Numerical Methods II: Temporal Discretizations / Stability

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Dynamical Core Model Intercomparison Project (DCMIP) 2012 Summer School

Outline

1. *Introduction / Motivation*
2. *Explicit / Implicit Methods*
3. *Runge-Kutta Methods*
4. *Lagrangian / Semi-Lagrangian Methods*
5. *Numerical Stability*

Part 1

Introduction

- *Dynamic Evolution of the Atmosphere*

Last Time: Spatial Discretizations

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?

1D Advection Equation

Eulerian Frame

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

We considered this term.

This Time: Temporal Discretizations

Atmospheric Modeling – Question Two

- How do we best represent the dynamic evolution of the atmosphere? (how to deal with time?)

Let's look at this term.

1D Advection Equation

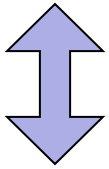
Eulerian Frame

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

Spatial and Temporal Discretizations

Atmospheric Modeling – Question One

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



These questions are inherently linked

Atmospheric Modeling – Question Two

- How do we best represent the dynamic evolution of the atmosphere? (how to deal with time?)

Spatial and Temporal Discretizations

- Last time we discretized the spatial component of the equations:

$$\frac{\partial q_j}{\partial t} = F_j(\mathbf{q})$$

Time evolution of data point j.

Some function applied to all other data points.

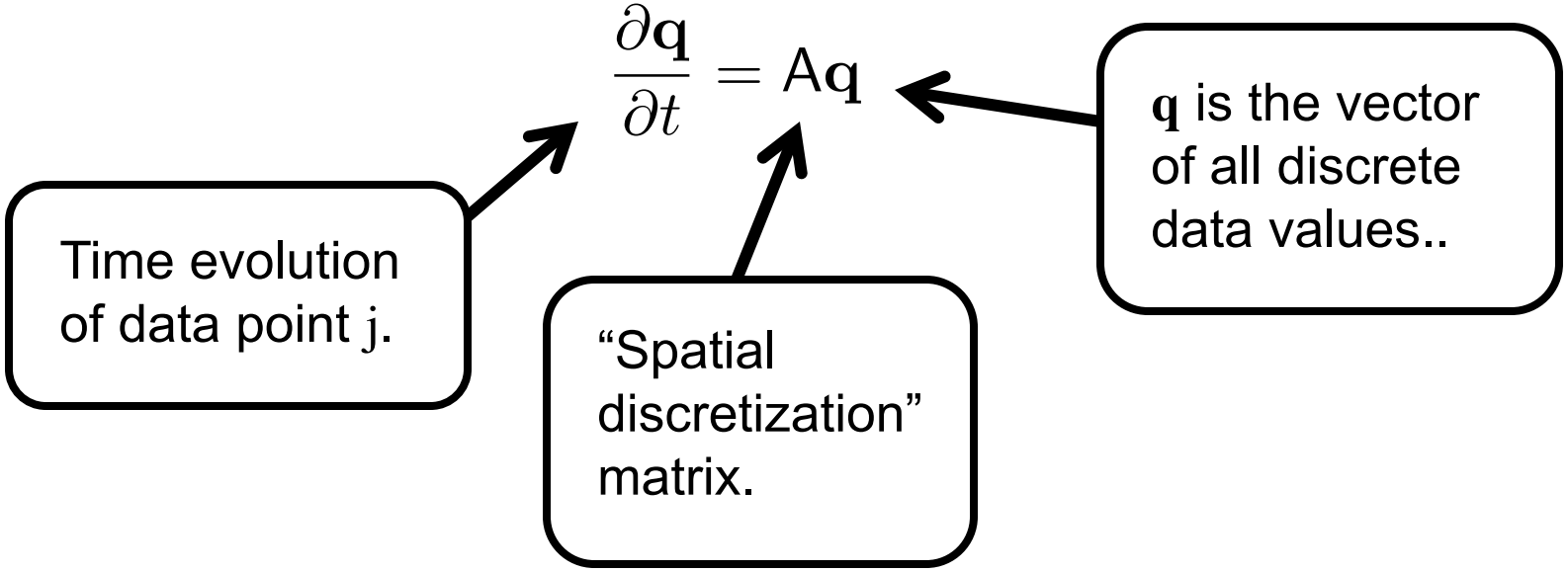
$\mathbf{q}$ is the vector of all discrete data values..

- Example from finite-differences:

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

Spatial and Temporal Discretizations

- All the methods discussed yesterday are ***linear:***
  For a linear differential equation (e.g. advection equation)
  the function f can be represented as a matrix multiply.



Spatial and Temporal Discretizations

- Example from finite-differences:

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

1D Evolution Equation

$$\frac{\partial \mathbf{q}}{\partial t} = \mathsf{A}\mathbf{q}$$

$$\mathsf{A} = \frac{u}{2\Delta x} \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & +1 \\ +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 & 0 \end{pmatrix}$$

Spatial and Temporal Discretizations

- Example from finite-differences:

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

1D Evolution Equation

$$\frac{\partial \mathbf{q}}{\partial t} = \mathrm{A}\mathbf{q}$$

Matrix is mostly zeroes!

$$\mathrm{A} = \frac{u}{2\Delta x} \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & +1 \\ +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 & 0 \end{pmatrix}$$

Banded structure!

Application to Spatial Discretizations

- An evolution matrix which consist mostly of zeroes are referred to as ***sparse*** matrices.

- Finite-difference, finite-volume, spectral element methods all (typically) lead to a sparse evolution matrix.

- The spectral transform method leads to a ***dense*** evolution matrix. That is, there are very few zeros.

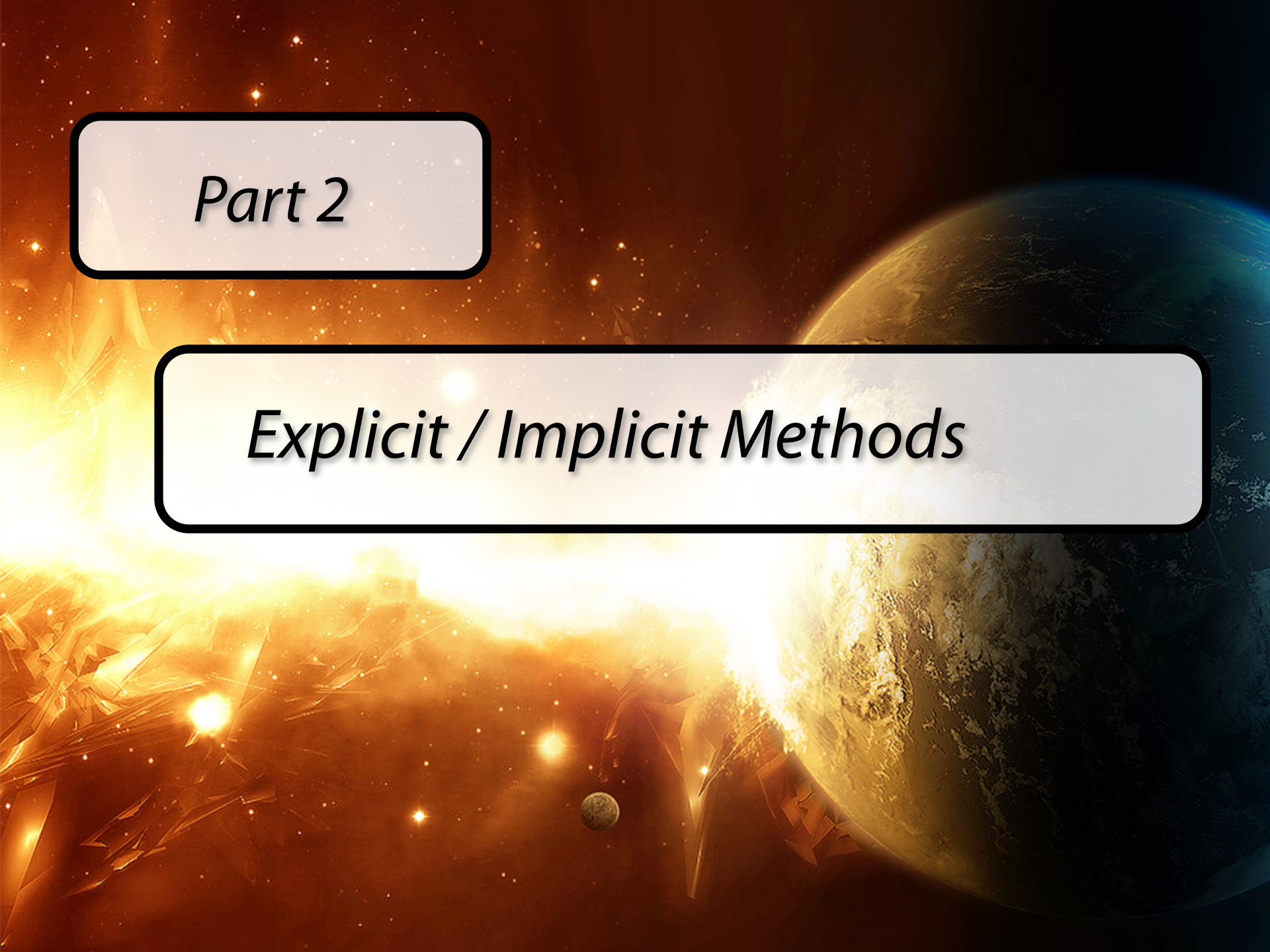
Application to Spatial Discretizations

- As the accuracy of a numerical method increases, there are fewer zeros in the evolution matrix (they make use of more information).

- That is, accuracy implies the need for a dense matrix.

- **But!** A more dense matrix is more computationally expense to apply in calculations.

- Hence, there is a trade-off between accuracy and efficiency.


Part 2
Explicit / Implicit Methods

The Time Step

Linear Discretization

$$\frac{\partial \mathbf{q}}{\partial t} = \mathrm{A}\mathbf{q}$$

Non-Linear Discretization

$$\frac{\partial \mathbf{q}}{\partial t} = \mathbf{F}(\mathbf{q})$$

Integrate these discretizations with respect to time:

Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^{n} = \int_{t^n}^{t^{n+1}} \mathrm{A}\mathbf{q} dt$$

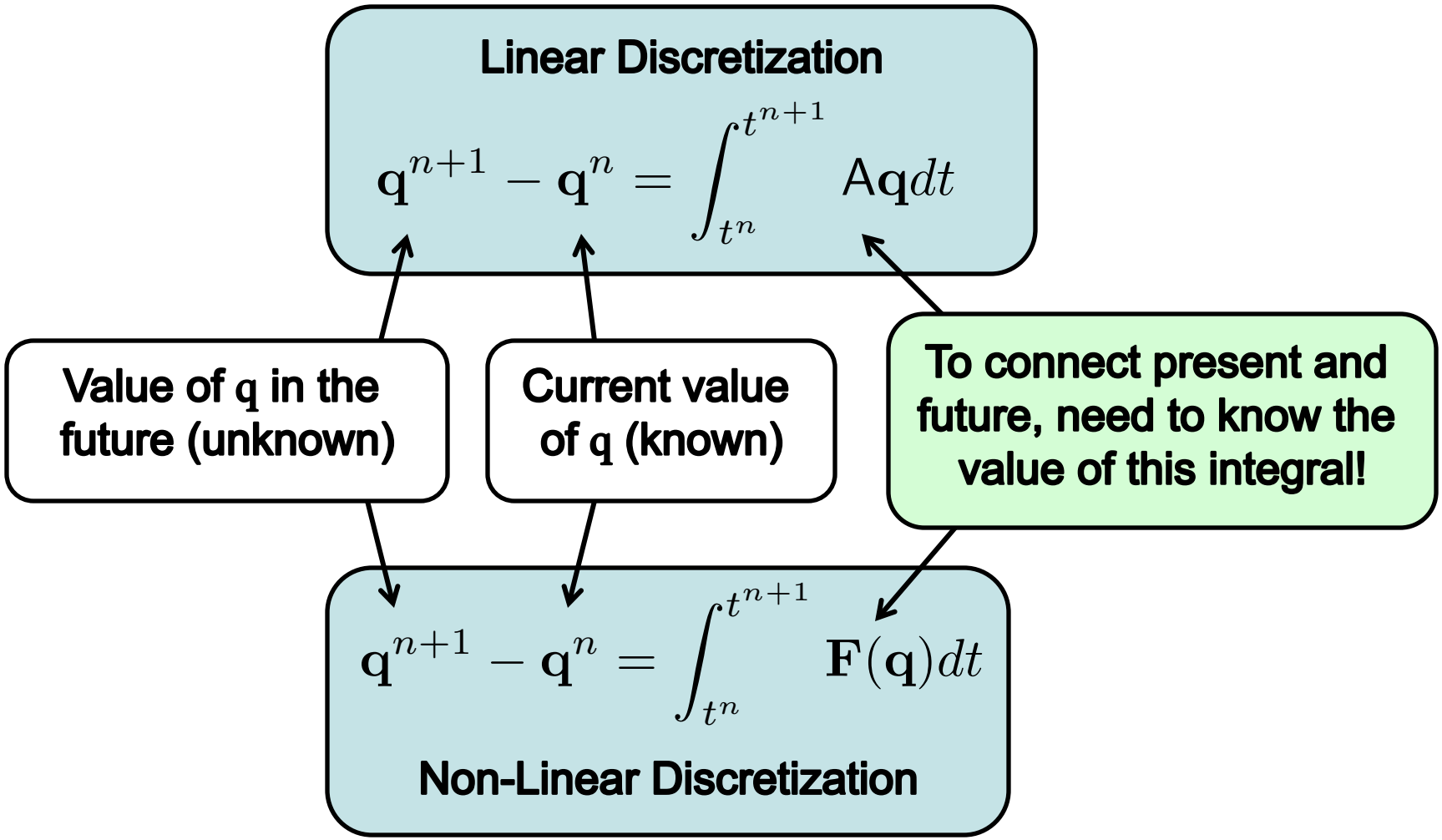
Non-Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^{n} = \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$

Current value of $\mathbf{q}$ (known)

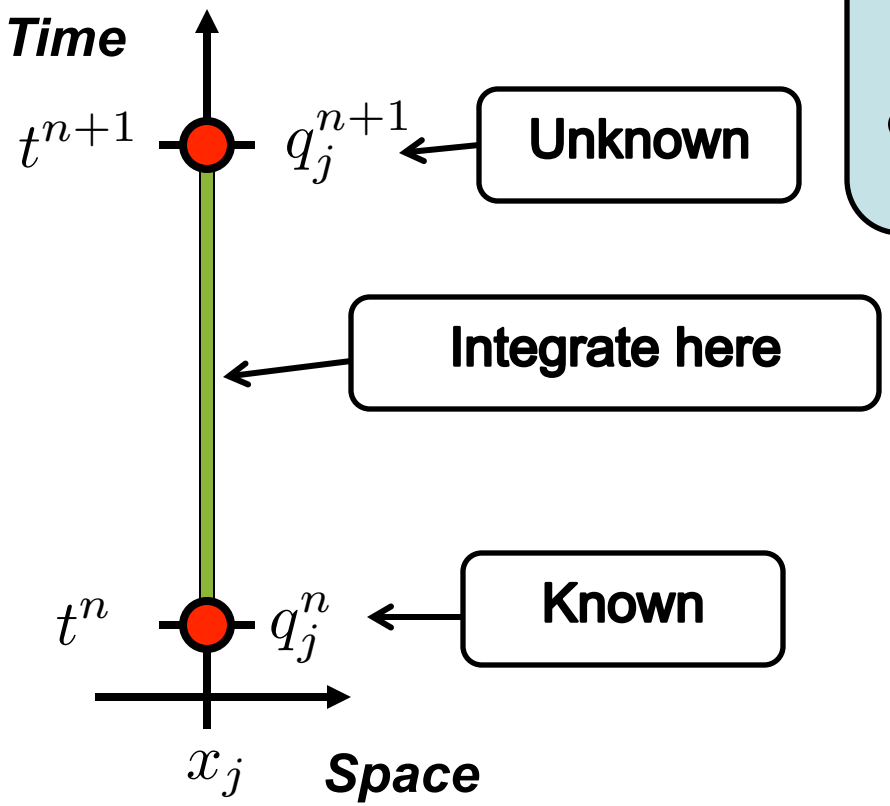
Value of $\mathbf{q}$ in the future (unknown)

The Time Step



The Time Step

Consider the non-linear discretization of the evolution equation.



Non-Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$

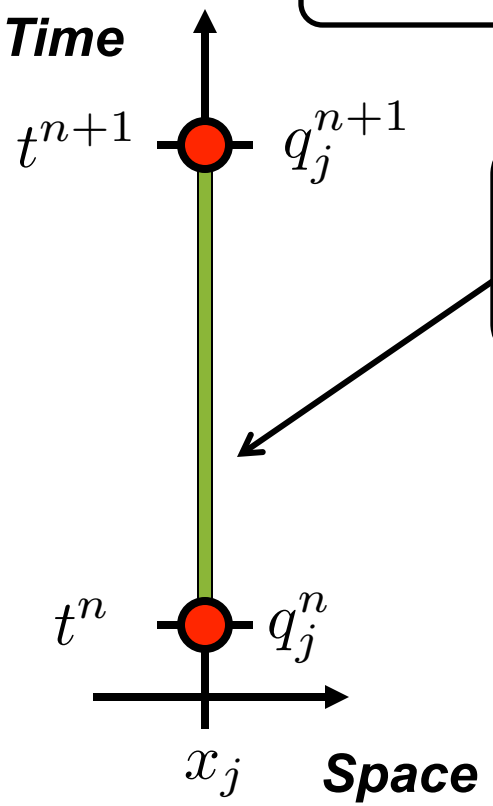
A First Explicit Scheme

Non-linear discretization.

$$\Delta t = t^{n+1} - t^n$$

Non-Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$



$$\int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt \approx \Delta t \; \mathbf{F}(\mathbf{q^n})$$

Forward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \; \mathbf{F}(\mathbf{q}^n)$$

A First Explicit Scheme

Non-linear discretization.

$$\Delta t = t^{n+1} - t^n$$

Non-Linear Discretization

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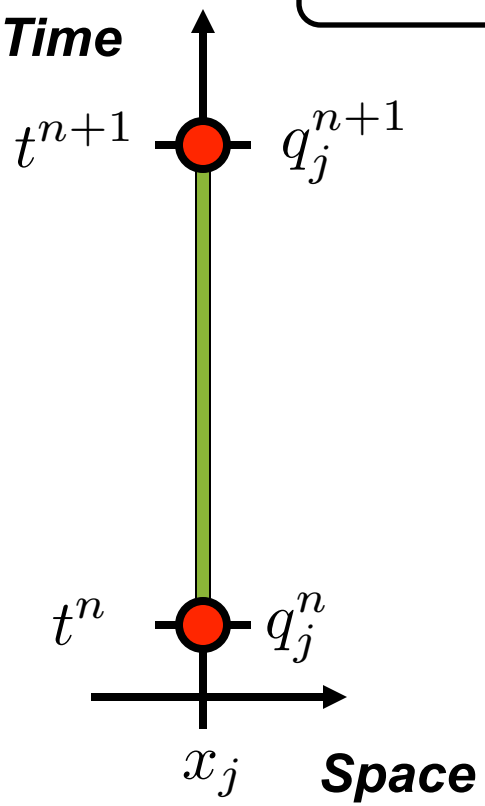


Forward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t\ \mathbf{F}(\mathbf{q}^n)$$

Unknown **Known**

Under the explicit discretization, the unknown is written ***explicitly*** in terms of known values.

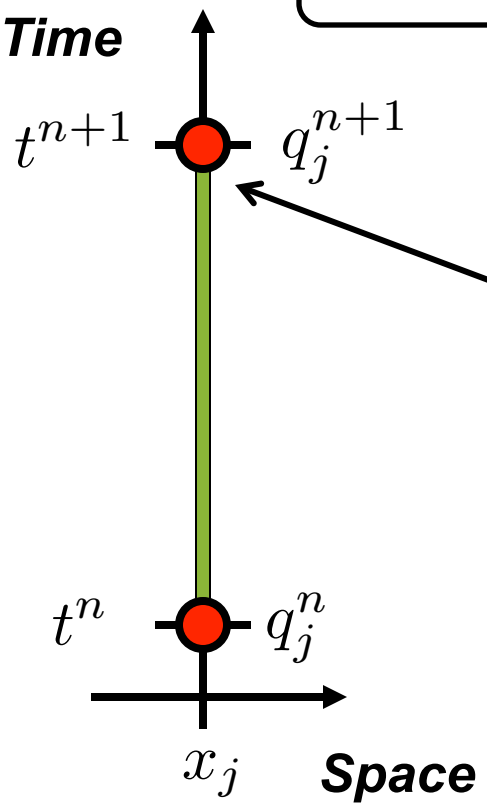
A First Implicit Scheme

Non-linear discretization.

$$\Delta t = t^{n+1} - t^n$$

Non-Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$



$$\int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt \approx \Delta t \; \mathbf{F}(\mathbf{q}^{n+1})$$

Backward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \; \mathbf{F}(\mathbf{q}^{n+1})$$

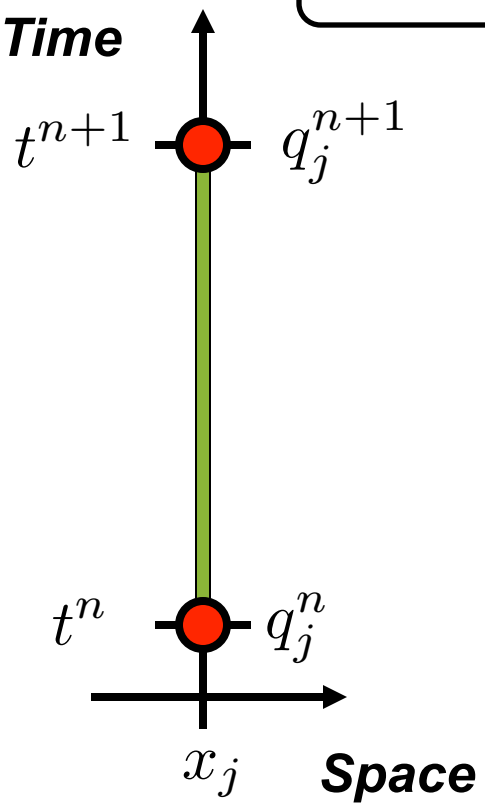
A First Implicit Scheme

Non-linear discretization.

$$\Delta t = t^{n+1} - t^n$$

Non-Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$



Backward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t\ \mathbf{F}(\mathbf{q}^{n+1})$$

Unknown **Known** **Unknown**

Under the implicit discretization, one needs to solve a system of equations to find $\mathbf{q}^{n+1}$.

A First Implicit Scheme

In the linear case, the backward Euler method simplifies to

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \; \mathrm{A} \; \mathbf{q}^{n+1}$$

Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \int_{t^n}^{t^{n+1}} \mathrm{A}\mathbf{q} dt$$

We can directly rewrite this in terms of $\mathbf{q}^{n+1}$:

$$\mathbf{q}^{n+1} = (I - \Delta t \; \mathrm{A})^{-1} \mathbf{q}^n$$

Need to solve a linear system!

Solving the linear system is potentially an expensive operation.

A First Implicit Scheme

Backward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \, \mathbf{F}(\mathbf{q}^{n+1})$$

Non-Linear Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$

In the non-linear case, we can also linearize the update:

$$\mathbf{F}(\mathbf{q}^{n+1}) \approx \mathbf{F}(\mathbf{q}^n) + \frac{d\mathbf{F}}{d\mathbf{q}}(\mathbf{q}^{n+1} - \mathbf{q}^n)$$

Linearly Implicit Backward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \left(I - \Delta t \frac{d\mathbf{F}}{d\mathbf{q}}(\mathbf{q}^n) \right)^{-1} \mathbf{F}(\mathbf{q}^n)$$

Again need to solve a linear system!

Implicit / Explicit Methods

Q: Clearly the explicit method is significantly more straightforward to evaluate. Why would we choose an implicit method?

A: Stability! We will see this more later, but the basic difference is as follows:

Forward Euler Method

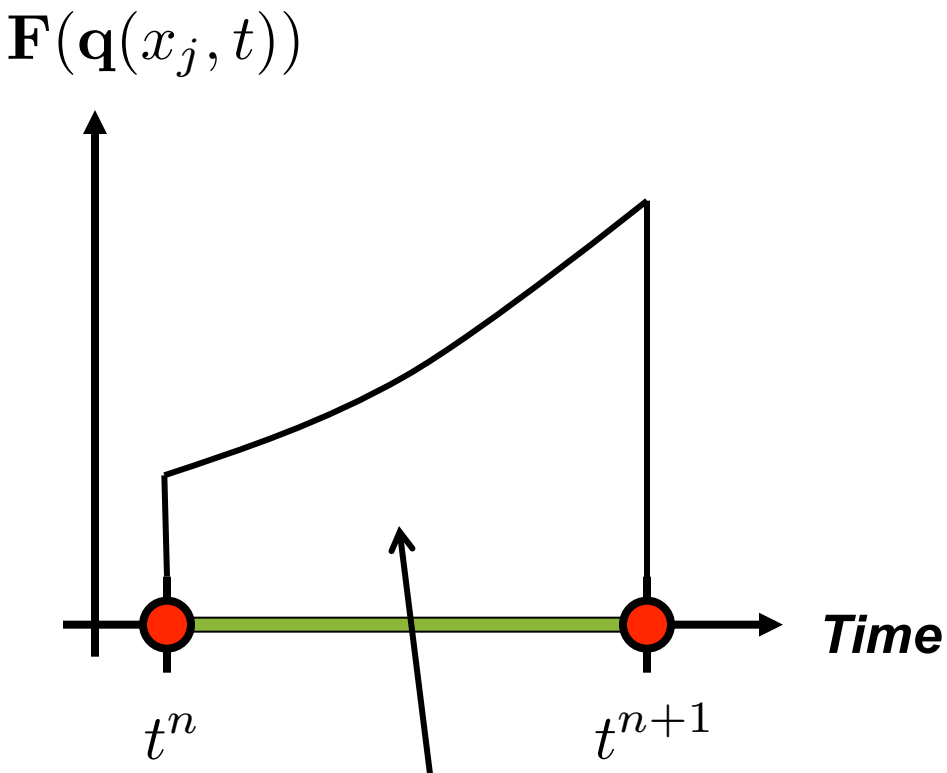
$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \; \mathbf{F}(\mathbf{q}^n)$$

Backward Euler Method

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \; \mathbf{F}(\mathbf{q}^{n+1})$$

- ***Implicit schemes*** have no limit on the size of the time step size Δt. However, a larger time step size is less accurate. Also: Implicit schemes generally require global communication.
- ***Explicit schemes*** impose a (strict) limit on the time step size Δt. Exceeding this limit will cause the method to "blow up".

Accuracy



Time Integral

$$\int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}(x_j,t))dt$$

Area under the $\mathbf{F}$ curve determines how to update $\mathbf{q}$

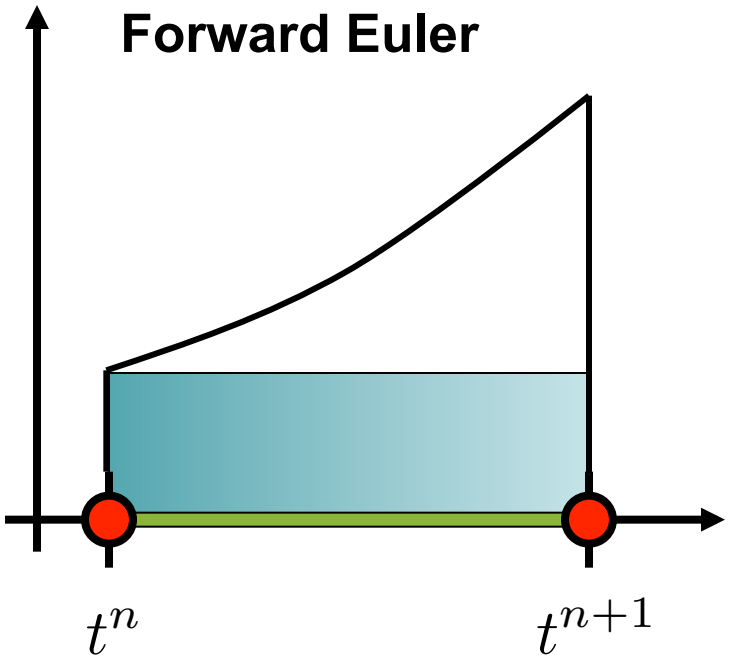
Accuracy

Time Integral

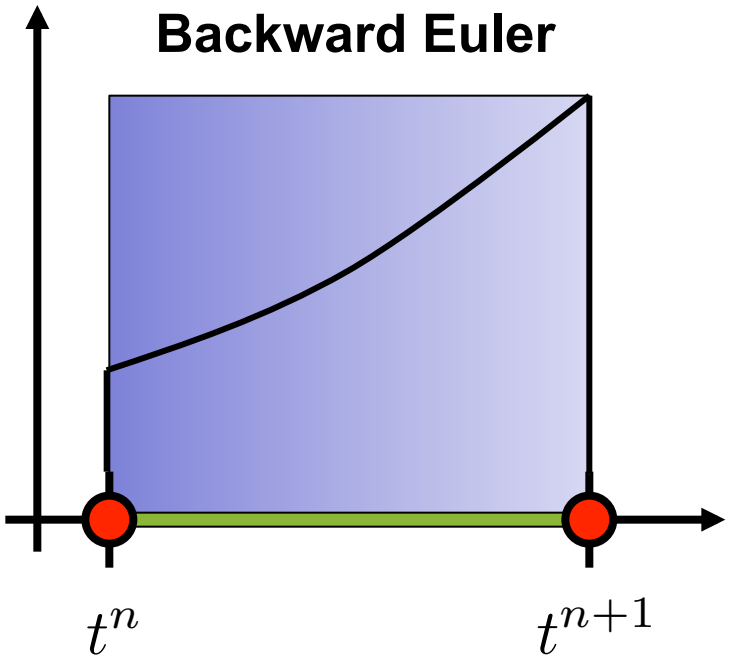
$$\int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q}(x_j,t))dt$$

$\mathbf{F}(\mathbf{q}(x_j,t))$

Forward Euler



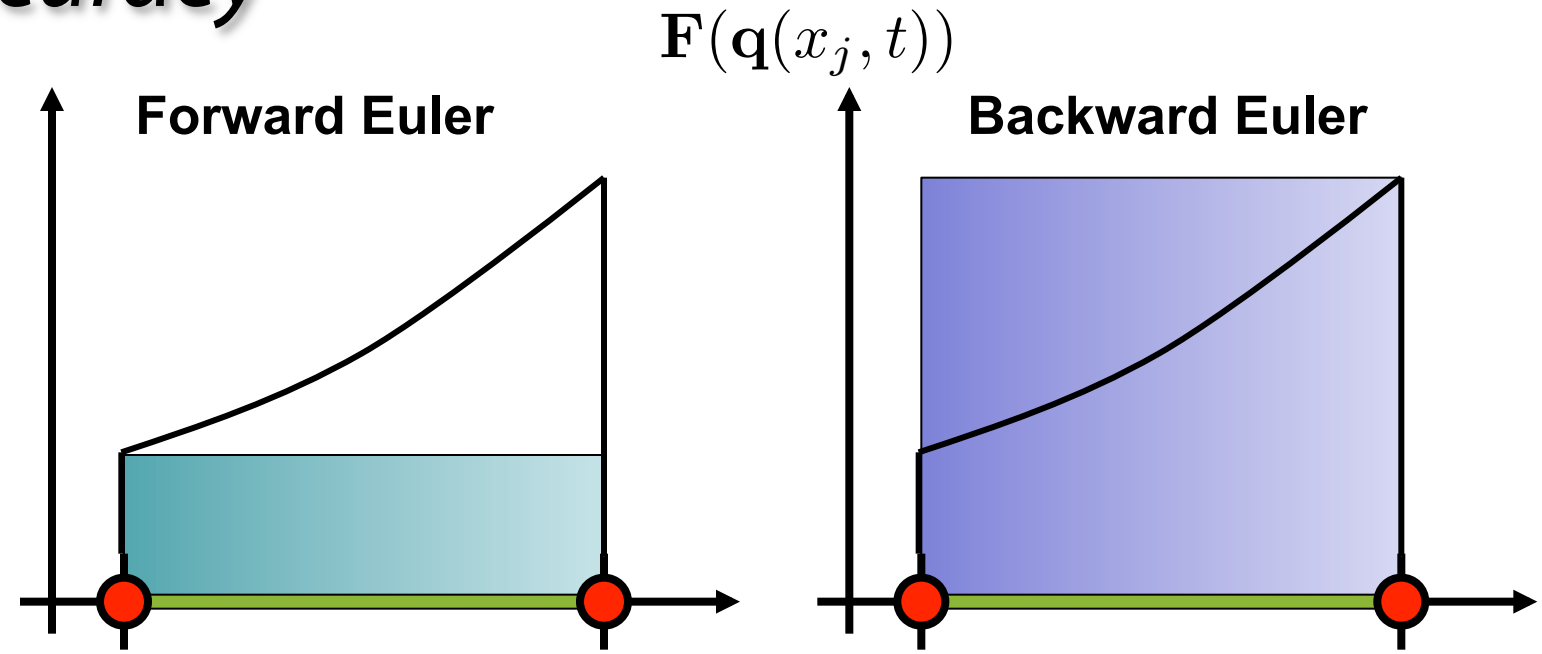
Backward Euler



$$\int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q})dt \approx \Delta t\ \mathbf{F}(\mathbf{q}^n)$$

$$\int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q})dt \approx \Delta t\ \mathbf{F}(\mathbf{q}^{n+1})$$

Accuracy

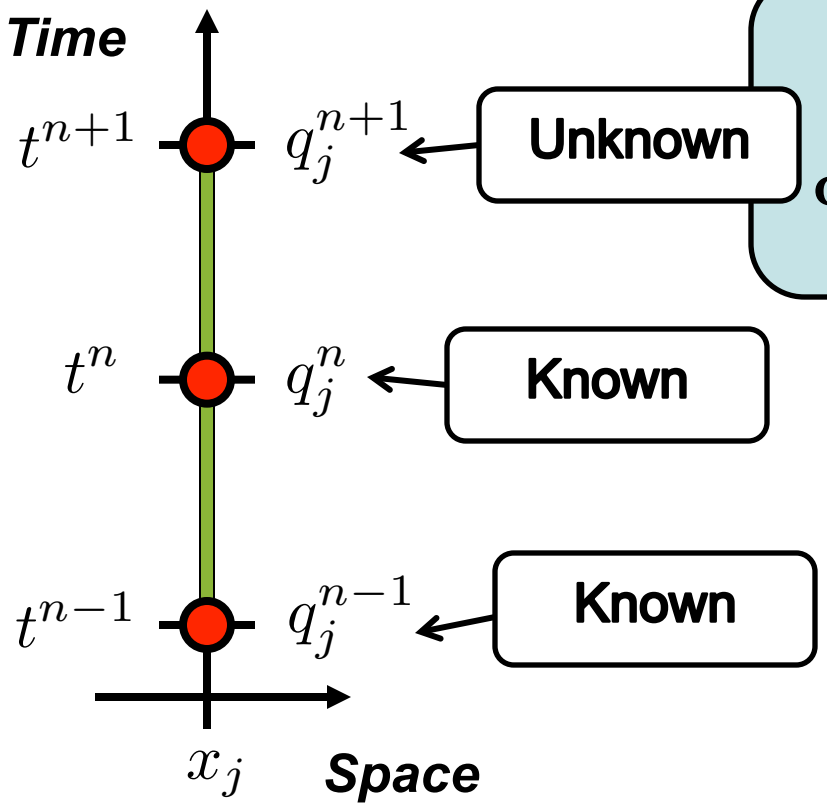


Both the forward Euler method and backward Euler method are ***first-order accurate***: They are only exact when $\mathbf{F}$ is a constant.

First-order accuracy is typically insufficient. We need to do better.

Leap Frog

The leap frog scheme is a traditional ***second-order accurate explicit method***. This means that the integral is exact if $\mathbf{F}$ is either constant or linear in time.



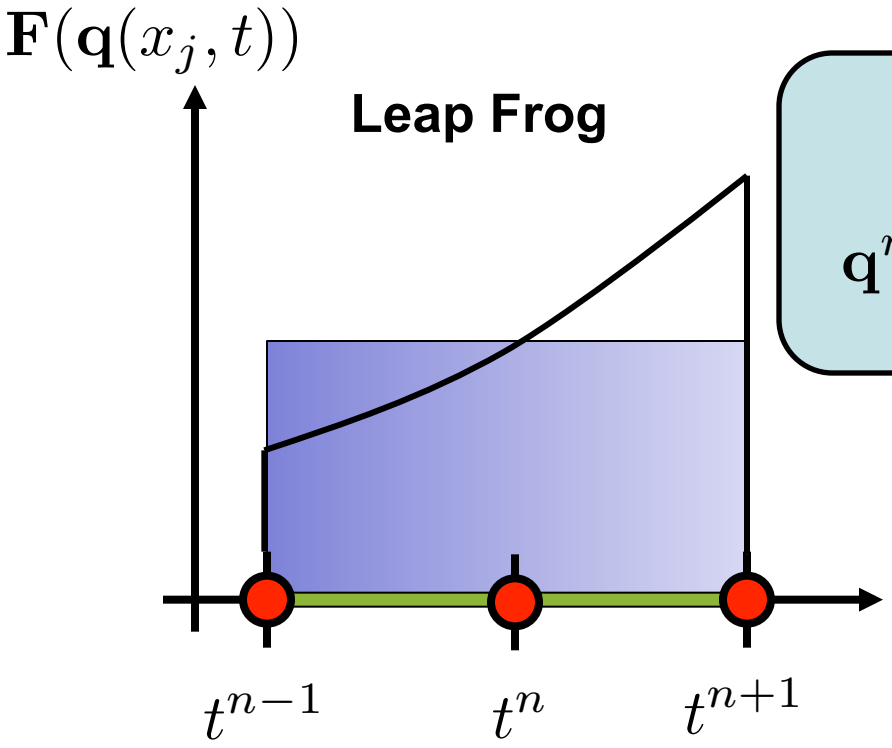
Two-Step Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^{n-1} = \int_{t^{n-1}}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$

Leap frog requires knowledge of $\mathbf{q}$ from two time levels prior to the unknown level.

Accuracy of Leap Frog

Second-order accuracy for the leap frog method is attained by using the *midpoint value*.

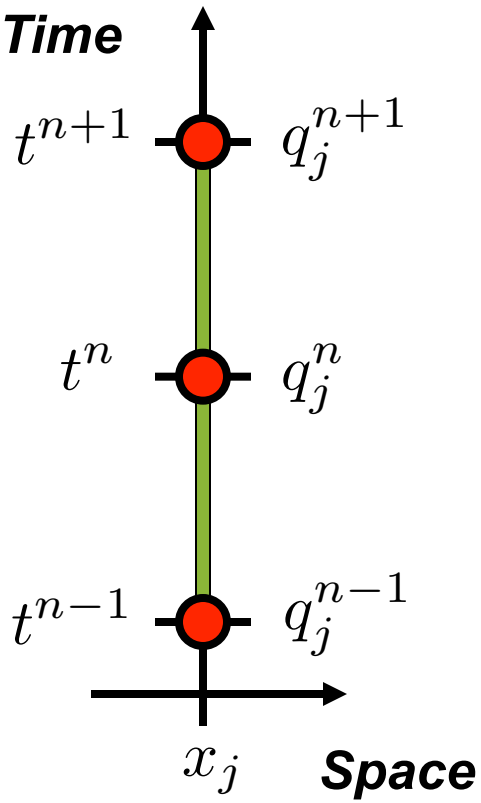


Two-Step Discretization

$$\mathbf{q}^{n+1} - \mathbf{q}^{n-1} = \int_{t^{n-1}}^{t^{n+1}} \mathbf{F}(\mathbf{q}) dt$$

Leap Frog

The leap frog scheme has traditionally been used in combination with the spectral transform method.



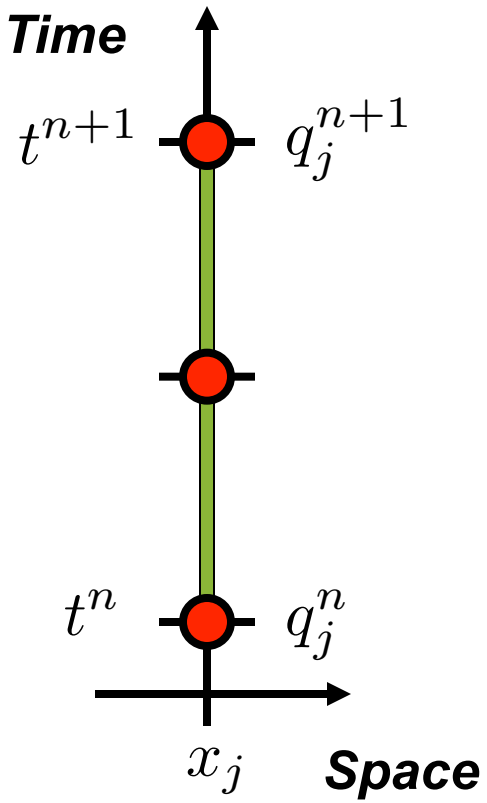
The leap frog scheme possesses a ***computational mode*** since the odd and even time levels can separate.

This is usually fixed by using off-centering (Asselin filtering)


Part 3
Runge-Kutta Methods

Runge-Kutta Methods

Runge-Kutta methods are a popular method for attaining high-order accuracy in time without the need to store data from multiple time steps.



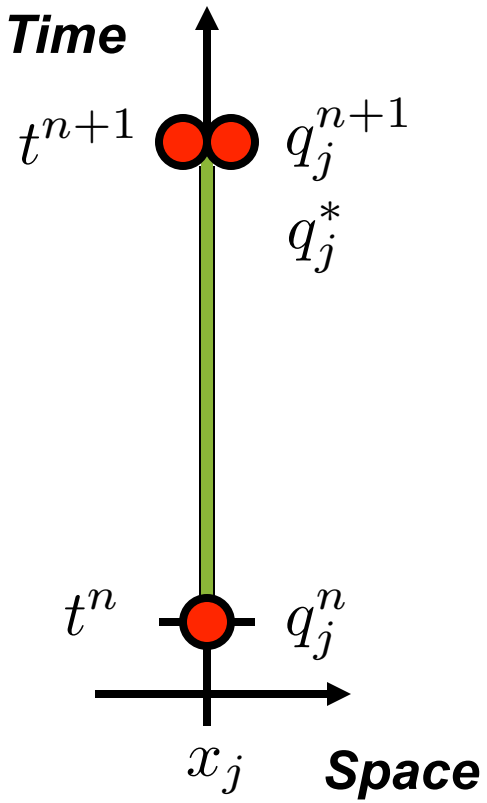
Non-Linear Discretization

$$\frac{\partial \mathbf{q}}{\partial t} = \mathbf{F}(\mathbf{q})$$

- Runge-Kutta methods are multi-stage, which means in order to advance by Δt the function $\mathbf{F}$ must be evaluated multiple times.

Predictor / Corrector

The second-order accurate predictor-corrector method is one of the most basic Runge-Kutta methods.



A first-order approximation to q_j^{n+1} is first computed (prediction step):

$$\mathbf{q}^* = \mathbf{q}^n + \Delta t \; \mathbf{F}(\mathbf{q}^n)$$

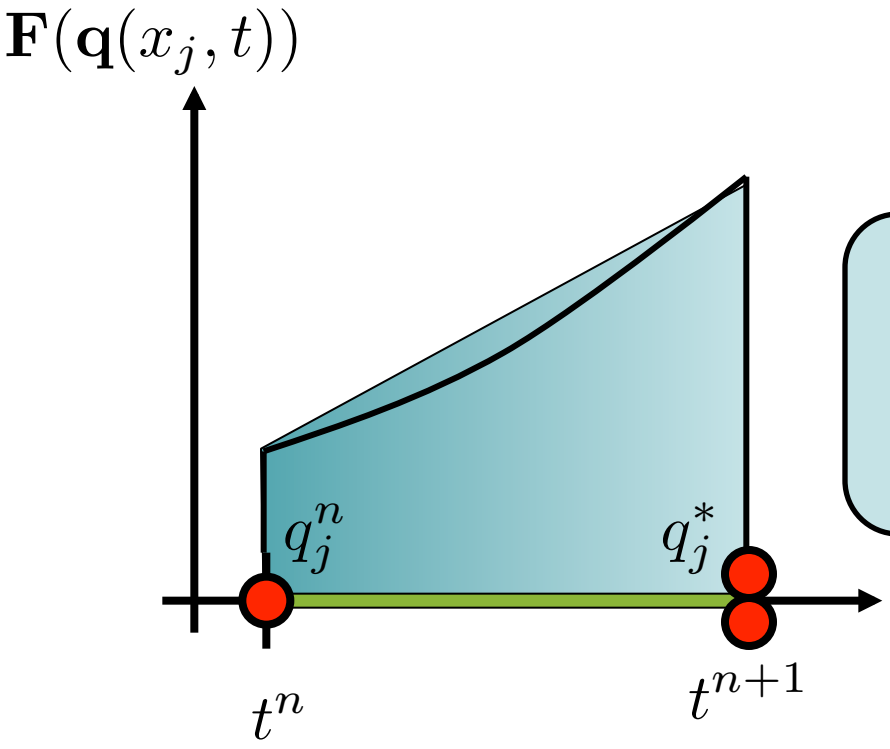
A second-order *correction* is then computed:

$$\mathbf{q}^{n+1} = \frac{1}{2}\mathbf{q}^n + \frac{1}{2}\mathbf{q}^* + \frac{\Delta t}{2} \; \mathbf{F}(\mathbf{q}^*)$$

Predictor / Corrector

The predictor corrector scheme can also be written as follows:

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \frac{\Delta t}{2}\mathbf{F}(\mathbf{q}^n) + \frac{\Delta t}{2}\mathbf{F}(\mathbf{q}^*)$$



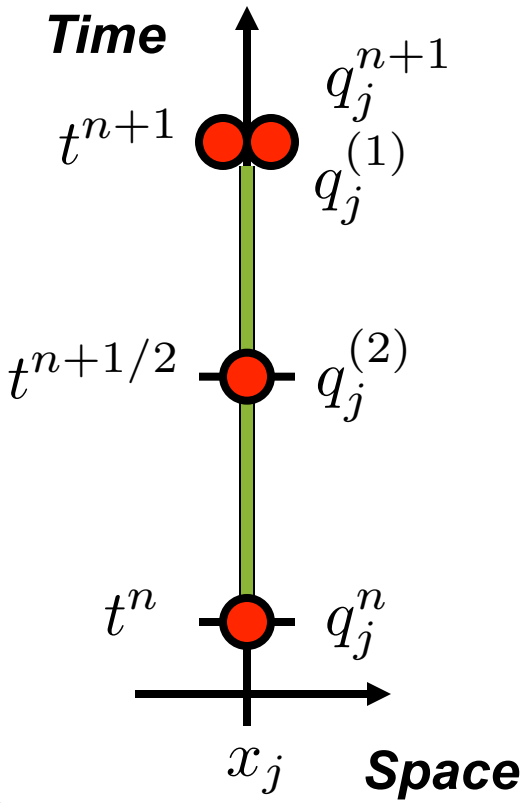
Trapezoid rule for integration

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q})dt$$

Non-Linear Discretization

Strong Stability Preserving RK3 (SSPRK3)

One of the more popular Runge-Kutta methods is the SSPRK3 scheme, which is a third-order accurate, three stage Runge-Kutta method.



Stage one:

$$\mathbf{q}_j^{(1)} = \mathbf{q}_j^n + \Delta t \mathbf{F}(\mathbf{q}^n)$$

Stage two:

$$\mathbf{q}_j^{(2)} = \frac{3}{4}\mathbf{q}_j^n + \frac{1}{4}\mathbf{q}_j^{(1)} + \frac{\Delta t}{4}\mathbf{F}(\mathbf{q}^{(1)})$$

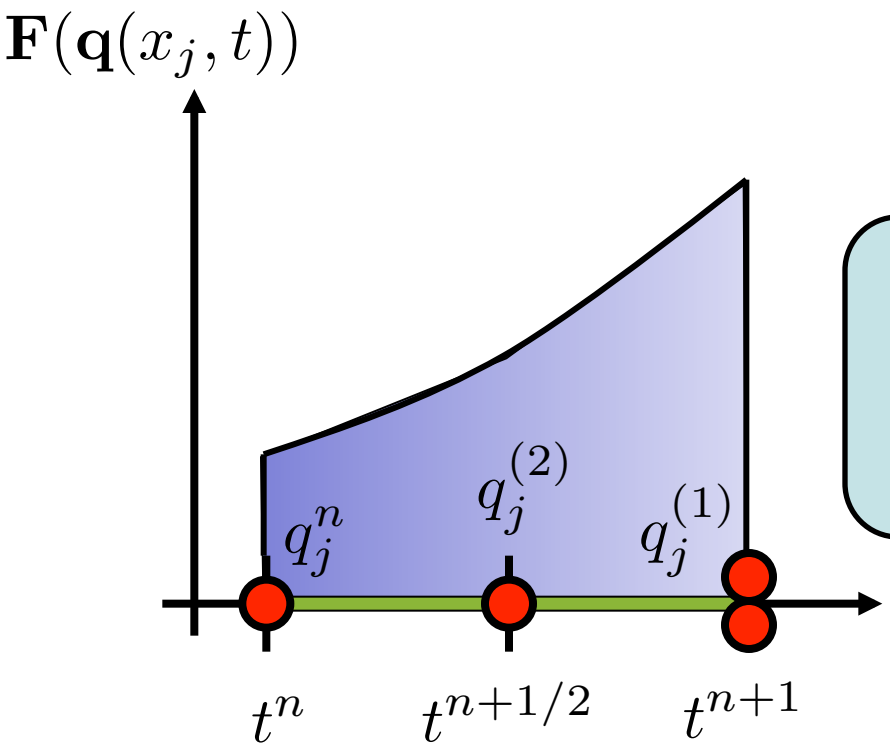
Final update:

$$\mathbf{q}_j^{n+1} = \frac{1}{3}\mathbf{q}_j^n + \frac{2}{3}\mathbf{q}_j^{(2)} + \frac{2\Delta t}{3}\mathbf{F}(\mathbf{q}^{(2)})$$

Strong Stability Preserving RK3 (SSPRK3)

Writing as a one-stage update equation:

$$\mathbf{q}_j^{n+1} = \mathbf{q}_j^n + \frac{\Delta t}{6}\left[\mathbf{F}(\mathbf{q}^n) + 4\,\mathbf{F}(\mathbf{q}^{(2)}) + \mathbf{F}(\mathbf{q}^{(1)})\right]$$



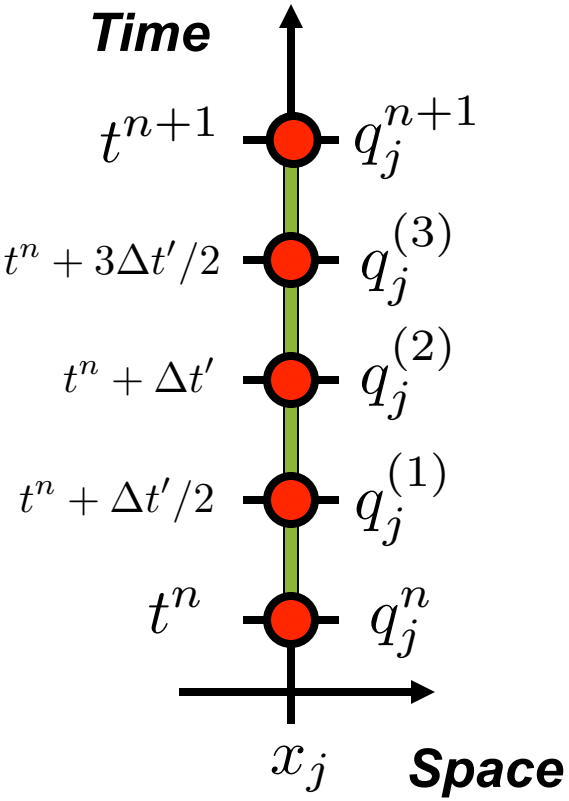
Simpson's rule for integration

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \int_{t^n}^{t^{n+1}} \mathbf{F}(\mathbf{q})\,dt$$

Non-Linear Discretization

Synchronized Leap Frog

The CAM Spectral Element (CAM-SE) model uses a Runge-Kutta scheme closely modeled on the leap frog scheme discussed earlier:



$$\mathbf{q}^{(0)} = \mathbf{q}_j^n$$

Stage one:

$$\mathbf{q}_j^{(1)} = \mathbf{q}_j^n + \frac{\Delta t'}{2}\mathbf{F}(\mathbf{q}_j^n)$$

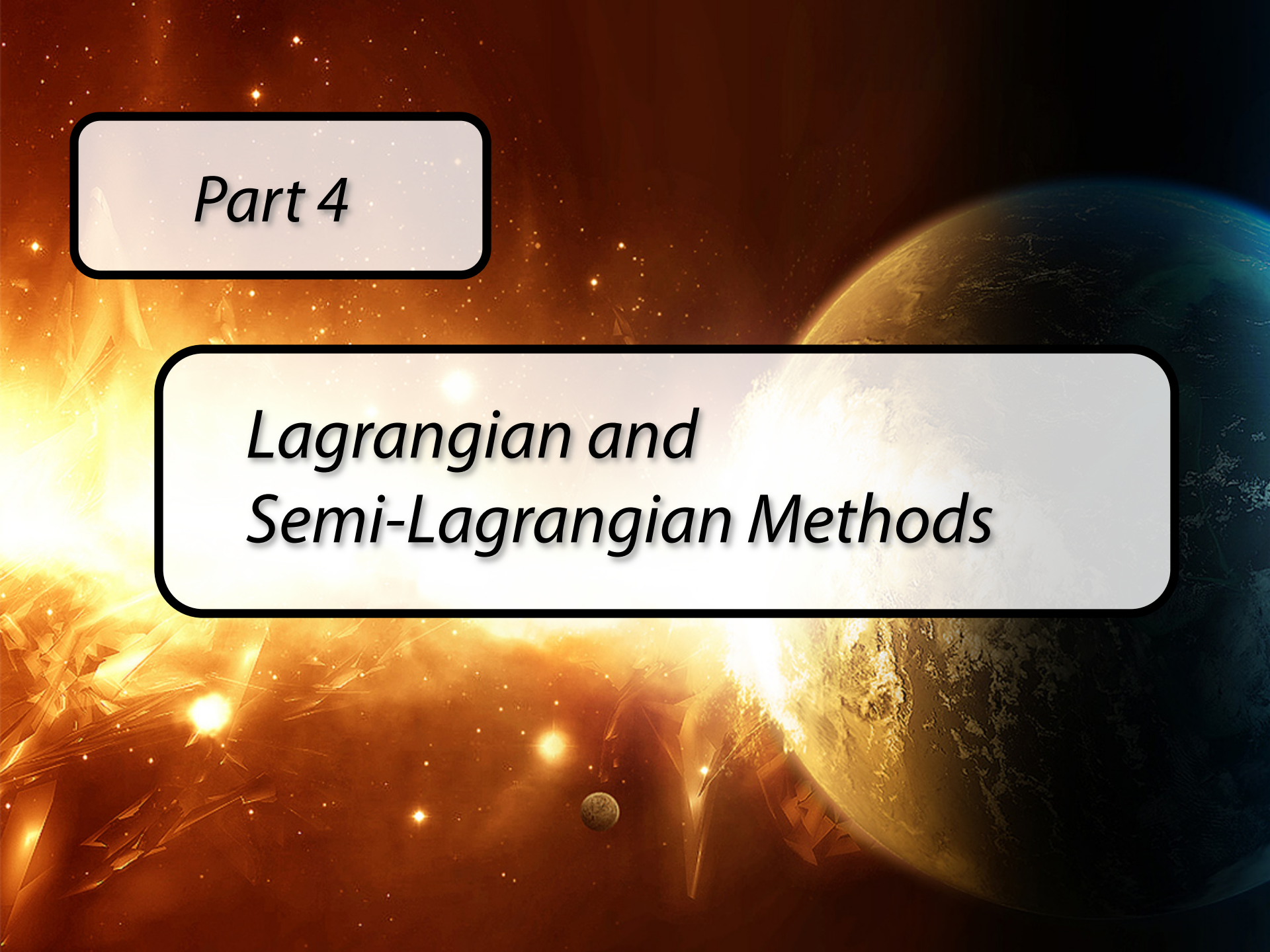
Stage k+1:

$$\mathbf{q}^{(k+1)} = \mathbf{q}_j^{(k-1)} + \Delta t'\mathbf{F}(\mathbf{q}_j^{(k)})$$

Final update:

$$\mathbf{q}^{n+1} = \mathbf{q}^{(N)}$$

Overall 2nd order


Part 4
Lagrangian and
Semi-Lagrangian Methods

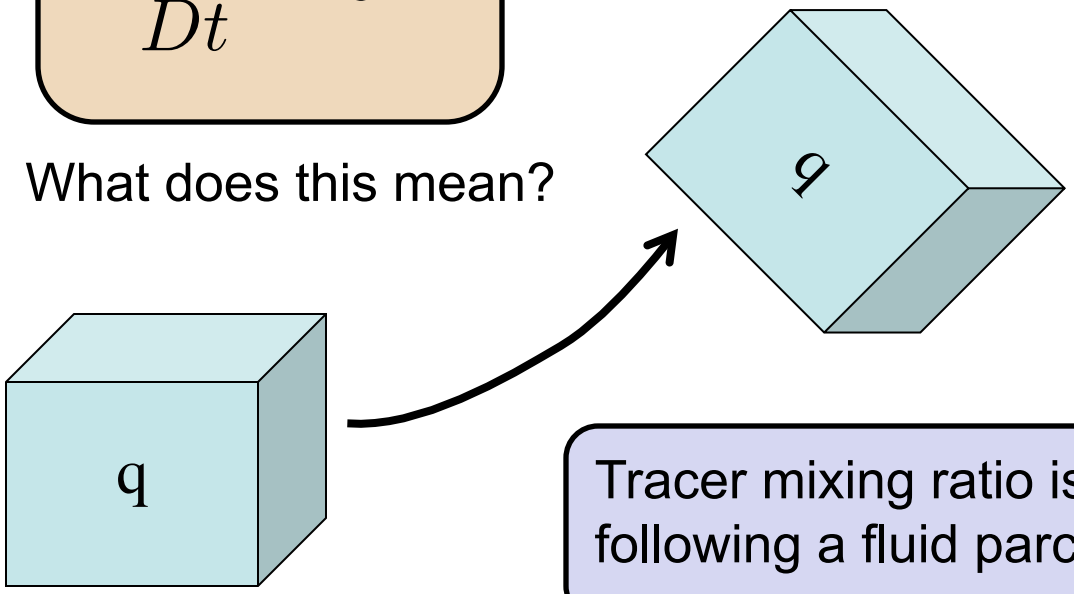
Advection of a Tracer

Recall Lagrangian reference frame (follows a fluid parcel).

Lagrangian Frame

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

What does this mean?



Tracer mixing ratio is constant following a fluid parcel.

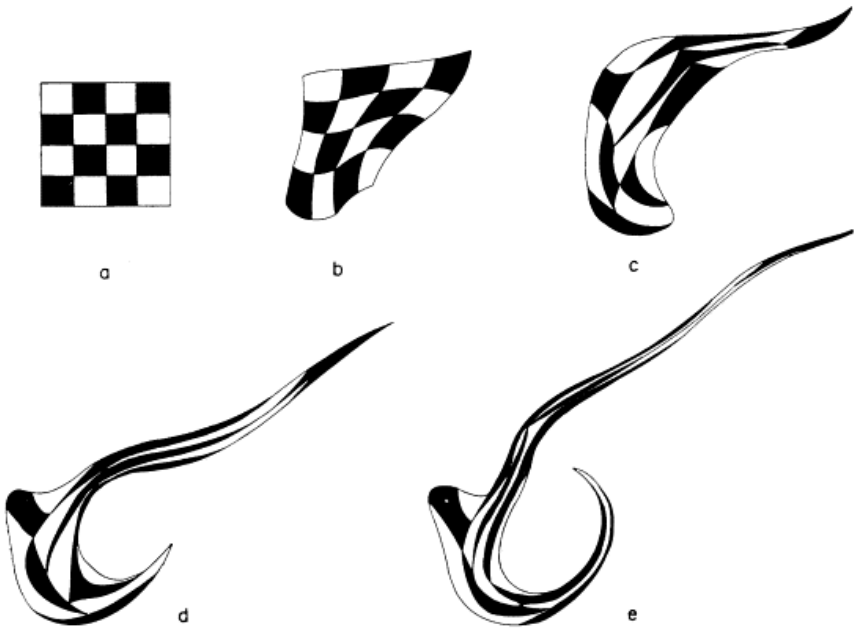
Fully Lagrangian Transport Methods

- The Lagrangian frame is, in some sense, the most natural way to think about the advection equation.

- **But:** In practice it is difficult to follow around fluid parcels in presence of deforming flow.

Lagrangian Frame

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

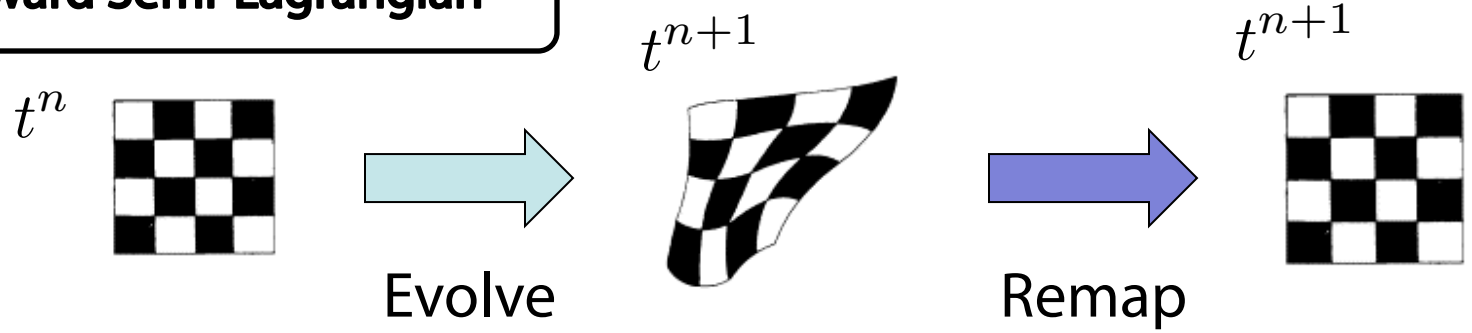


Source: R.A. Pielke and M. Uliasz (1997).

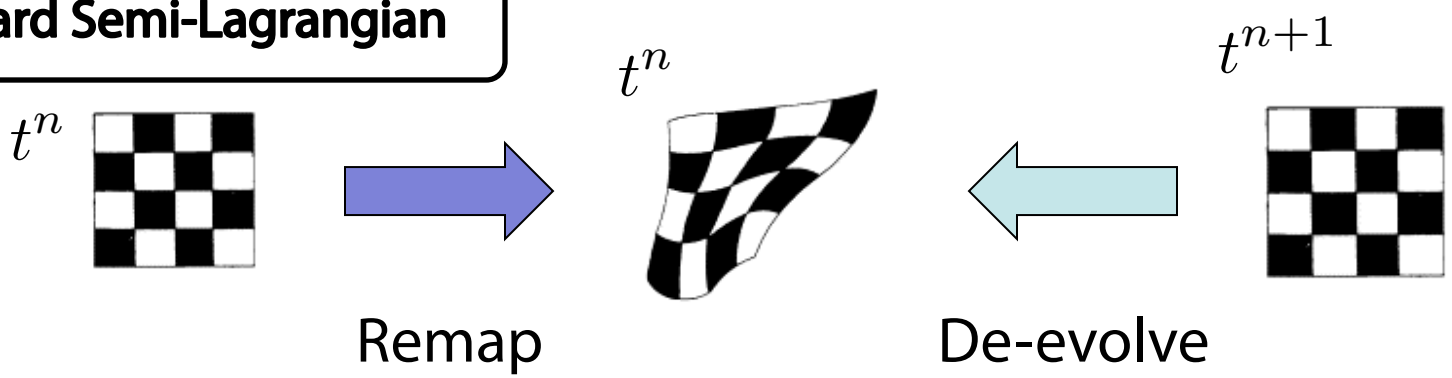
Semi-Lagrangian Transport Methods

- **Instead:** Semi-Lagrangian methods follow a fluid parcel in time, then remap to a regular mesh.

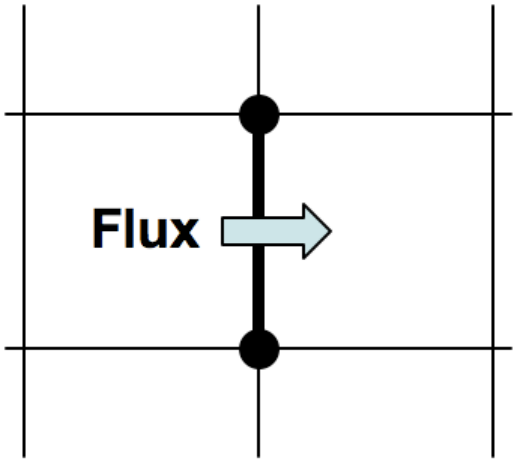
Forward Semi-Lagrangian



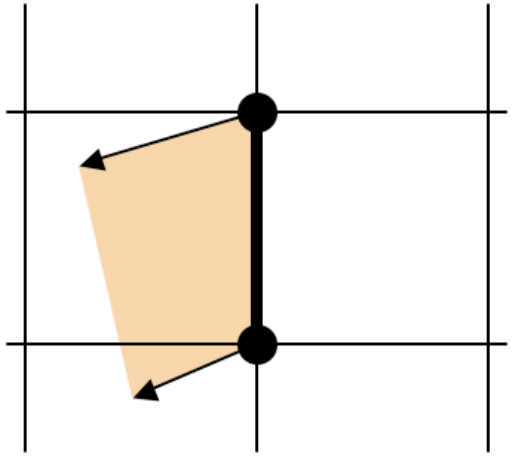
Backward Semi-Lagrangian



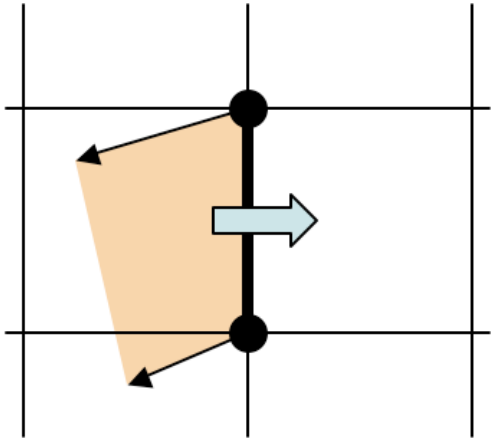
Flux-Form Semi-Lagrangian Transport



The flux across the highlighted edge is desired.

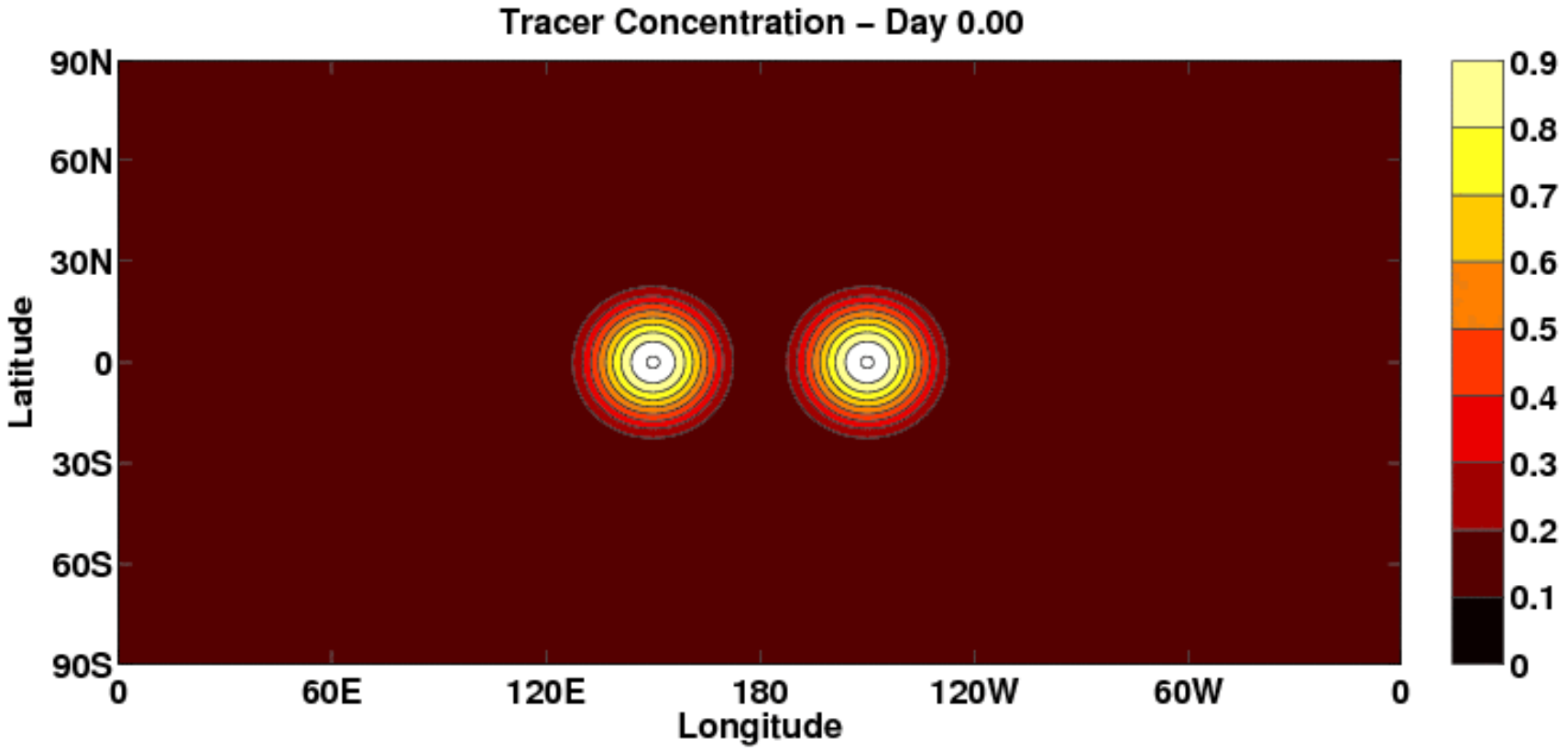


Step 1: Project velocity field backwards in time to obtain a "flux area."



Step 2: Integrate over the flux area to obtain the flux through the edge.

Deformational Flow Test



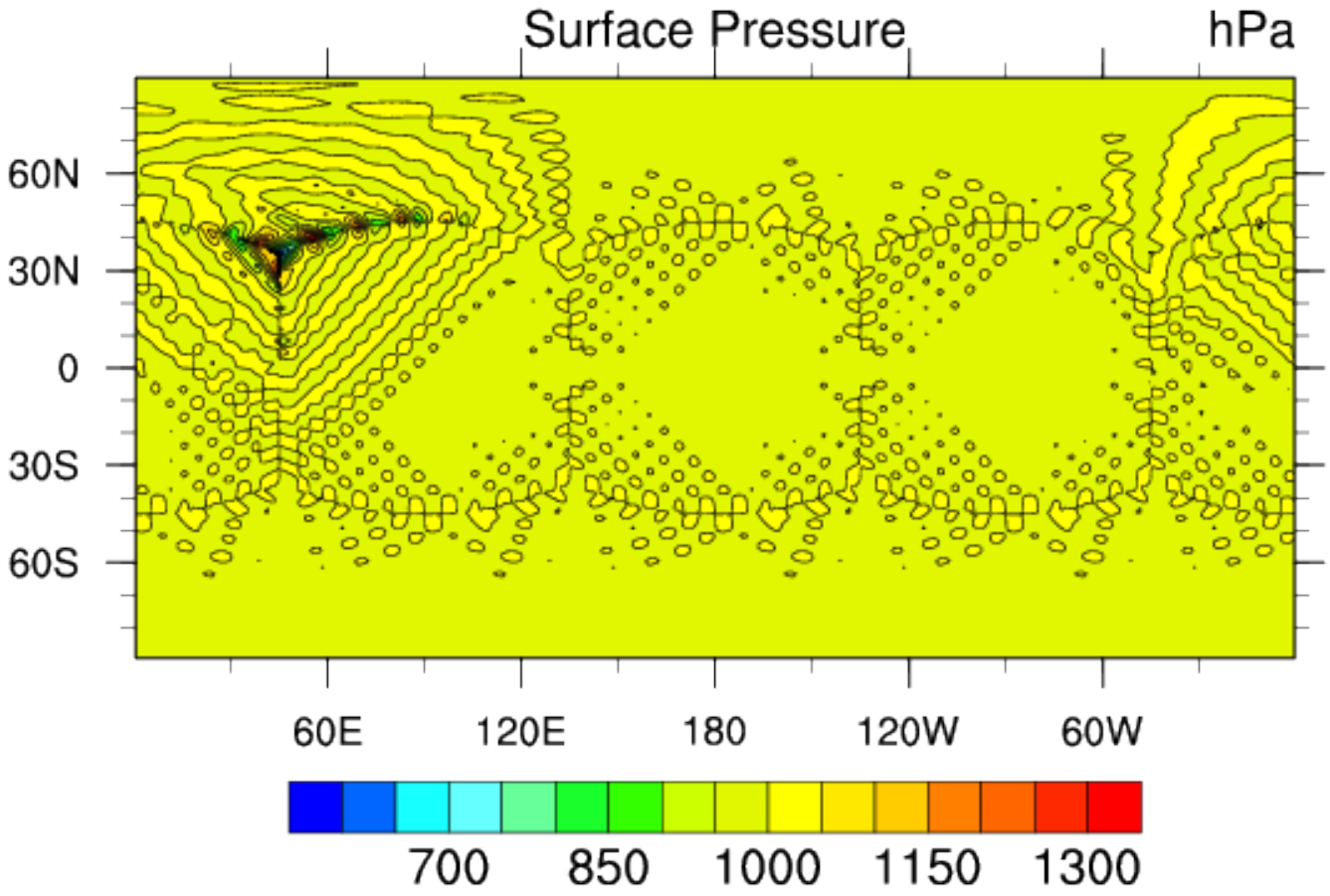
Part 5

Stability

- *Eigenmode Analysis*

Introduction to Stability

Numerical instability in a high-frequency computational mode:



Introduction to Stability

Apply both time and space discretization:

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

- Recall definition of eigenvectors of B: If $\mathbf{v}$ is an eigenvector of B, then it satisfies $\mathrm{B}\mathbf{v} = \lambda\mathbf{v}$ where λ is the (complex) eigenvalue associated with $\mathbf{v}$.

Computational modes

- **Theory:** If B is well behaved, then it will have N eigenvector / eigenvalue pairs, where N is the number of free parameters.

$$\mathbf{q}^{n} = \sum_{i=1}^{N} a_i^n \mathbf{v}_i$$

Introduction to Stability

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

$\mathbf{v}_i$ eigenvectors of B, with associated eigenvalues λ_i.

$$\mathbf{q}^{n} = \sum_{i=1}^{N} a_i^n \mathbf{v}_i$$

- Substitute this solution into the update equation:

$$\mathbf{q}^{n+1} = \sum_{i=1}^{N} a_i^n \mathrm{B}\mathbf{v}_i$$

- Use properties of eigenvectors:

$$\mathbf{q}^{n+1} = \sum_{i=1}^{N} \lambda_i a_i^n \mathbf{v}_i$$

Introduction to Stability

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

$\mathbf{v}_i$ eigenvectors of B, with associated eigenvalues λ_i.

$$\mathbf{q}^{n} = \sum_{i=1}^{N} a_i^n \mathbf{v}_i \qquad \mathbf{q}^{n+1} = \sum_{i=1}^{N} a_i^{n+1} \mathbf{v}_i$$

where $a_i^{n+1} = \lambda_i a_i^n$

Each mode is amplified by its corresponding eigenvalue.

Introduction to Stability

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

$\mathbf{v}_i$ eigenvectors of B, with associated eigenvalues λ_i.

$$\mathbf{q}^{n} = \sum_{i=1}^{N} a_i^n \mathbf{v}_i \qquad \mathbf{q}^{n+1} = \sum_{i=1}^{N} a_i^{n+1} \mathbf{v}_i$$

where $a_i^{n+1} = \lambda_i a_i^n$

Take absolute values: $|a_i^{n+1}| = |\lambda_i| \; |a_i^n|$

What happens if

$|\lambda_i| > 1?$ $|\lambda_i| < 1?$

Introduction to Stability

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

$\mathbf{v}_i$ eigenvectors of B, with associated eigenvalues λ_i.

$|\lambda_i| > 1$ Instability! The corresponding computational mode will blow up.

$|\lambda_i| \leq 1$ Stable! The corresponding computational mode will either maintain its amplitude, or will decay with time (lose energy?)

Stability: An Example

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

Example: Forward Euler plus upwinding (first-order finite volume).

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

Corresponding evolution matrix:

$$\mathrm{B} = \begin{pmatrix} 1-\nu & & & \dots & \nu \\ \nu & 1-\nu & & & \\ & \nu & 1-\nu & & \\ & & \ddots & \ddots & \end{pmatrix}$$

Eigenvectors and eigenvalues:

$$(\mathbf{v}_k)_j = \exp(ijk) \qquad \lambda_k = 1 - \nu(1 + \exp(-ik))$$

Stability: An Example

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

Example: Forward Euler plus upwinding (first-order finite volume).

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Eigenvectors and eigenvalues:

$$(\mathbf{v}_k)_j = \exp(ijk) \qquad \lambda_k = 1 - \nu(1 + \exp(-ik))$$

Absolute value of eigenvalues:

$$|\lambda_k|^2 = 1 - 2\nu(\nu - 1)(\cos(k) - 1)$$

Maximum eigenvalue:

$$\max_k |\lambda_k|^2 = 1 + 4\nu(\nu - 1)$$

Stability: An Example

Linear Update Equation

$$\mathbf{q}^{n+1} = \mathrm{B}\mathbf{q}^{n}$$

Example: Forward Euler plus upwinding (first-order finite volume).

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

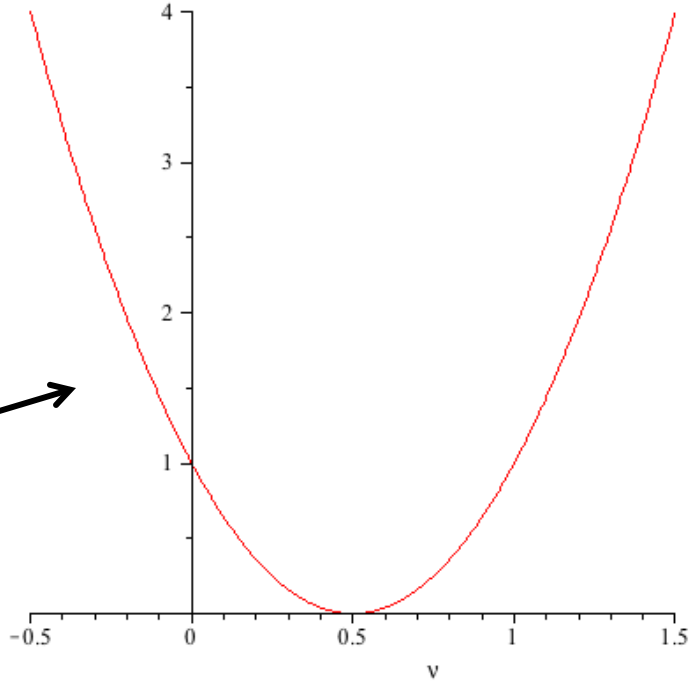
Maximum eigenvalue:

$$\max_k |\lambda_k|^2 = 1 + 4\nu(\nu - 1)$$

Stable as long as

$$0 \le \nu \le 1$$

(CFL Condition)




Thank You