Time Integration Schemes

Bill Skamarock NCAR/MMM

skamaroc@ucar.edu

Outline

1. Canonical equations for scheme analyses.
2. Time-integration schemes used in NWP models.
3. Leapfrog scheme.
4. Semi-implicit schemes.
5. Runge-Kutta schemes.
6. Combining the schemes
7. Summary

Canonical Equations for Scheme Analyses

Navier-Stokes equations:

- Transport
  - Linear (e.g. scalar advection with uniform flow)
  - Nonlinear (e.g. momentum)
- Wave Propagation
- Dissipation
  - Energy and Enstrophy

Canonical Equations for Scheme Analyses

Possible canonical equations:

Oscillation equation $$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

Exponential decay $$\frac{\partial \psi}{\partial t} = -\lambda\psi$$

Exponential growth $$\frac{\partial \psi}{\partial t} = \lambda\psi$$

Nonlinear ODEs $$\frac{\partial \psi}{\partial t} = F_n(\psi)$$

where κ is real and λ is positive and real

Canonical Equations for Scheme Analyses

Navier-Stokes equations:

- Transport
  - Linear
  - Nonlinear
- Wave Propagation

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

- Dissipation
  - Energy and Enstrophy

$$\frac{\partial \psi}{\partial t} = -\lambda\psi$$

Canonical Equations for Scheme Analyses

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

Linear oscillation equation

$$\psi(t) = \psi(t_o)\, e^{i\kappa(t-t_o)}$$
$$= \psi(t_o)\ [\cos(\kappa(t-t_o)) + i \sin(\kappa(t-t_o))]$$

$$\frac{\partial \psi}{\partial t} = -\lambda\psi$$

Exponential decay equation

$$\psi(t) = \psi(t_o)\, e^{-\lambda(t-t_o)}$$

Canonical Equations for Scheme Analyses

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

κ is a frequency (T^{-1})
(phase speed/wavelength)

Atmosphere - consider the shortest resolvable wavelengths

Transport velocities: maximum O(100 ms^{-1})
Gravity wave phase speeds, internal waves: < 100 ms^{-1}
Deep gravity wave phase speeds: > 100-300 ms^{-1}
(e.g. external modes in pressure coordinate models)
Sound (acoustic) waves: 300 ms^{-1}

Canonical Equations for Scheme Analyses

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

κ is a frequency (T^{-1})
(phase speed/wavelength)

$$\frac{\partial \psi}{\partial t} = i\kappa_s\psi + i\kappa_f\psi$$

where

$$\kappa_s = \text{ slow-mode frequency}$$
$$\kappa_f = \text{ fast-mode frequency}$$

Canonical Equations for Scheme Analyses

$$\frac{\partial \psi}{\partial t} = -\lambda \psi$$

λ is a decay rate (T^{-1})
(viscosity/wavelength^2)

Atmosphere - Decay rates proportional to eddy turnover times:

Large scales: 1/days
PBL: 1/minutes

$$\frac{\partial \psi}{\partial t} = -\lambda_s \psi - \lambda_f \psi$$

where

$\lambda_s =$ slowly decay
$\lambda_f =$ fast decay

Time Integration Schemes Used in NWP Models.

ECMWF IFS, JMA GSM,

DWD GME, NCEP GFS

All these models use some form of Leapfrog semi-implicit (semi-Lagrangian) time integration.

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$ wave propagation

Leapfrog $\psi^{t+\Delta t} - \psi^{t-\Delta t} = 2\Delta t\, i\kappa_s \psi^t$

Semi-implicit $\psi^{t+\Delta t} - \psi^{t-\Delta t} = \Delta t\, i\kappa_f \left(\psi^{t-\Delta t} + \psi^{t+\Delta t}\right)$

Time Integration Schemes Used in NWP Models.

ECMWF IFS, JMA GSM,

DWD GME, NCEP GFS

Dissipation is either handled implicitly or using forward Euler (in the leapfrog context).

$$\frac{\partial \psi}{\partial t} = -\lambda \psi$$ dissipation

Forward Euler $$\psi^{t+\Delta t} - \psi^{t-\Delta t} = -2\Delta t\, \lambda_s \psi^{t-\Delta t}$$

Semi-implicit $$\psi^{t+\Delta t} - \psi^{t-\Delta t} = -\Delta t\, \lambda_f \left(\psi^{t-\Delta t} + \psi^{t+\Delta t}\right)$$

Time Integration Schemes Used in NWP Models.

UKMO Unified model, GRAPES

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$ wave propagation

<u>Predictor-Corrector</u> $$\psi^{t+\Delta t} - \psi^{t} = \Delta t\, i\kappa_s \frac{1}{2}\left(\psi^{t} + \tilde{\psi}^{t+\Delta t}\right)$$

<u>Semi-implicit</u> $$\psi^{t+\Delta t} - \psi^{t} = \Delta t\, i\kappa_f \frac{1}{2}\left(\psi^{t} + \psi^{t+\Delta t}\right)$$

$$\frac{\partial \psi}{\partial t} = -\lambda\psi$$ dissipation

<u>Forward Euler</u> $$\psi^{t+\Delta t} - \psi^{t} = -\Delta t\, \lambda_s \psi^{t}$$

<u>Semi-implicit</u> $$\psi^{t+\Delta t} - \psi^{t} = -\Delta t\, \lambda_f \frac{1}{2}\left(\psi^{t} + \psi^{t+\Delta t}\right)$$

Time Integration Schemes Used in NWP Models.

MM5, ARPS, COAMPS

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$ wave propagation

Leapfrog (advection, gravity waves)

$$\psi^{t+\Delta t} - \psi^{t-\Delta t} = 2\Delta t \, i\kappa_s \psi^t$$

Forward-backward (acoustic modes)

$$\psi_1^{\tau+\Delta\tau} - \psi_1^{\tau} = \Delta\tau \, i\kappa_f \psi_2^{\tau}, \quad \psi_2^{\tau+\Delta\tau} - \psi_2^{\tau} = \Delta\tau \, i\kappa_f \psi_1^{\tau+\Delta\tau}$$

Time Integration Schemes Used in NWP Models.

MM5, ARPS, COAMPS

Dissipation is either handled implicitly or using forward Euler (in the leapfrog context).

$$\frac{\partial \psi}{\partial t} = -\lambda \psi$$

<u>Leapfrog</u> $$\psi^{t+\Delta t} - \psi^{t-\Delta t} = -2\Delta t \, \lambda_s \psi^{t-\Delta t}$$

<u>Semi-implicit</u> $$\psi^{t+\Delta t} - \psi^{t-\Delta t} = -\Delta t \, \lambda_f \left(\psi^{t-\Delta t} + \psi^{t+\Delta t} \right)$$

Time Integration Schemes Used in NWP Models.

WRF (ARW), COSMO, NICAM

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$ wave propagation

Runge-Kutta (advection)

RK3

$$\psi^{*} = \psi^{t} + \frac{\Delta t}{3} i\kappa_s \psi^{t}$$

$$\psi^{**} = \psi^{t} + \frac{\Delta t}{2} i\kappa_s \psi^{*}$$

$$\psi^{t+\Delta t} = \psi^{t} + \Delta t i\kappa_s \psi^{**}$$

RK2

$$\psi^{*} = \psi^{t} + \frac{\Delta t}{2} i\kappa_s \psi^{t}$$

$$\psi^{t+\Delta t} = \psi^{t} + \Delta t i\kappa_s \psi^{*}$$

Forward-backward (acoustic modes)

$$\psi_1^{\tau+\Delta\tau} - \psi_1^{\tau} = \Delta\tau\, i\kappa_f \psi_2^{\tau}, \quad \psi_2^{\tau+\Delta\tau} - \psi_2^{\tau} = \Delta\tau\, i\kappa_f \psi_1^{\tau+\Delta\tau}$$

Time Integration Schemes Used in NWP Models.

WRF (ARW), COSMO, NICAM

Dissipation is either handled implicitly or using forward Euler or using Runge-Kutta.

$$\frac{\partial \psi}{\partial t} = -\lambda \psi$$

<u>Forward Euler</u> $\psi^{t+\Delta t} - \psi^t = -\Delta t \, \lambda_s \psi^t$

<u>Semi-implicit</u> $\psi^{t+\Delta t} - \psi^t = -\Delta t \, \lambda_f \frac{1}{2} \left(\psi^t + \psi^{t+\Delta t} \right)$

Leapfrog Time Integration

<u>continuous</u>

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

$$\psi(t) = \psi(t_o)\, e^{i\kappa(t-t_o)}$$

$$\psi(t) = A_e\, e^{i\kappa(t-t_o)}$$

Stability:
continuous solutions do not grow

$$|\psi(t)| = |\psi(t_o)\, e^{i\kappa(t-t_o)}| = |\psi(t_o)|$$

<u>discrete</u>

$$\psi^{t+\Delta t} - \psi^{t-\Delta t} = 2\Delta t\, i\kappa\psi^t$$

assume solutions of the form

$$\psi^{t+\Delta t} = A\, e^{i\theta}\psi^t$$

$$A^2 - 2i\kappa\Delta t A - 1 = 0$$

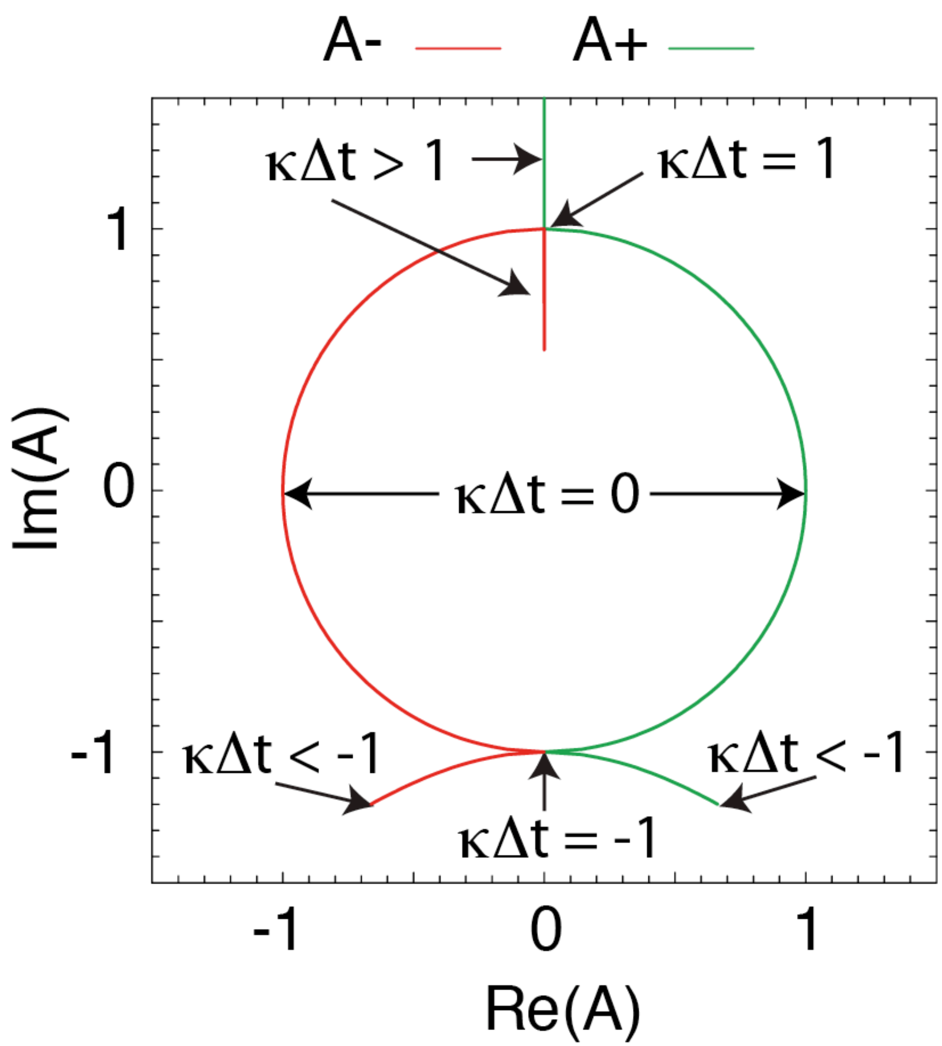
$$A = i\kappa\Delta t \pm \left(1 - \kappa^2\Delta t^2\right)^{1/2}$$

Leapfrog Time Integration

$$A = i\kappa\Delta t \pm \left(1 - \kappa^2 \Delta t^2\right)^{1/2}$$

Two roots:
A+ physical mode
A- computational mode
(parasitic mode or root)

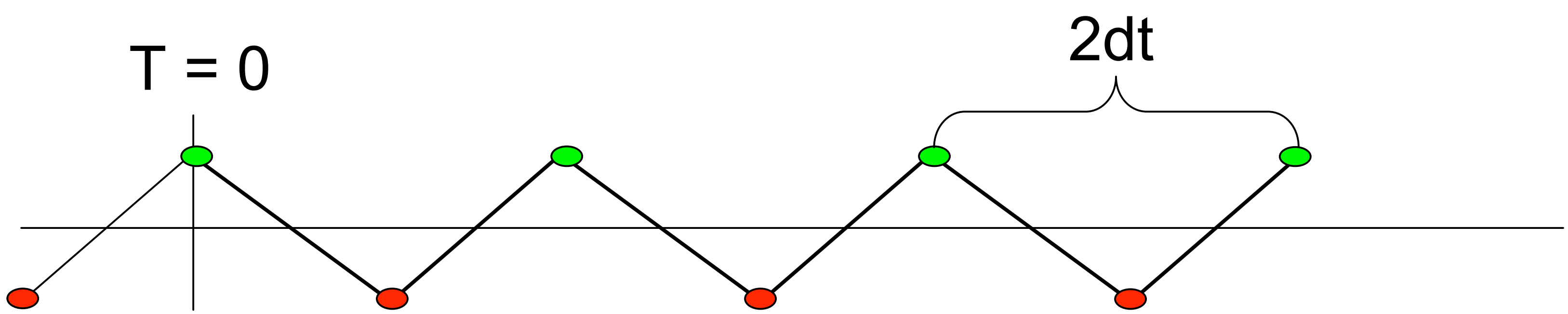
Stability: $|\kappa\Delta t| < 1$



Leapfrog Time Integration

Relevance of the computational mode? $A = i\kappa\Delta t \pm \left(1 - \kappa^2\Delta t^2\right)^{1/2}$

Consider $\kappa\Delta t = 0, \;\; A = \pm 1$ → $\psi^{t+\Delta t} = \psi^{t-\Delta t}$

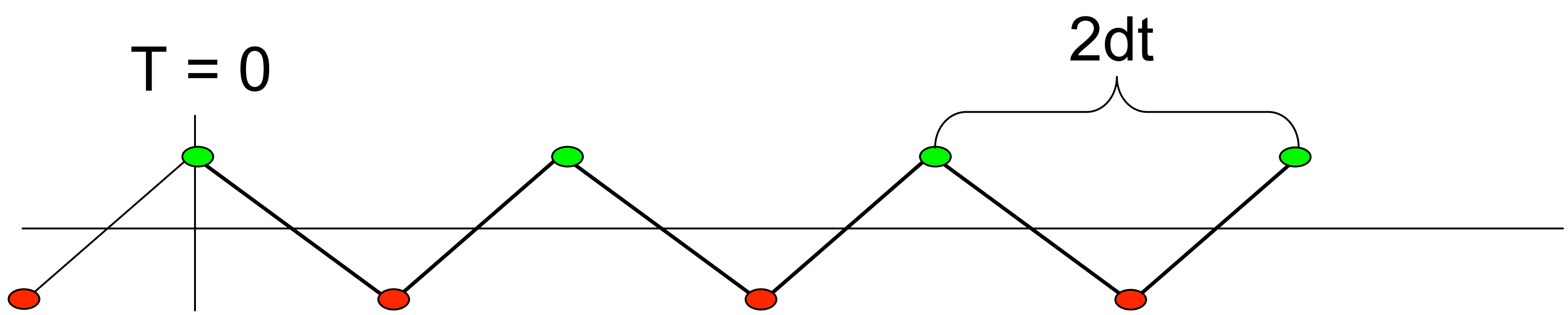


Odd and even timestep are decoupled.

The amplitude of the computational mode depends on starting procedure. In practice, nonlinearities will put energy into the computation mode during an integration.

Leapfrog Time Integration

Controlling the computational mode



Asselin filter

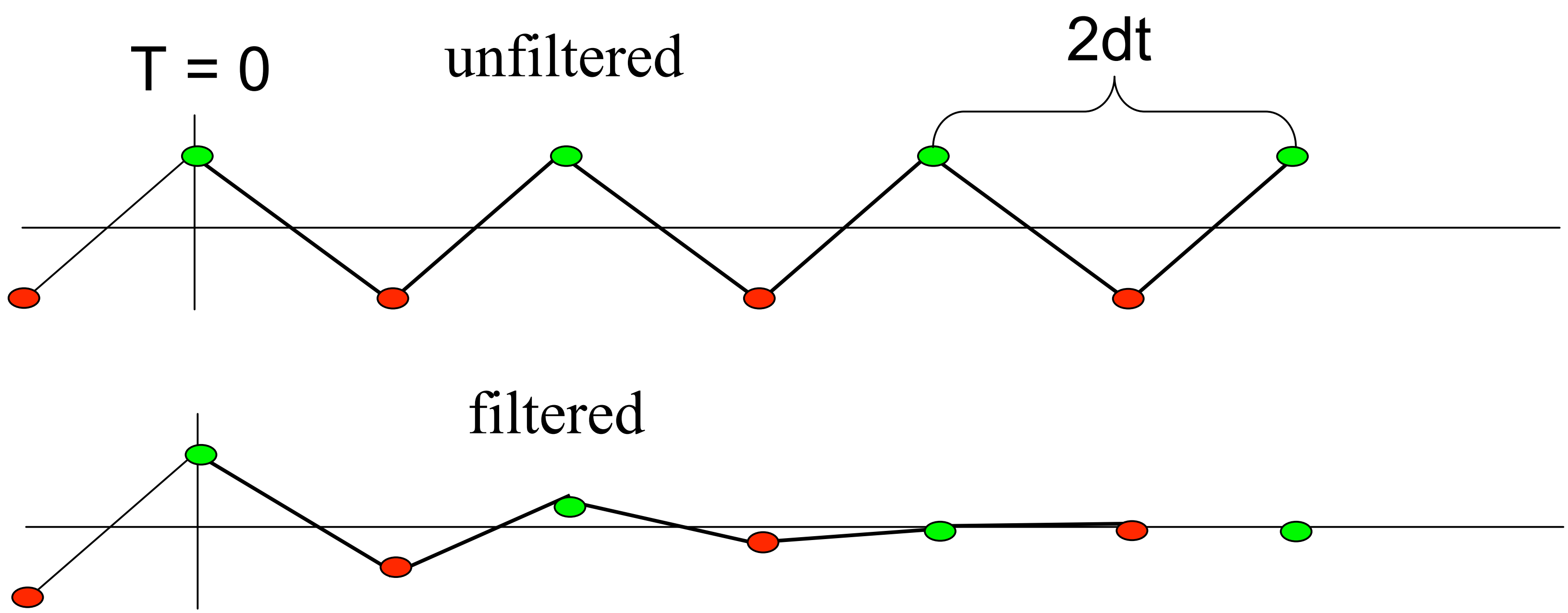
$$\overline{\psi^{t-\Delta t}} = \psi^{t-\Delta t} + \gamma\left(\overline{\psi^{t-2\Delta t}} - 2\psi^{t-\Delta t} + \psi^{t}\right)$$

Asselin-filtered leapfrog

$$\psi^{t+\Delta t} - \overline{\psi^{t-\Delta t}} = 2\Delta t\, i\kappa\psi^{t}$$

Leapfrog Time Integration

Controlling the computational mode



Drawbacks: damping - first order in time (error $O(dt)$, not $O(dt^2)$)
Asselin filter damps all modes!

Semi-Implicit Time Integration
- The Implicit Component -

continuous

$$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

$$\psi(t) = \psi(t_o)\, e^{i\kappa(t-t_o)}$$

$$\psi(t) = A_e\, e^{i\kappa(t-t_o)}$$

Stability:
continuous solutions do not grow

$$|\psi(t)| = |\psi(t_o)\, e^{i\kappa(t-t_o)}| = |\psi(t_o)|$$

Implicit

$$\psi^{t+\Delta t} - \psi^t = \Delta t\, i\kappa \frac{1}{2}\left(\psi^t + \psi^{t+\Delta t}\right)$$

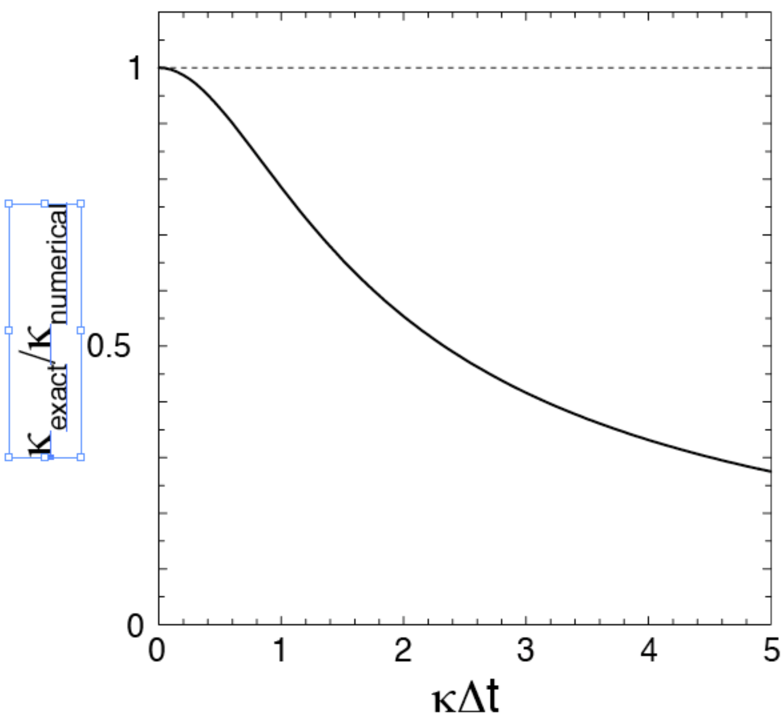
$$A = \frac{1 + i\kappa\Delta t}{1 - i\kappa\Delta t} \equiv 1$$

Stable for all timesteps
with no damping!

Semi-Implicit Time Integration
- The Implicit Component -

$$\psi^{t+\Delta t} - \psi^t = \Delta t \, i\kappa \frac{1}{2} \left(\psi^t + \psi^{t+\Delta t} \right)$$

Drawbacks of centered implicit integration



(1) Phase Errors
stability gained by reducing the frequency.

(2) Need to solve 3D elliptic equation

Semi-Implicit Time Integration
- The Implicit Component -

Offcentering is used to stabilize the integration

Replace $$\psi^{t+\Delta t} - \psi^{t} = \Delta t \, i\kappa \frac{1}{2}\left(\psi^{t} + \psi^{t+\Delta t}\right)$$

with $$\psi^{t+\Delta t} - \psi^{t} = \Delta t \, i\kappa \left((1-\beta)\psi^{t} + \beta\psi^{t+\Delta t}\right)$$

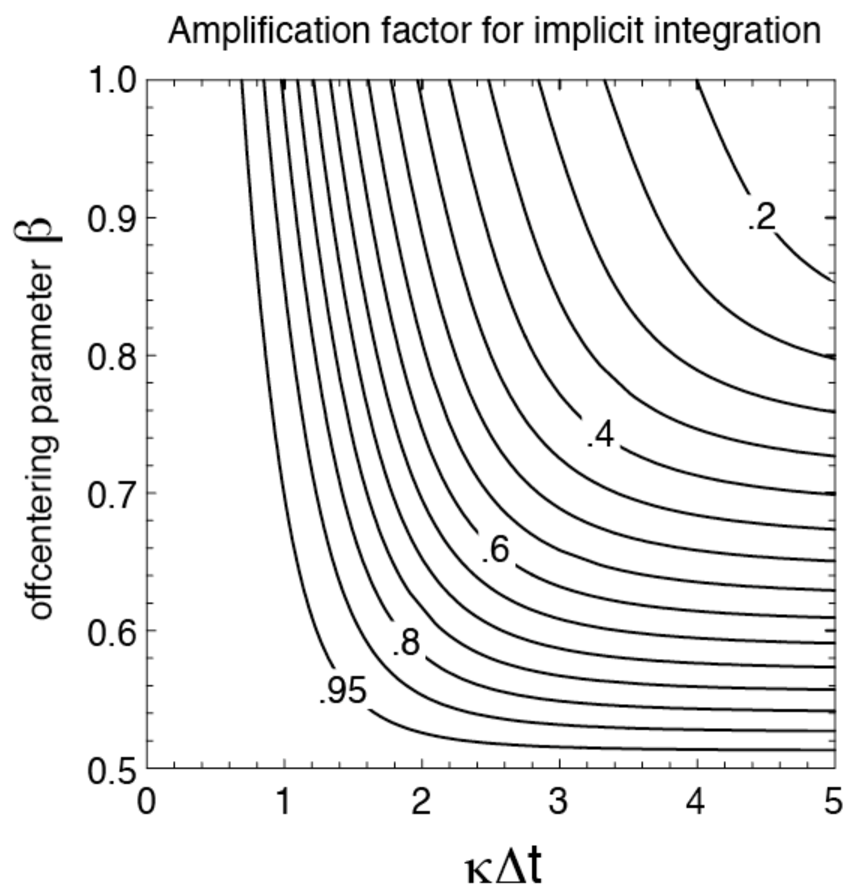
Amplitude $$|A|^2 = \frac{1 + i(1-\beta)\kappa\Delta t}{1 + i\beta\kappa\Delta t} \leq 1 \quad \text{for } \beta \geq 1/2$$

Semi-Implicit Time Integration
- The Implicit Component -

Amplitude $$|A|^2 = \frac{1 + i(1-\beta)\kappa\Delta t}{1 + i\beta\kappa\Delta t} \leq 1 \quad \text{for } \beta \geq 1/2$$

Consequences:

In semi-Lagrangian semi-implicit (SLSI) models that use large timesteps, physically relevent modes may be strongly damped.



Runge-Kutta Time Integration

(1) $$\frac{\partial \psi}{\partial t} = i\kappa\psi$$

(2) $$\frac{\partial \psi}{\partial t} = -\lambda\psi$$

<u>RK3</u>

$$\psi^* = \phi^t + \frac{\Delta t}{3} i\kappa_s \psi^t$$
$$\psi^{**} = \phi^t + \frac{\Delta t}{2} i\kappa_s \psi^*$$
$$\psi^{t+\Delta t} = \phi^t + \Delta t i\kappa_s \psi^{**}$$

Stable for the oscillation eqn (1) and decay eqn (2).

<u>RK2</u>

$$\psi^* = \phi^t + \frac{\Delta t}{2} i\kappa_s \psi^t$$
$$\psi^{t+\Delta t} = \phi^t + \Delta t i\kappa_s \psi^*$$

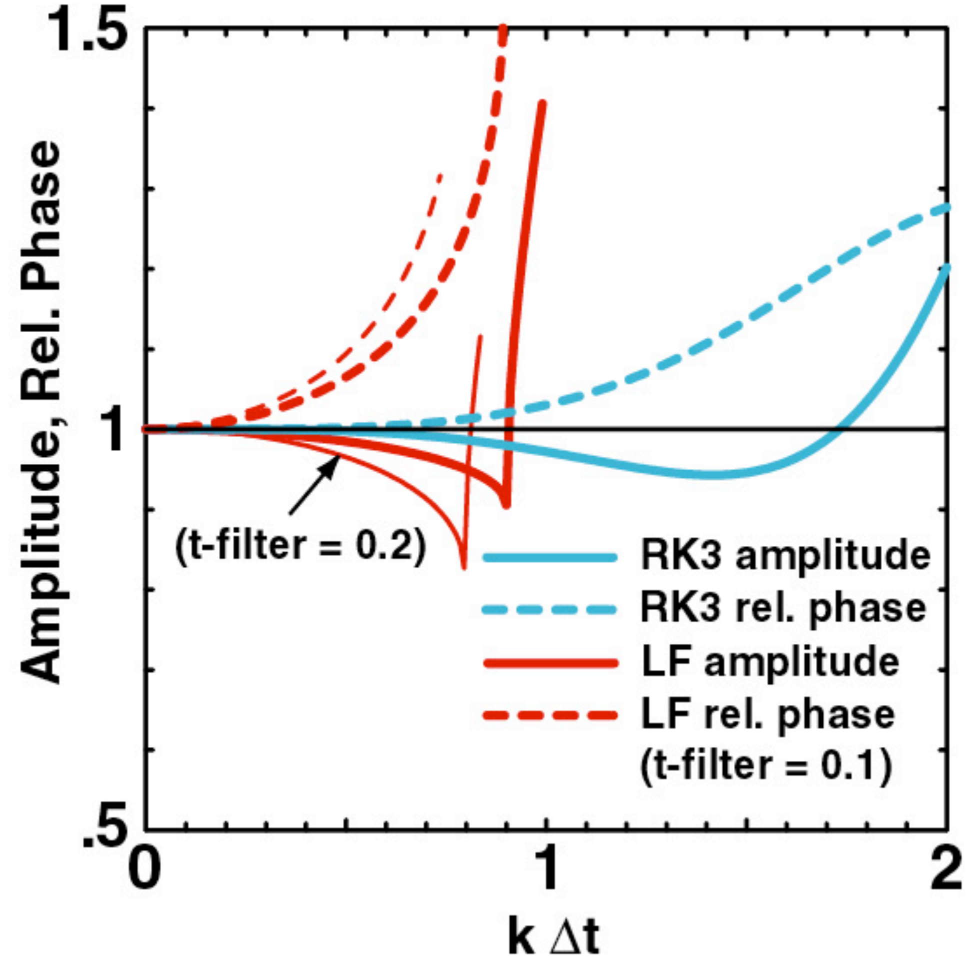
Unstable for the oscillation eqn (1). Stable for the decay eqn (2).

RK2 transport must be dissipative!

Runge-Kutta Time Integration

$$\phi_t = ik\phi; \quad \phi^{n+1} = A\phi^n; \quad |A| = 1 - \frac{(k\Delta t)^4}{24}$$

From the ARW tutorial.



Combining Time-Integration Schemes

Canonical equation

$$\frac{\partial \psi}{\partial t} = i\kappa_s \psi + i\kappa_f \psi$$

where

$$\kappa_s = \text{ slow-mode frequency}$$

$$\kappa_f = \text{ fast-mode frequency}$$

Example:

Linearized acoustic-mode equations

$$u_t + c_s p_x + U u_x = 0$$

$$p_t + c_s u_x + U p_x = 0$$

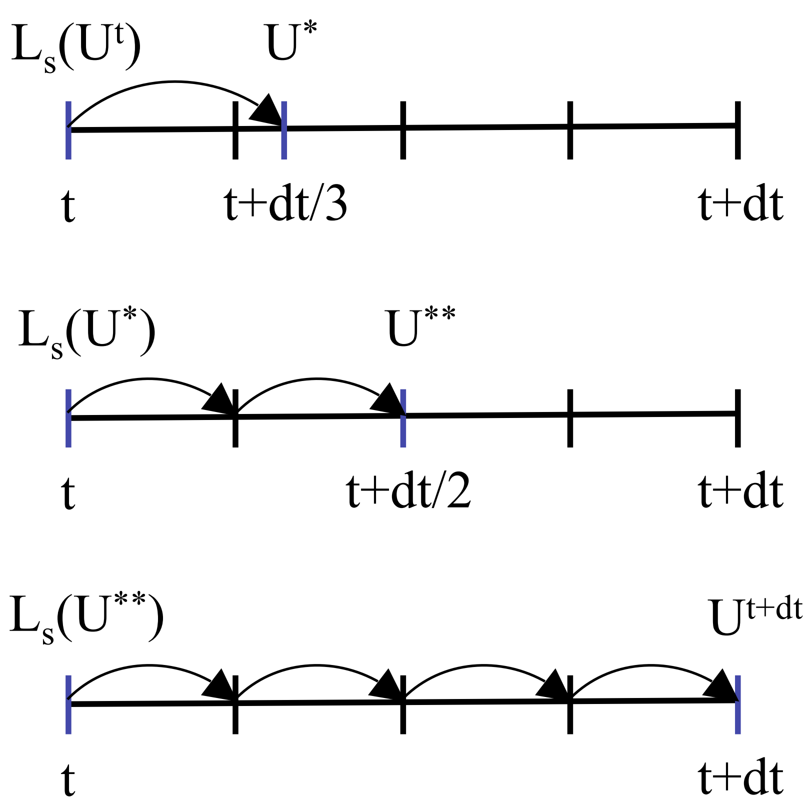
Assume solutions of the form e^{ikx}

$$\frac{\partial \vec{\psi}}{\partial t} = \mathbf{A}_f \vec{\psi} + \mathbf{A}_s \vec{\psi}$$

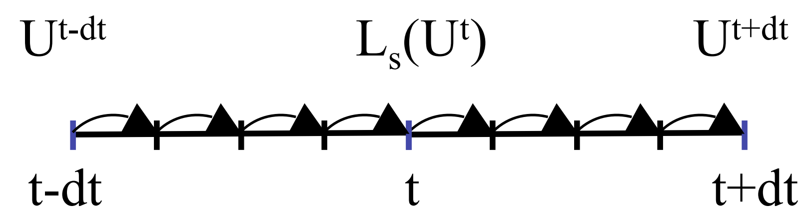
Split-Explicit time integration
ARW RK3 and Leapfrog

$$U_t = L_{fast}(U) + L_{slow}(U)$$

3rd order Runge-Kutta, 3 steps



Leapfrog - 1 step

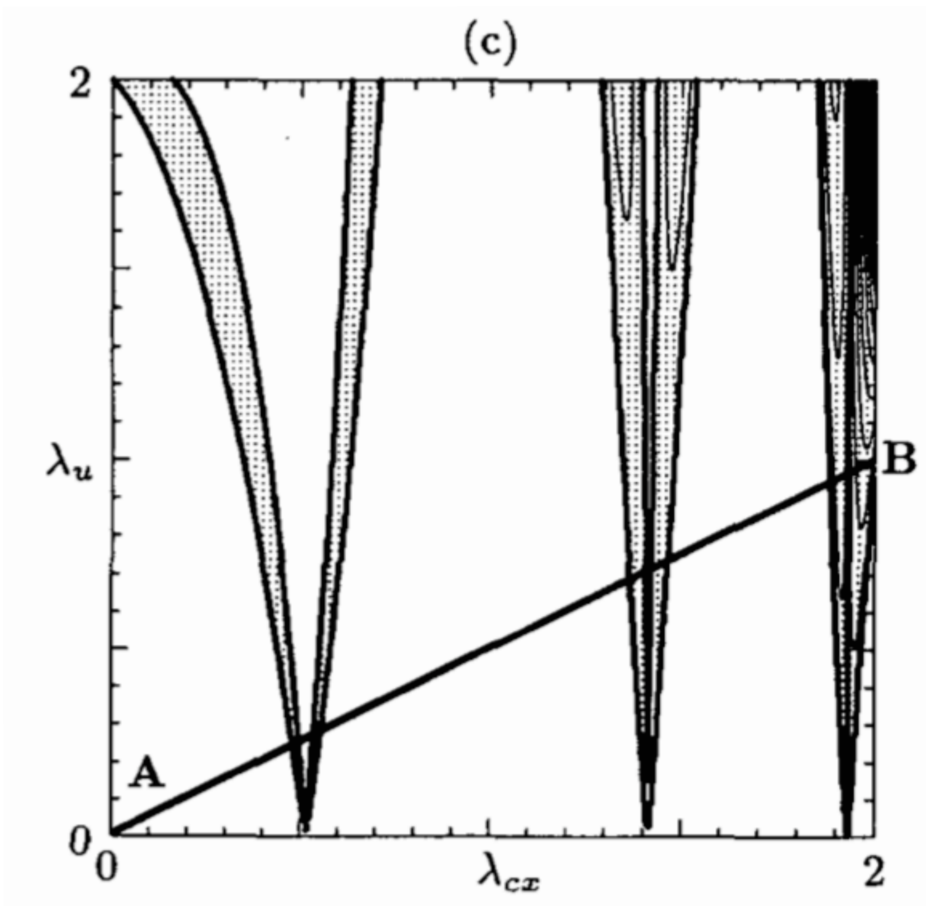


Acoustic mode integration:
forward-backward

$$\begin{aligned} u^{\tau+\Delta\tau} &= u^{\tau} - \Delta\tau c_s \delta_x p^{\tau} \\ &\quad + L_s(u^t, p^t) \\ p^{\tau+\Delta\tau} &= p^{\tau} - \Delta\tau c_s \delta_x u^{\tau+\Delta\tau} \\ &\quad + L_s(u^t, p^t) \end{aligned}$$

Split-Explicit time integration
ARW RK3 and Leapfrog

Leapfrog, n_s = 6
(shaded regions unstable; A > 1)

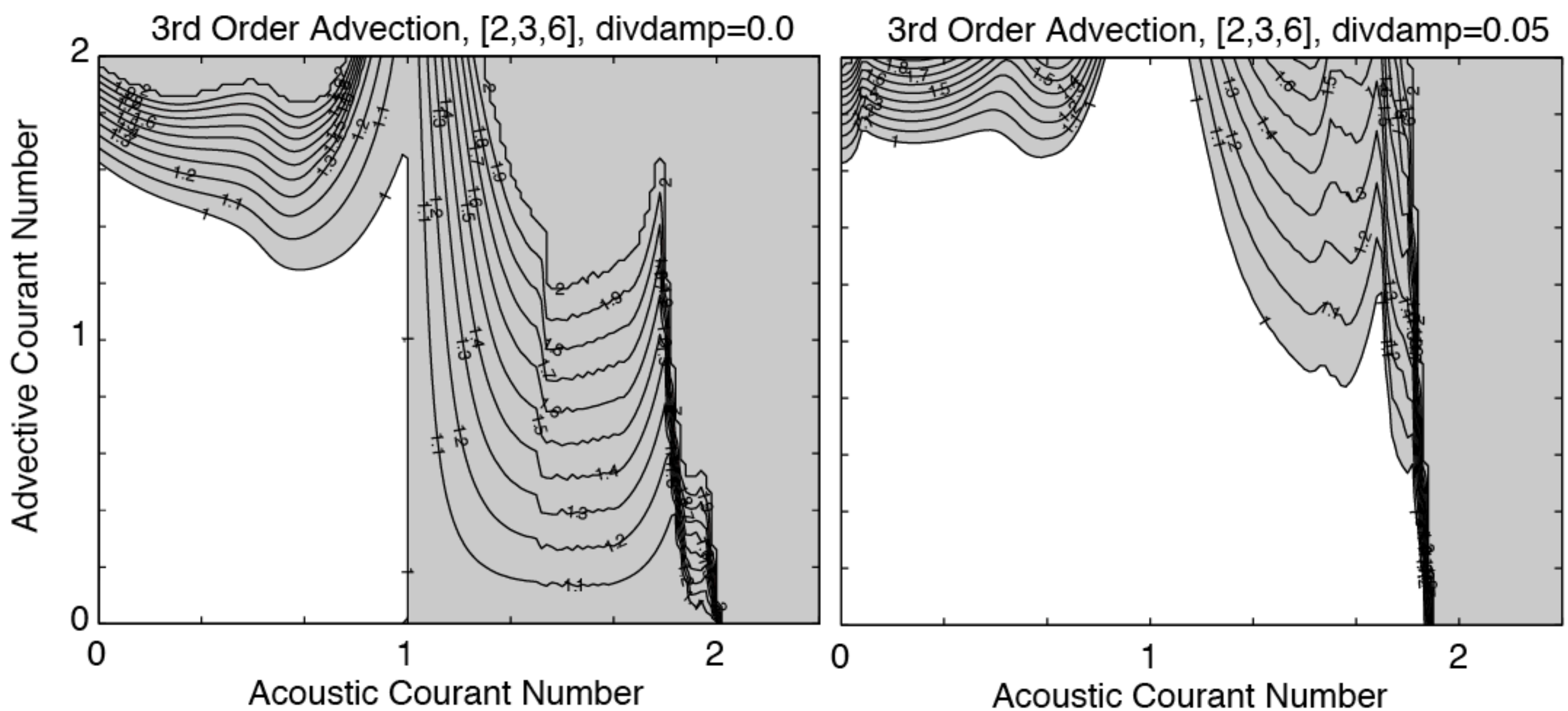


Perfect advection:
Unstable modes exist in Leapfrog and FB stable Courant numbers.

LF Asselin time filter removes these instabilities as does 3D divergence mode damping (acoustic mode damping).

Split-Explicit time integration
ARW RK3 and Leapfrog

RK3, n_s = 6
(shaded regions unstable; A > 1)

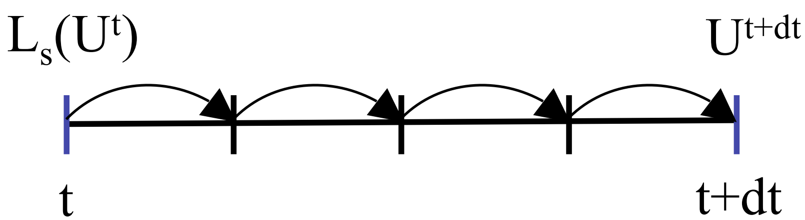


Perfect advection: Divergence damping helps stabilize the split scheme

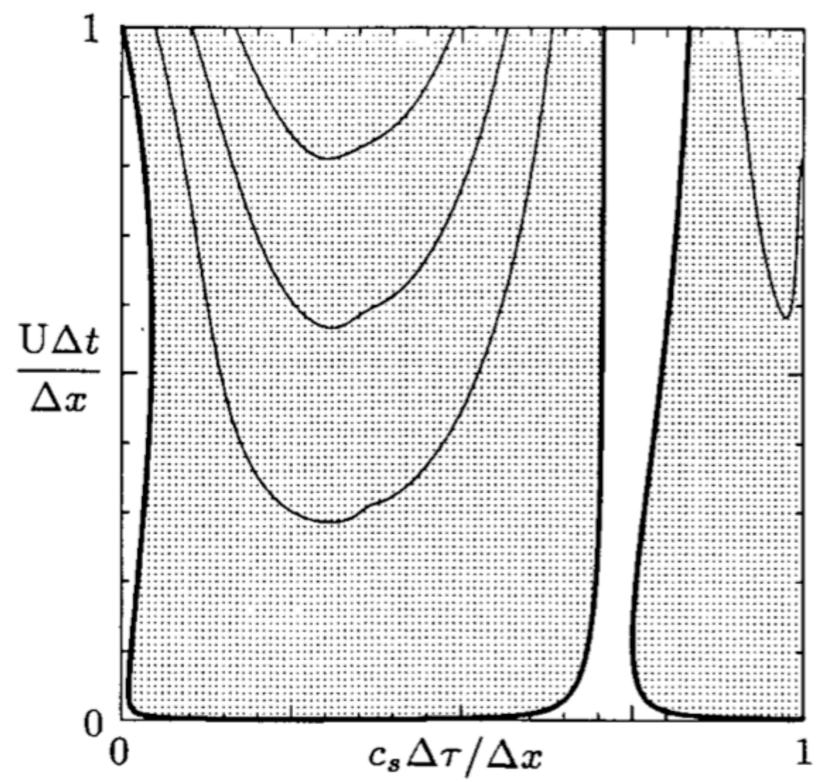
Split-Explicit Time Integration
Forward-In-Time Transport

$$U_t = L_{fast}(U) + L_{slow}(U)$$

FIT - 1 step



1st order Upwind, n_s = 6
(shaded regions unstable; A > 1)



Upwinding with FB scheme is unstable, divergence damping does not provide stability needed for applications.

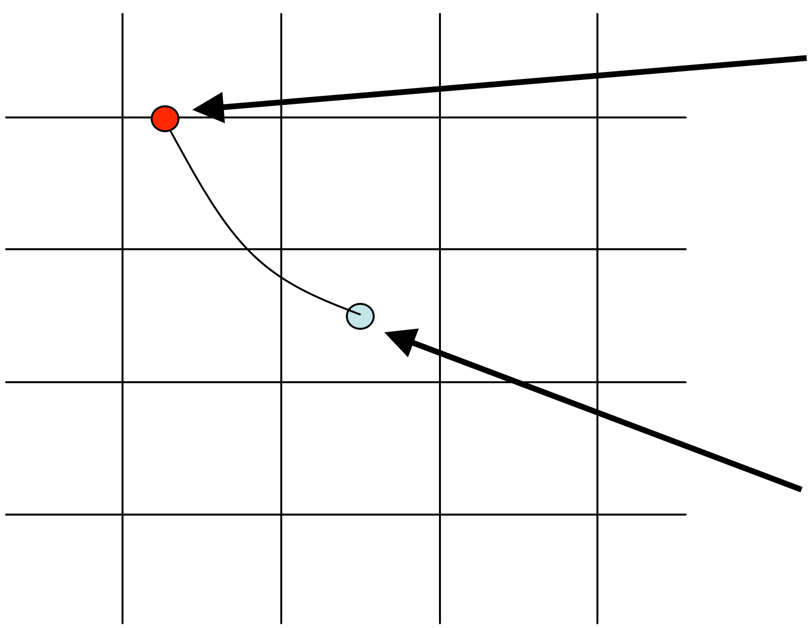
Semi-Lagrangian Semi-Implicit Time Integration (UKMO Unified Model)

Continuous linear acoustic equations

$$u_t + c_s p_x + U u_x = 0$$
$$p_t + c_s u_x + U p_x = 0$$

Discrete linear acoustic equations

$$u^{t+\Delta t} = u^t|_d - \Delta t c_s \left[\beta \delta_x p^{t+\Delta t} + (1-\beta)(\delta_x p^t)|_d\right]$$
$$p^{t+\Delta t} = p^t|_d - \Delta t c_s \left[\beta \delta_x u^{t+\Delta t} + (1-\beta)(\delta_x u^t)|_d\right]$$



Departure point following fluid trajectory - quantities needed here must be interpolated.

Grid-point value

Semi-Lagrangian Semi-Implicit Time Integration (UKMO Unified Model)

Continuous linear acoustic equations

$$u_t + c_s p_x + U u_x = 0$$
$$p_t + c_s u_x + U p_x = 0$$

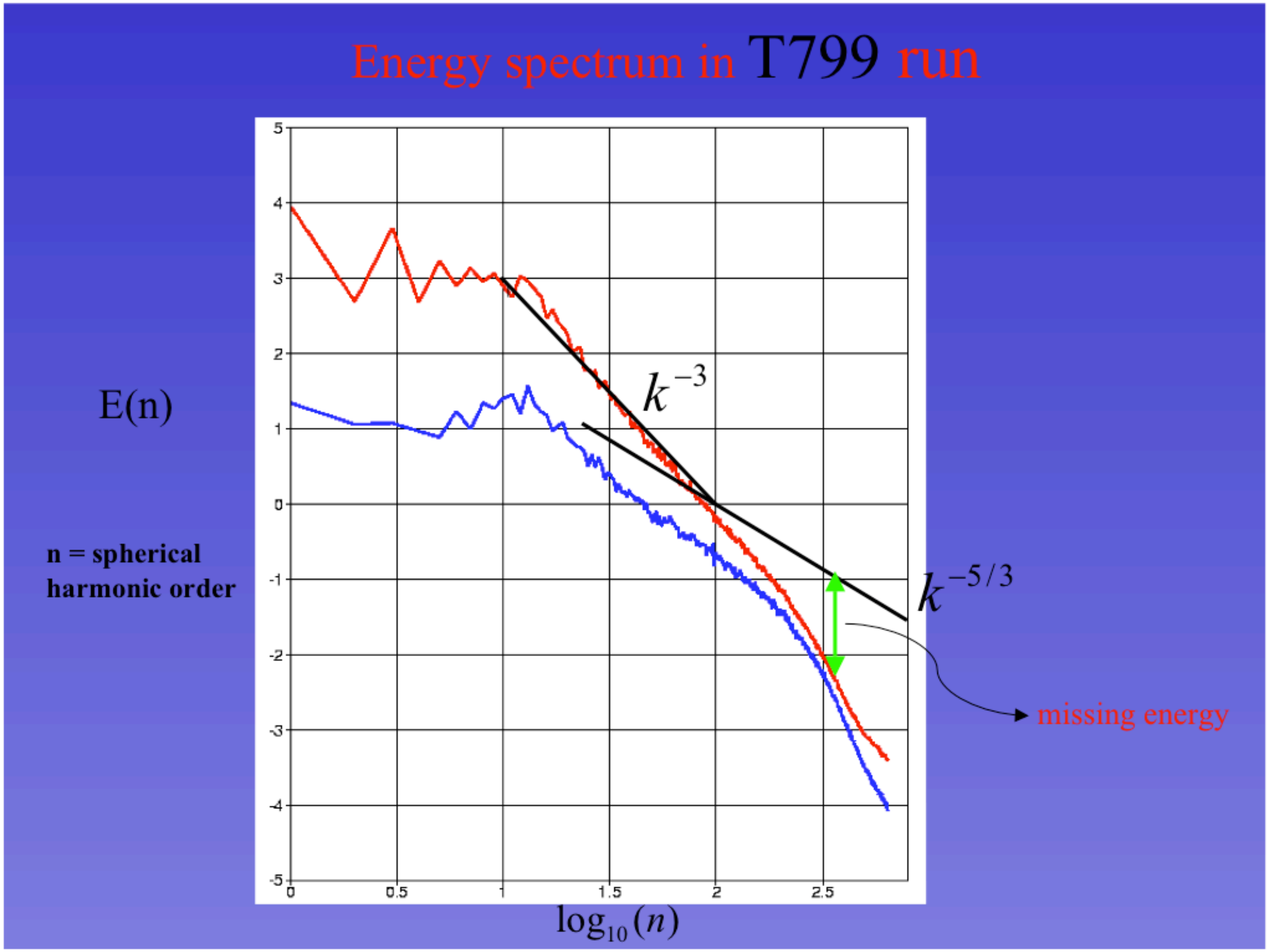
Discrete linear acoustic equations

$$u^{t+\Delta t} = u^t|_d - \Delta t c_s \left[\beta \delta_x p^{t+\Delta t} + (1-\beta)(\delta_x p^t)|_d\right]$$
$$p^{t+\Delta t} = p^t|_d - \Delta t c_s \left[\beta \delta_x u^{t+\Delta t} + (1-\beta)(\delta_x u^t)|_d\right]$$

For $\beta = 1/2$, the scheme is absolutely stable for all Δt for the *linear* problem

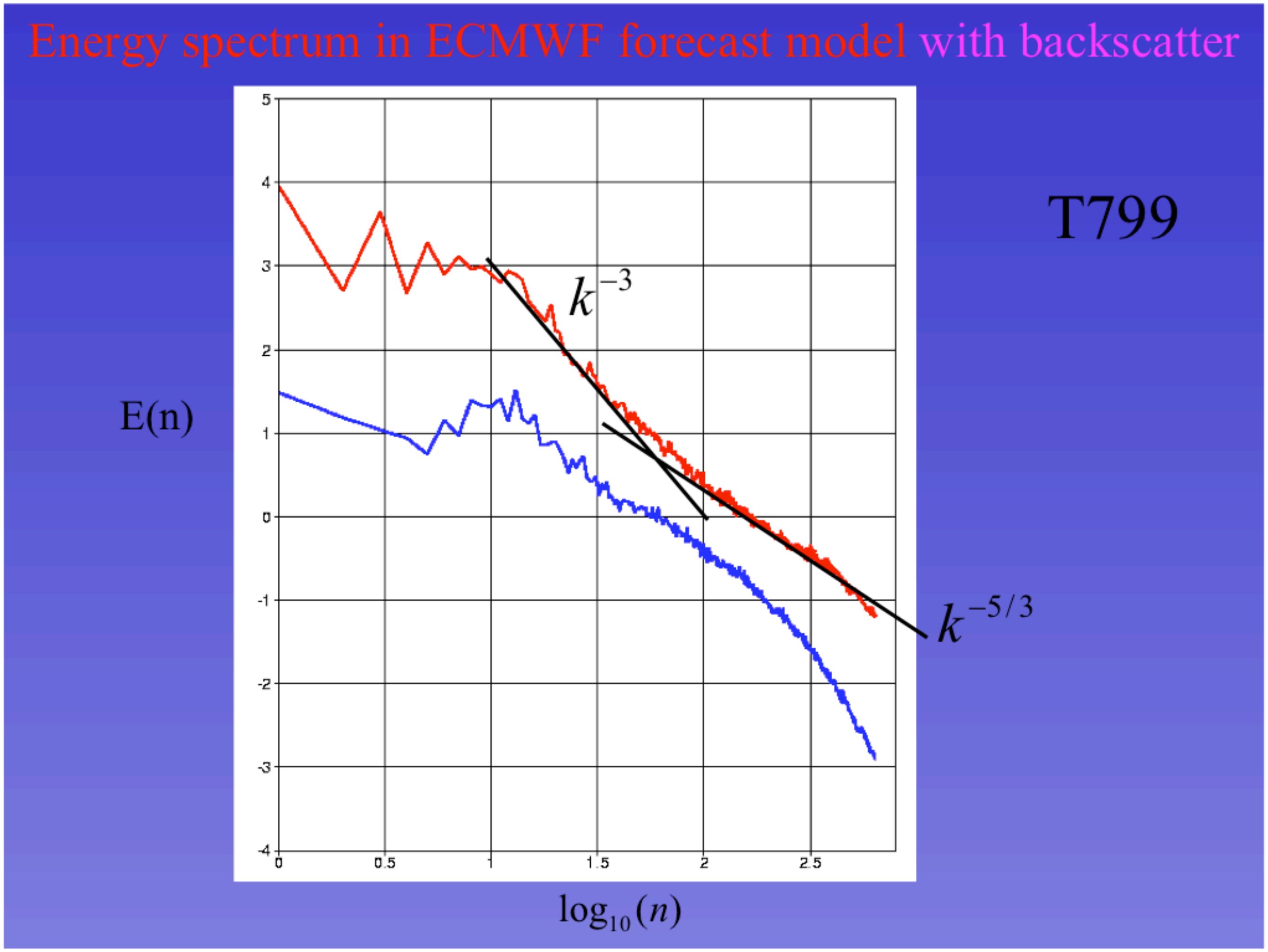
However, for the full nonlinear equations, truncation errors in the trajectory calculations, and nonlinear terms not included in the implicit formulation lead to the need for offcentering the implicit calculation. Typically $0.6 < \beta < 0.8$

Implicit-Scheme Damping - Does It Matter? ECMWF Model



(courtesy of Tim Palmer, 2004)

Implicit-Scheme Damping - Does It Matter? ECMWF Model



Correct mesoscale spectrum for the wrong reason?

Summary

- Linear analyses of the oscillation and decay equations reveal stability properties of the individual time integration schemes.
- When schemes are combined to integrate slow and fast modes, the stability of the combination is not necessarily indicated by the stability of the individual schemes.
- Most combined schemes need some form of filtering for stability.

References: For atmospheric models, see the textbook *Numerical Methods for Wave Equations in Geophysical Fluid Dynamics* by Dale Durran (Springer, 1998) and references therein.