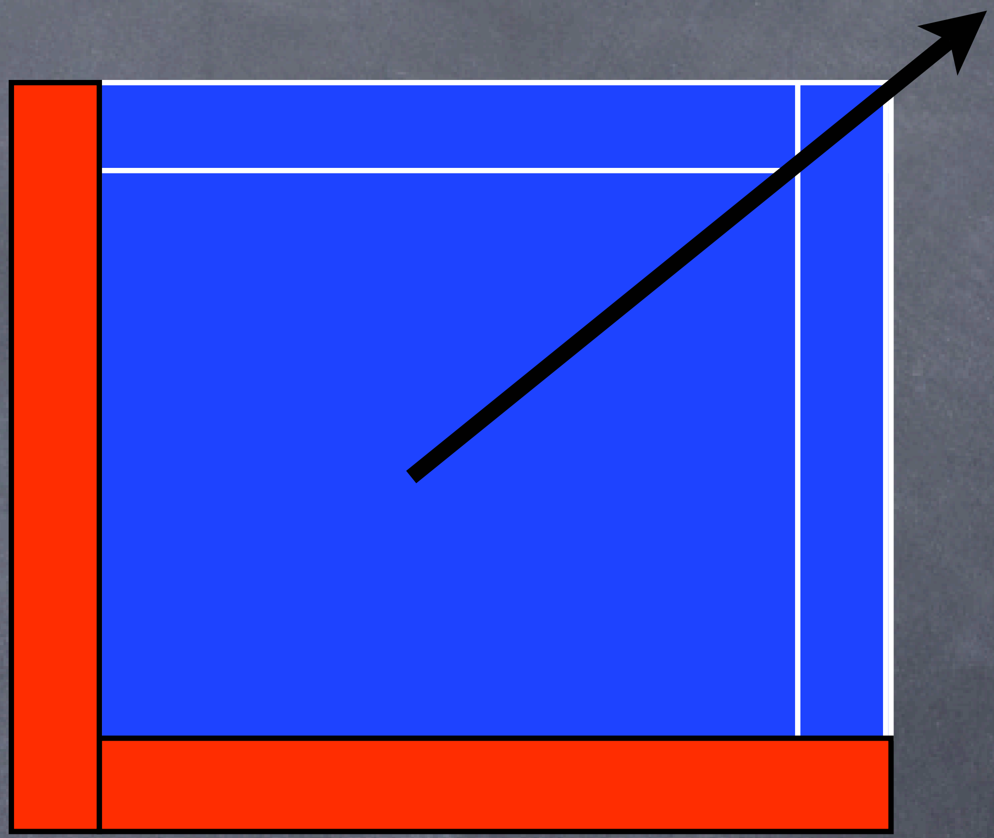

Flux is computed via quadrature methods with limiting on the reconstruction to produce a monotone (or otherwise limited) advection scheme.

# Limiting the reconstruction for monotone transport



# Even if we have the exact edge fluxes (and thus the exact cell mean tendency), we still have a problem ....

Assume the velocity (black arrrow) is transporting low concentration tracer (blue) out of the box and high concentration tracer (red) into the box. (assume constant density and nondivergent flow so that mass drops out).



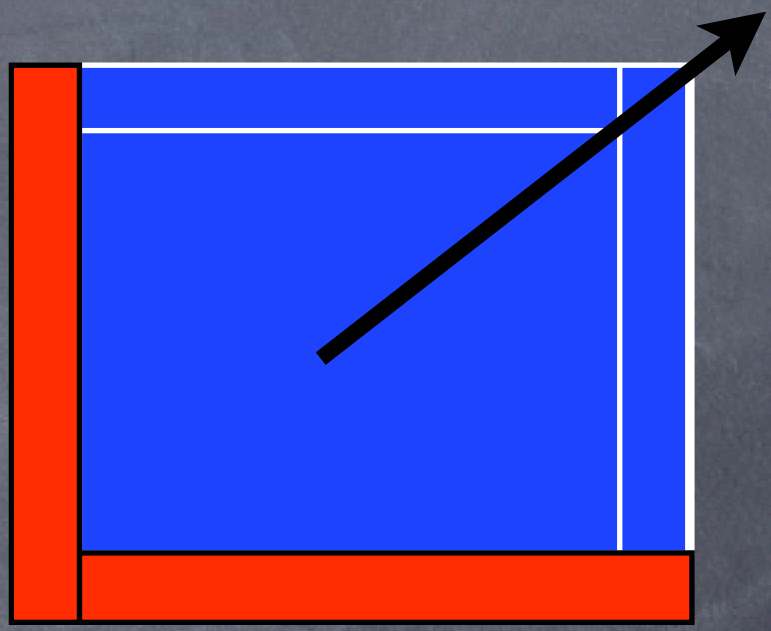
$$q^{new} = \frac{1}{A_{total}}\left[ (A_{total} - A_{red}) q^{blue} + A_{red} q^{red} \right]$$

The high concentration tracer coming into the box is **immediately mixed** with the the low concentration tracer left in the box.

On the next time step, the (now diluted) high tracer that came in the left side of the box will exit out the right side of the box, regardless of the size of the box!

This mixing occurs because we (generally) only keep track of the cell mean quantity, so one (rather expensive) way around this problem is to augment our cell-mean tracer equation with tracer-moment equations that allow us to retain the information that "red" is to the bottom-left.

In addition to conserving the zeroth-moment of the tracer field, we also conserve the first, or maybe even, the second moments. At this point the distinction between finite-volume and discontinuous Galerkin becomes unclear.



$$q(x,y) = m_0 K_0 + m_X K_X + m_Y K_Y + \ldots$$

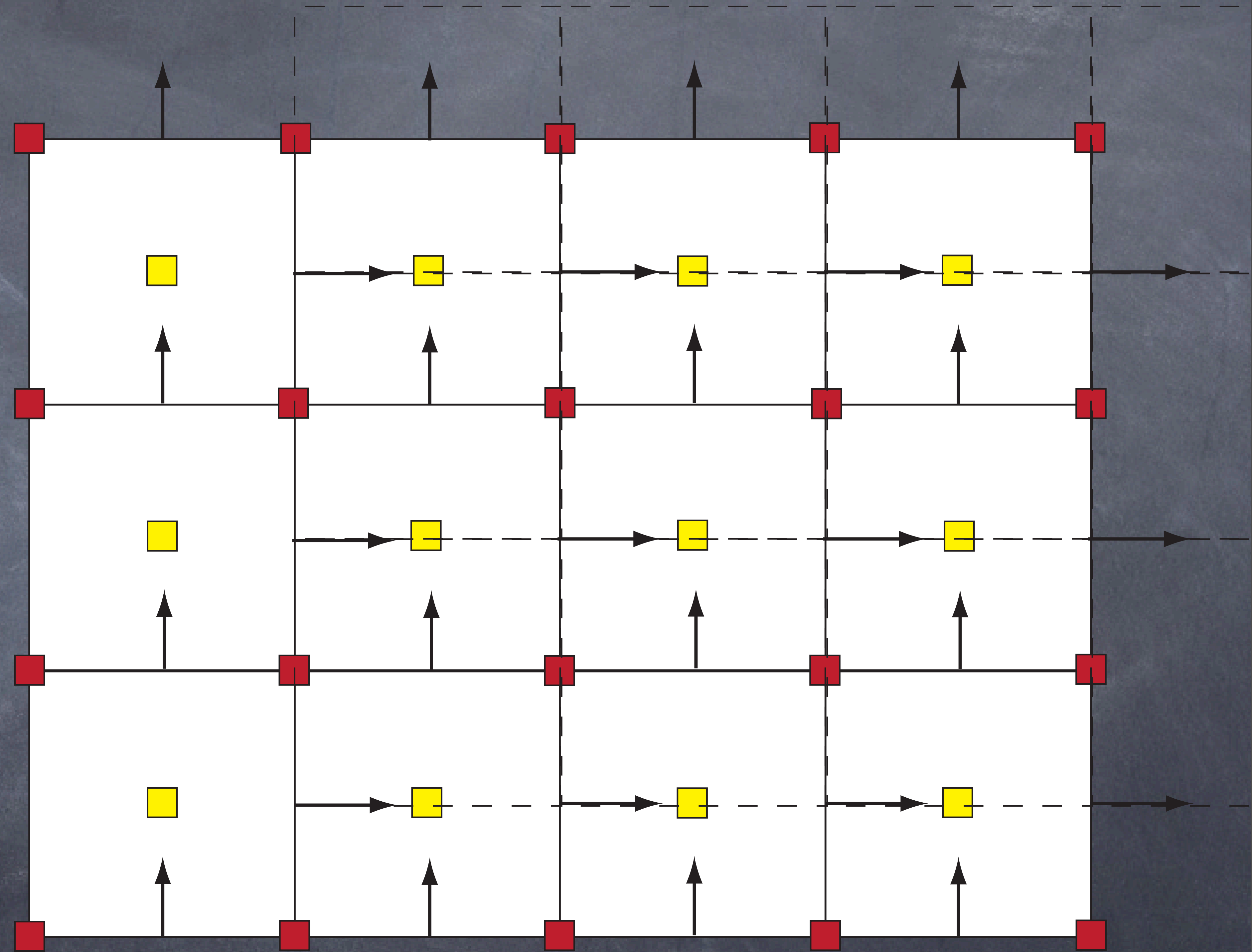
$$K_0 = 1, K_X = x - \bar{x}, K_Y = y - \bar{y}$$ ← our orthogonal basis

evolution equations for $m_0, m_X, m_Y, \ldots$

cell-mean value → $m_0$; tracer slope in x,y directions → $m_X, m_Y$

And finally, a tie back to Monday's discussion on F=ma and "slaving" the velocity field to our discrete vorticity equation.

# RECAP: What is the C-grid staggering?



mass point

northward velocity point

eastward velocity point

vorticity point

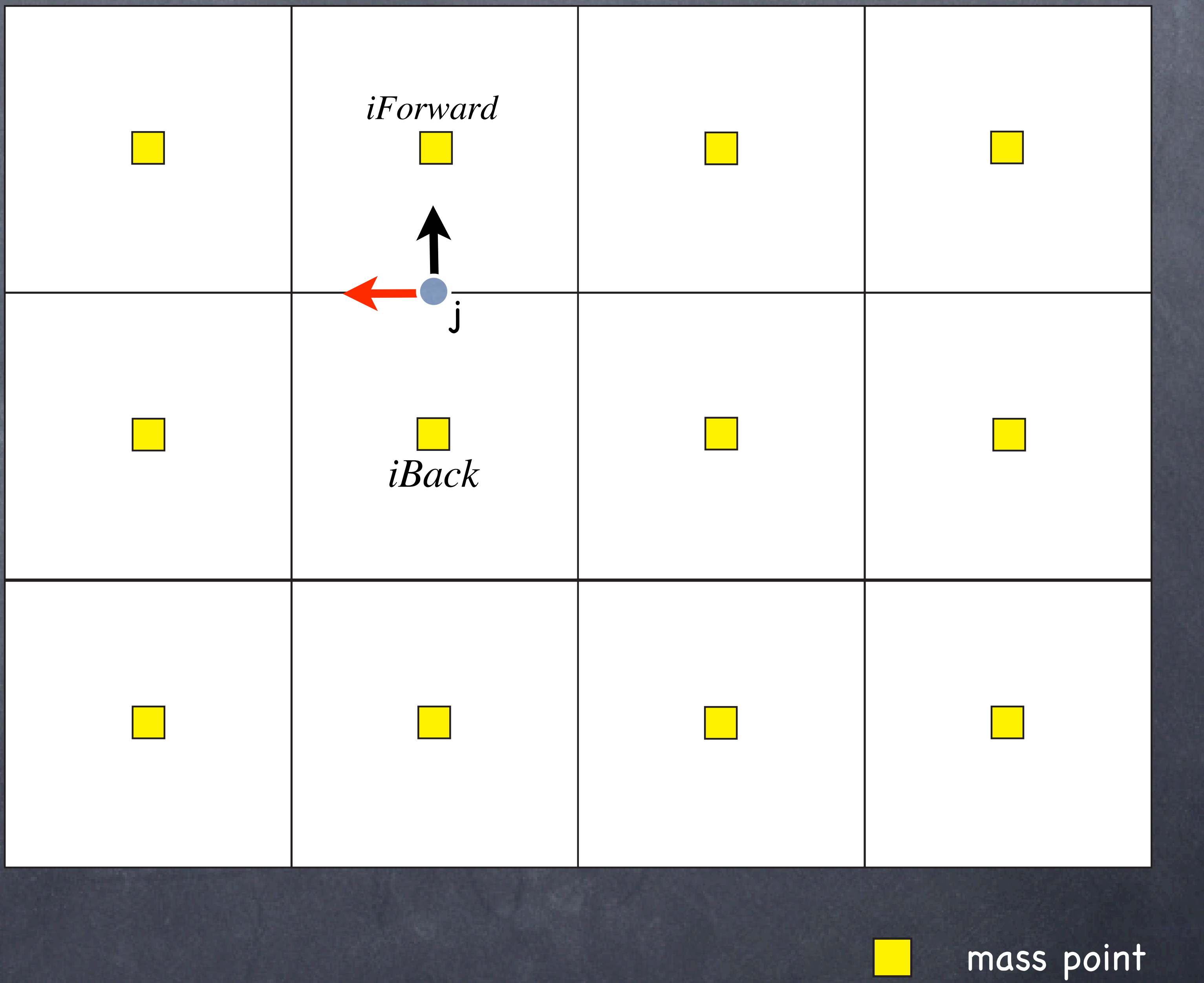
Define all prognostic velocity points as N (as in Normal) to a mass cell edge. In order to construct a full velocity vector, N will have be augmented with T (as in Tangent) to a mass cell edge, defined positive in the k cross N direction.

The orthogonality constraint requires the line connecting two mass points to be orthogonal to the shared edge (and thus parallel to the projected velocity component.

# RECAP: The discrete momentum equation: everything with an overhat has to be defined

$$\frac{\partial N_j}{\partial t} = \hat{\eta}_j \hat{T}_j - \left\{ \left[ gh + gh_s + \hat{K} \right]_{iForward} - \left[ gh + gh_s + \hat{K} \right]_{iBack} \right\} / dc_j$$

- $dc_j$ distance between iForward and iBack
- $\hat{\eta}_j$ absolute vorticity
- $\hat{T}_j$ reconstructed, tangent velocity, for here simply state $\hat{T}_j = f(N_j)$.
- $gh + gh_s + \hat{K}$ sum of potential and kinetic energy



# The discrete vorticity equation:

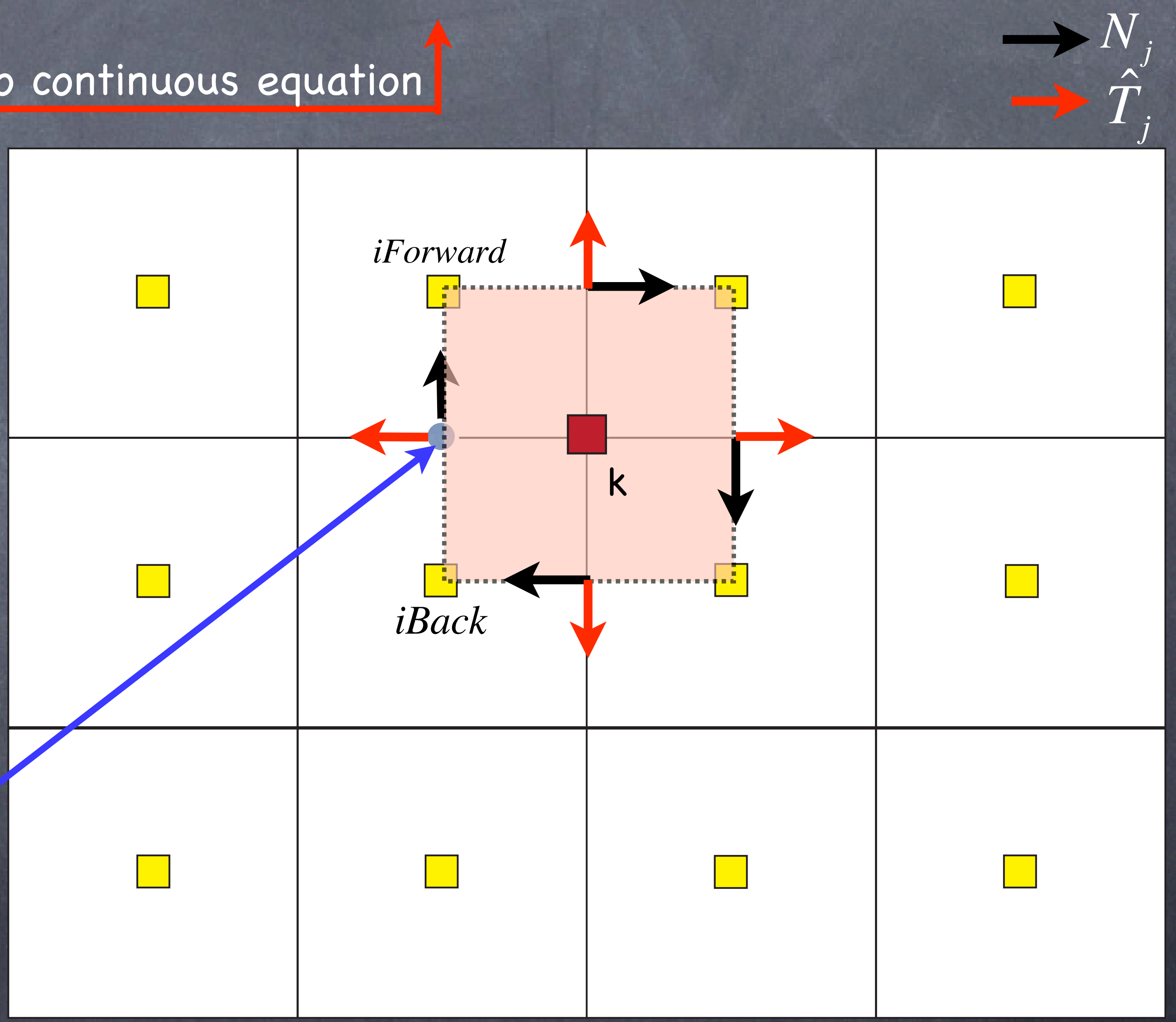
taking the curl of the momentum equation.

$$\frac{1}{A_k}\sum_{j=1}^{nedges} dc_j \left\{ \frac{\partial N_j}{\partial t} = \hat{\eta}_j \hat{T}_j - \left\{ \left[ gh + gh_s + \hat{K} \right]_{iForward} - \left[ gh + gh_s + \hat{K} \right]_{iBack} \right\} / dc_j \right\}$$

$$\frac{\partial \eta_k}{\partial t} + \frac{1}{A_k}\sum_{j=1}^{nedges} \hat{\eta}_j \hat{T}_j dc_j = 0 \qquad \frac{\partial \eta}{\partial t} + \nabla \cdot (\eta \underset{\sim}{u}) = 0$$

nice analog to continuous equation

needs to be determined for use in the momentum equation. → $\hat{\eta}_j$



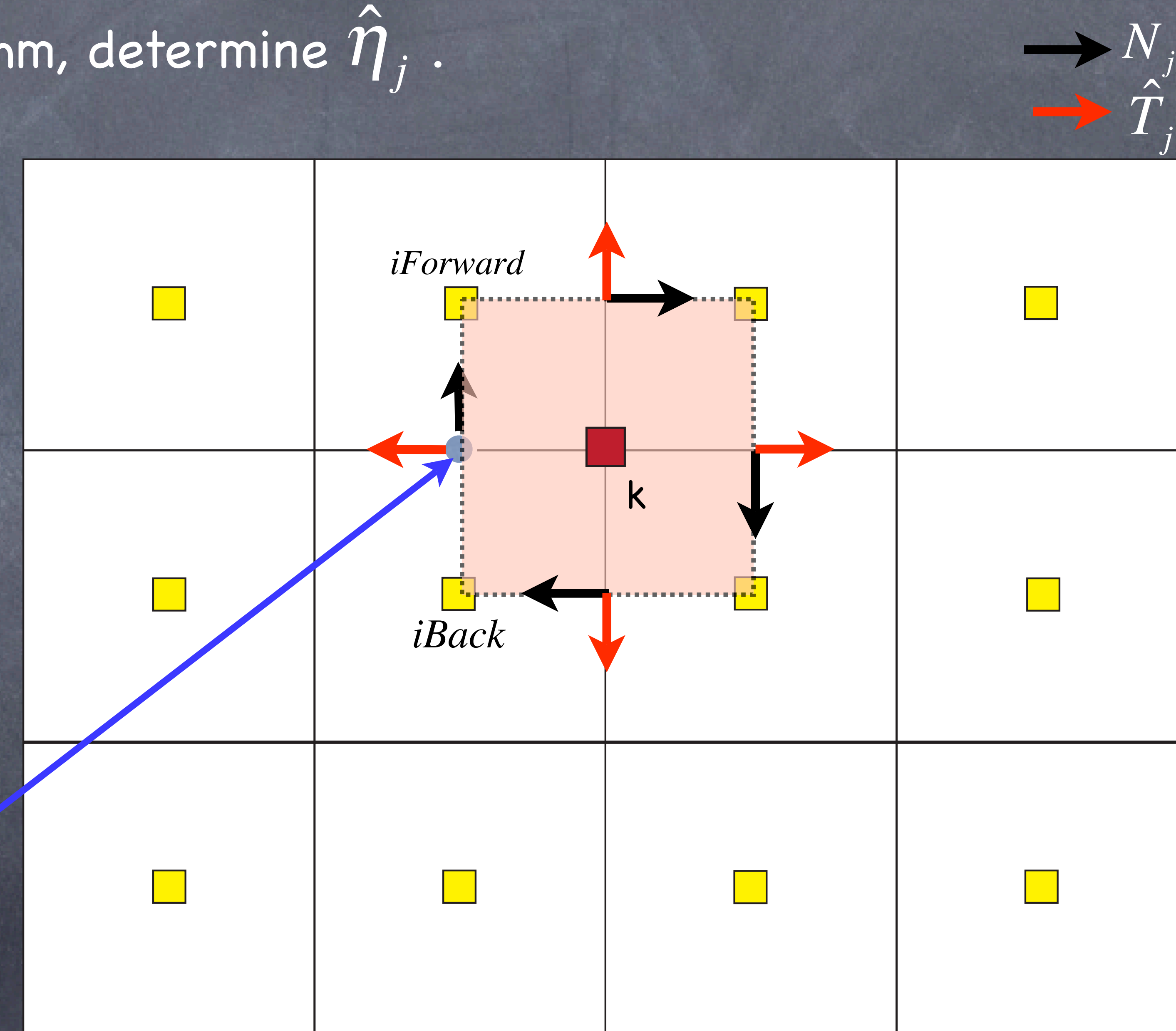
# Transport-based approach for slaving velocity to an evolving vorticity field.

1) At t=0, given the velocity field determine absolute vorticity at k points.

2) Reconstruct T velocities (shown in red).

3) Using your favorite transport algorithm, determine $\hat{\eta}_j$ .

4) Use this $\hat{\eta}_j$ in the momentum eq.




At the end of the time step (n +1), the curl of the velocity field at n+1 plus the Coriolis parameter is equal (i.e. within machine round-off error) to the absolute vorticity at n+1.

$\hat{\eta}_j$

# Summary, 1 of 3

Applying (or choosing) transport algorithms in the context of a full climate simulation (particularly with chemistry) is still part science and part art.

On the one hand, high order reconstructions will inevitably lead to over/under shoots. The primary question to ask is: How will these over/under shoots impact the chemistry component, the cloud parameterization and so on. Is the simulation really "accurate" if the high-order transport algorithm damages the quality of the parameterizations?

On the other hand, limiting (either via fluxes or reconstruction) will inevitably lead to something close to 1st-order accuracy when the limiting is active. The primary question to ask is: How important is enforcing mononicity, positive definite or other bounds on the transport? Is a smooth simulation of tracer transport worth the reduction in formal accuracy?

# Summary, 2 of 3

Climate simulations with 10 to 100 tracer quantities are now common, and the number will only grow in time. There is no reason to think that the same algorithm to compute $\hat{q}$ is appropriate for all tracer fields. Different schemes, along with different limiting options, will likely lead to a better overall simulation per computational cost.

If the above is considered, attention needs to be given to insure mass/tracer consistency for all tracers. Are all transport methods consistent with the single mass evolution equation?

# Summary, 3 of 3

Monotone (or otherwise) limited transport schemes add diffusion that is variable in time and space. A "good" transport scheme will add that diffusion only when and where it is required. By construction, flux-limited transport schemes enhance the down-gradient flux.

Many (most?) discrete models of tracer transport include ad hoc horizontal mixing, such as Laplacian or biharmonic smoothing that are generally active at all time at all places. The use of flux-limited transport can reduce the need for ad hoc smoothing.

(Conjecture): When flux-limited advection schemes are paired with non-diffusive, back-scattering turbulent closure models (such as the Lagrangian Averaged Navier Stokes (LANS) closure) we have a robust (and complete) model of tracer transport at the grid scale. The LANS model limits the accumulation of power of at the grid scale via backscattering and the flux-limiting dissipates the remaining power above some threshold.

# Flux-limiting combined with non-diffusive closures

To be added.