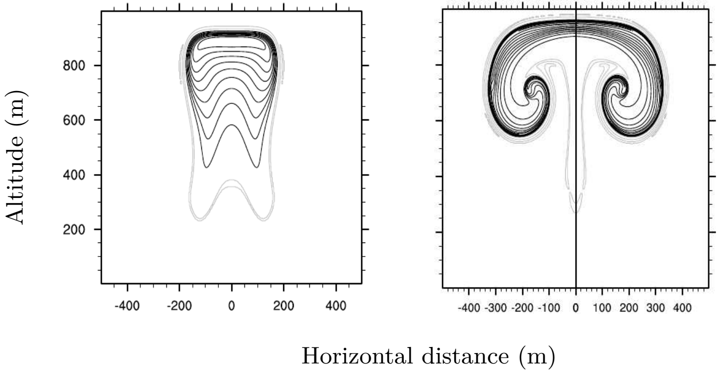
Horizontally-explicit vertically-implicit (HEVI) time-stepping methods for NWP and climate models

Sarah-Jane Lock

Why bother?



[left:] Fig. 1(d) & [right:] Fig. 2(d), Ullrich & Jablonowski (2012, MWR), courtesy Paul Ullrich

Outline

- Overview of the problem for time-stepping schemes
- Review of established HEVI methods
- Introduce ideas for a new HEVI approach
- Show some analyses of Runge-Kutta HEVI schemes:
    - linear analyses
    - numerical results

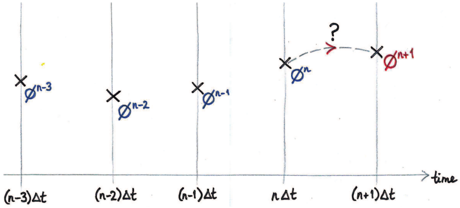
Time discretisation

Consider the atmospheric system as

$$\frac{\partial F}{\partial t} = g(F), \tag{1}$$

where $F = [\mathbf{u}, T, p]^{\mathrm{T}}$.

For the discretised model, how do we use past solutions to approximate (1)?



LHS: $\frac{\partial F}{\partial t} \approx \frac{\phi^{n+1} - ?}{\alpha \Delta t}$

RHS: $g(F) \approx g\left(\phi^{?}\right)$

Time discretisation

The atmospheric model is better described by

$$\frac{\partial F}{\partial t} = f(F) + s(F),$$

where $||f|| \gg ||s||$.

The difference in scales comes from 2 aspects:

1. **continuous model:** solutions comprise fast *and* slow modes, i.e. **speed (**c**)**;
2. **discretised model:** grid-spacings differ: $\Delta x \gg \Delta z$, i.e. **mesh**.

The extent to which a time-stepping method can represent the model solution on a given mesh depends on

$$\Delta t.$$

Specifically, the *Courant* numbers

$$c_x \frac{\Delta t}{\Delta x}, \qquad c_z \frac{\Delta t}{\Delta z}$$

for a given model problem can be used to determine a discretisation method's

- accuracy, and
- stability.

What are these fast and slow modes?

Many global weather models are based on nonhydrostatic, compressible equations.

From dispersion relation analyses, we can identify the major (dry) dynamical processes to be (from slowest to fastest):

- rotation
- advection (U)
- gravity waves
- acoustic waves (c_s)

such that $c_s \gg U$,

$$\Rightarrow c_s \frac{\Delta t}{\Delta x} \gg U \frac{\Delta t}{\Delta x}.$$

$\Rightarrow$ Question becomes:

How do we handle the acoustic waves?

Approaches for handling the fast modes

Consider again the atmospheric model

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2. $\Delta x \gg \Delta z$.

We can:

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- tackle (1) & (2) with

  "semi-implicit" solutions (e.g. Tapp & White, 1976; Cullen, 1990)
  $\Rightarrow$ no stability limit on Δt for implicit solutions of fast modes
  $\Rightarrow$ computationally expensive 3D Helmholtz problem to solve (N. Wood and P. Benard talks);

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  (N. Wood and P. Benard talks);

- tackle (2) & accept horizontal constraint from (1) with

  a "HEVI" (horizontally-explicit vertically-implicit) approach.

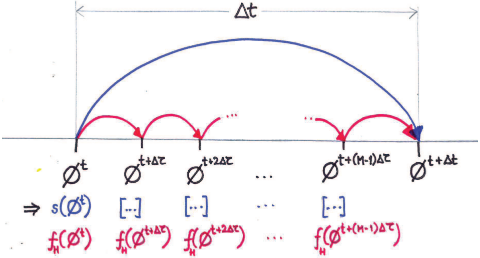
HEVI approaches: "Split-explicit" time-stepping

- **vertical:** implicit (trapezoidal) for fast modes ⇒ no stability limit on Δt; 1D (column) ⇒ tridiagonal problem ⇒ computationally cheap & no implications for parallelisation;
- **horizontal:** choose Δt appropriate for physically important modes; use **sub-steps** ($\Delta\tau = \Delta t / M$) to solve the fast modes.

Now, the atmospheric model is described by

$$\frac{\partial F}{\partial t} = f_V(F) + f_H(F) + s(F)$$

with fast contributions acting in the vertical (f_V) and horizontal (f_H).



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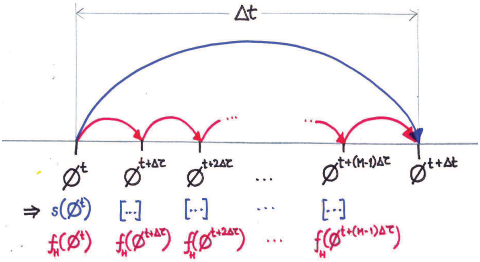

Efficiency comes from:

- $s(\phi)$: costly, but only once per Δt;
- $f(\phi)$: multiple computations, but cheap

HEVI approaches: Split-explicit time-stepping

Approach is well-established and widely used, e.g.:

- Klemp & Wilhelmson (1978), Skamarock & Klemp (1992, 1994)
- Wicker & Skamarock (2002), Klemp et al. (2007) $\rightarrow$ WRF
- Baldauf (2008, 2010) $\rightarrow$ COSMO model
- MPAS, NICAM ...

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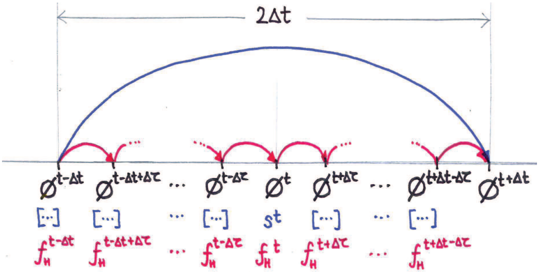
Choice of scheme for the slow modes varies:

- **leapfrog:**



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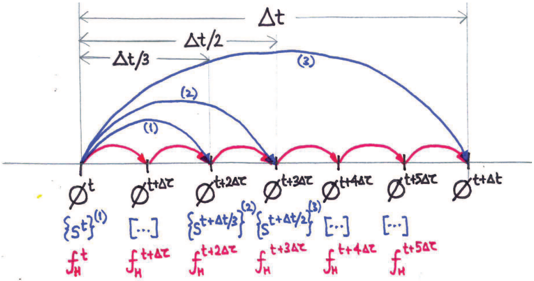
- **3rd-order 3-stage Runge-Kutta:**



HEVI schemes: recent ideas

Recent work has proposed a simpler approach:

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Why?

- Concern that deep atmosphere models, O(100 km), cannot benefit from efficiency gains with the split-explicit approach since $U \approx c_s$ in stratospheric polar jet (Gassmann, 2012)

$$\Rightarrow \Delta t \to \Delta\tau \quad (M \to 1)$$

- Split-explicit combination of schemes requires additional damping terms for stability (e.g. Baldauf, 2010)

New HEVI approaches

For a HEVI approach to solve

$$\frac{\partial F}{\partial t} = f(F) + s(F),$$

we need an implicit scheme to solve terms in f and an explicit scheme for terms in s, i.e. from wider literature:

"**IMEX**" (implicit-explicit) combination.

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- Current literature: very little analysis for the atmospheric system.
- Some very recent analyses:

- Durran & Blossey (2012): multi-step methods;
- Giraldo et al. (2013): multi-step & multi-stage methods;
- Ullrich & Jablonowski (2012): multi-stage (Runge-Kutta) methods;
- Weller, Lock, Wood (2013): multi-stage methods;
- Lock, Wood, Weller (QJRMS, accepted): multi-stage methods.

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Runge-Kutta HEVI schemes

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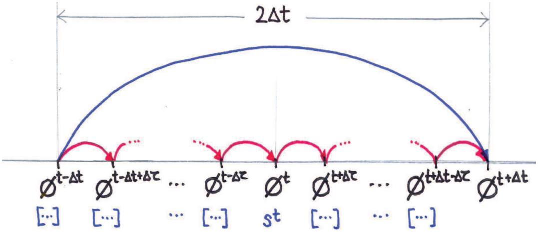
e.g. leapfrog = **multi-step**: **NOT**



Multi-**step** methods have computational modes:

- can be inherently well-behaved (damped) (see e.g. Durran & Blossey, 2012);
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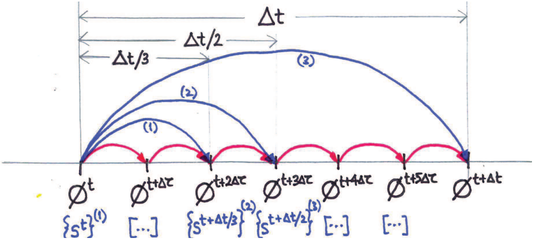
e.g. 3rd-order **3-stage** Runge-Kutta:



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Multi-**stage** methods don't support inherent computational modes.

Analyses of Runge-Kutta HEVI schemes

Our analyses include:

- identifying a number of Runge-Kutta (RK) IMEX schemes from the literature;
- linear analysis of a system supporting acoustic waves, considering errors in:
  - amplitude, and
  - phase;
- numerical experiments for a system supporting acoustic and gravity waves: considering errors and rates of convergence.

RK IMEX schemes

Consider the system

$$\mathbf{y}_t = \mathbf{s}(\mathbf{y}, t) + \mathbf{f}(\mathbf{y}, t),$$

with s slow terms and f fast terms.

RK IMEX schemes

The ν-stage RK IMEX scheme that steps system

$$\mathbf{y}_t = \mathbf{s}(\mathbf{y}, t) + \mathbf{f}(\mathbf{y}, t),$$

from time $t = n\Delta t$ to $t = (n+1)\Delta t$ is described by:

$$\mathbf{y}^{(j)} = \mathbf{y}^n + \Delta t \sum_{k=1}^{j-1} \tilde{a}_{jk} \mathbf{s}\left(\mathbf{y}^{(k)}, t + \tilde{c}_k \Delta t\right) + \Delta t \sum_{l=1}^{j} a_{jl} \mathbf{f}\left(\mathbf{y}^{(l)}, t + c_l \Delta t\right), \quad j = 1, \nu,$$

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t \sum_{j=1}^{\nu} \tilde{\omega}_j \mathbf{s}\left(\mathbf{y}^{(j)}, t + \tilde{c}_j \Delta t\right) + \Delta t \sum_{j=1}^{\nu} \omega_j \mathbf{f}\left(\mathbf{y}^{(j)}, t + c_j \Delta t\right)$$

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or by the double Butcher tableau:

$$\begin{array}{c|ccc} \tilde{c}_1 & \tilde{a}_{11} & \cdots & \tilde{a}_{1\nu} \\ \vdots & \vdots & & \vdots \\ \tilde{c}_\nu & \tilde{a}_{\nu 1} & \cdots & \tilde{a}_{\nu\nu} \\ \hline & \tilde{\omega}_1 & \cdots & \tilde{\omega}_\nu \end{array} \qquad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1\nu} \\ \vdots & \vdots & & \vdots \\ c_\nu & a_{\nu 1} & \cdots & a_{\nu\nu} \\ \hline & \omega_1 & \cdots & \omega_\nu \end{array}$$

where

$$\tilde{a}_{jk} = 0,\ k \geq j, \quad a_{jk} = 0,\ k > j;$$

$$\tilde{c}_j = \sum_{k=1}^{j-1} \tilde{a}_{jk}, \quad c_j = \sum_{k=1}^{j} a_{jk};$$

$$\sum \tilde{\omega}_j = \sum \omega_j = 1.$$

RK IMEX schemes

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we can easily identify:

- order of accuracy (explicit / implicit / overall) (e.g. Pareschi & Russo, 2005)
- time-level “splitting”: none / partial / complete
- implicit final stage for balanced solution (e.g. Ascher et al., 1997)
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We use a naming convention (Pareschi & Russo, 2005):

$$[\text{NAME}]k\,(s,\sigma,p)$$

for a k-order explicit scheme, with overall s implicit stages, σ explicit stages and p-order accuracy.

Linear analysis

We consider HEVI solution of a system of acoustic waves:

$$
\begin{aligned}
\frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} &= 0 \\
\frac{\partial w}{\partial t} + \frac{\partial P}{\partial z} &= 0 \\
\frac{\partial P}{\partial t} + c_s^2 \left(\underbrace{\frac{\partial u}{\partial x}}_{\text{explicit}} + \underbrace{\frac{\partial w}{\partial z}}_{\text{implicit}} \right) &= 0
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U-Forward,

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"UFPreF":
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but alternatively,

$$\frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = 0$$
$$\frac{\partial w}{\partial t} + \frac{\partial P}{\partial z} = 0$$
$$\frac{\partial P}{\partial t} \underbrace{\qquad}_{\text{explicit}} + \underbrace{c_s^2 \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right)}_{\text{implicit}} = 0$$

"UFPreB":
U-Forward,
P-Backward*

*Allusion to "forward-backward" scheme (Mesinger, 1977)

Solutions to the acoustic system

We rewrite the system as

$$\underline{\mathbf{F}}_t = -H_1\underline{\mathbf{F}}_x - H_2\underline{\mathbf{F}}_x - V\underline{\mathbf{F}}_z, \tag{2}$$

where subscripts denote partial derivatives, and

$$\underline{\mathbf{F}} = \begin{pmatrix} u \\ w \\ P \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad H_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ c_s^2 & 0 & 0 \end{pmatrix}, \quad V = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & c_s^2 & 0 \end{pmatrix}.$$

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Substituting (3) into (2) yields dispersion relation $\omega = \pm c_s\sqrt{k_x^2 + k_z^2}, 0$.

$\Rightarrow$ We know how the system truly amplifies between times t and $t+\Delta t$:

$$\underline{\mathbf{F}}(t+\Delta t) = A_0\underline{\mathbf{F}}(t) \quad \Rightarrow \quad A_0 = \mathrm{e}^{-i\omega\Delta t},$$

which has neutral amplitude $|A_0| = 1$ and phase $\theta_0 = -\omega\Delta t$.

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For analysing the time-stepping methods, we assume continuous spatial derivatives, i.e. from (3):

$$\underline{\mathbf{F}}_x = ik_x\underline{\mathbf{F}}, \quad \underline{\mathbf{F}}_z = ik_z\underline{\mathbf{F}}.$$

Then (2) becomes

$$\underline{\mathbf{F}}_t = -ik_x H_1\underline{\mathbf{F}} - ik_x H_2\underline{\mathbf{F}} - ik_z V\underline{\mathbf{F}}.$$

Numerical amplification factors for the acoustic system

Using a ν-stage RK IMEX scheme to solve

$$\underline{\mathbf{F}}_t = -ik_x H_1 \underline{\mathbf{F}} - ik_x H_2 \underline{\mathbf{F}} - ik_z V \underline{\mathbf{F}},$$

we can define numerical amplification factors for the $j = 1 : \nu$ sub-stages as

$$\underline{\mathbf{F}}^{(j)} = \mathbf{A}^{(j)} \underline{\mathbf{F}}^n$$

and for the final stage, from $t = n\Delta t$ to $t = (n+1)\Delta t$, as

$$\underline{\mathbf{F}}^{n+1} = \mathbf{A} \underline{\mathbf{F}}^n.$$

So, ...

Numerical amplification factors for the acoustic system

We construct amplification factors for a ν-stage RK IMEX scheme for:

UFPreF:

$$\begin{aligned}\mathbf{A}^{(j)} &= \mathbf{I} - \Delta t \sum_{k=1}^{j-1} \tilde{a}_{jk} ik_x (H_1 + H_2) \mathbf{A}^{(k)} - \Delta t \sum_{l=1}^{j} a_{jl} ik_z V \mathbf{A}^{(l)}, \quad j = 1, \nu; \\ \mathbf{A} &= \mathbf{I} - \Delta t \sum_{j=1}^{\nu} \tilde{w}_j ik_x (H_1 + H_2) \mathbf{A}^{(j)} - \Delta t \sum_{j=1}^{\nu} w_j ik_z V \mathbf{A}^{(j)},\end{aligned}$$

UFPreB:

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where $H_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $H_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ c_s^2 & 0 & 0 \end{pmatrix}$, $V = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & c_s^2 & 0 \end{pmatrix}$

Numerical amplification factors for the acoustic system

We construct amplification factors for a ν-stage RK IMEX scheme for:

UFPreF:

$$\mathbf{A}^{(j)} = \mathbf{I} - \Delta t \sum_{k=1}^{j-1} \tilde{a}_{jk}\, ik_x \,(H_1 + H_2)\,\mathbf{A}^{(k)} - \Delta t \sum_{l=1}^{j} a_{jl}\, ik_z\, V\,\mathbf{A}^{(l)}, \quad j = 1, \nu;$$

$$\mathbf{A} = \mathbf{I} - \Delta t \sum_{j=1}^{\nu} \tilde{w}_j\, ik_x \,(H_1 + H_2)\,\mathbf{A}^{(j)} - \Delta t \sum_{j=1}^{\nu} w_j\, ik_z\, V\,\mathbf{A}^{(j)},$$

UFPreB:

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Note: $\mathbf{A}$ is a 3×3 complex matrix — its eigenvalues $(\lambda_1, \lambda_2, \lambda_3)$ describe the amplification factors of the three system modes: two acoustic and one non-divergent

Linear analyses

We numerically generate values for $\mathbf{A}$ (and $\Rightarrow (\lambda_1, \lambda_2, \lambda_3)$) and consider:

- amplitude errors: $\Rightarrow$ instability?
- phase errors: $\Rightarrow$ implied direction of group velocity?

We consider the acoustic Courant number ($C_{s,x} \equiv c_s k_x \Delta t$, $C_{s,z} \equiv c_s k_z \Delta t$) ranges:

- $C_{s,x} \equiv \Delta t^* \in [0, 2.5]$
  since we anticipate the explicit scheme to limit stability at $C_{s,x} \approx 1$,
  $\Rightarrow$ time-step for resolving waves with c_s over given Δx; and
- $\dfrac{C_{s,z}}{\Delta t^*} = \dfrac{k_z}{k_x} \in [10^{-2}, 10^4]$,
  since we need stability to be ensured using Δt^* for the largest vertical Courant numbers, which depend on model resolution.

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  since we need stability to be ensured using Δt^* for the largest vertical Courant numbers, which depend on model resolution. Typically:

$$\Delta x \approx \begin{cases} 10^3\,\mathrm{m}, \text{ for high-res weather} \\ 10^5\,\mathrm{m}, \text{ for climate} \end{cases} \quad \text{and } \Delta z = \begin{cases} \Delta z_B \approx 10\ \mathrm{m}, & \text{model bottom} \\ \Delta z_T \approx 10^3 \mathrm{m}, & \text{model top} \end{cases}$$

$\Rightarrow$ to resolve the largest $C_{s,z}$ with Δt^*, we must consider

$$\frac{\max C_{s,z}}{\Delta t^*} = \frac{k_{z\max}}{k_{x\max}} = \frac{\Delta x}{\Delta z_{\min}} \le \begin{cases} 10^2 \text{ for high-res weather} \\ 10^4 \text{ for climate} \end{cases}$$

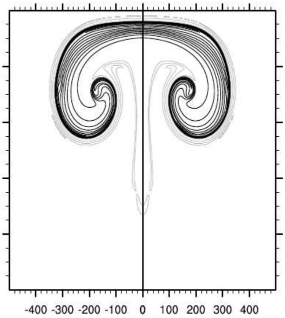
Example amplitude and phase errors: UJ3(1,3,2)

From Ullrich & Jablonowski (2012): "Strang carryover":

0	0					
0	0	0				
1	0	1	0			
1/2	0	1/4	1/4	0		
1	0	1/6	1/6	2/3	0	
1	0	1/6	1/6	2/3	0	0
	0	1/6	1/6	2/3	0	0

0	0					
1/2	1/2	0				
1/2	1/2	0	0			
1/2	1/2	0	0	0		
1/2	1/2	0	0	0	0	
1	1/2	0	0	0	0	1/2
	1/2	0	0	0	0	1/2

- SPP 3rd order;
- 1 implicit stage;
- 3 explicit stages;
- overall, 2nd order;
- time-levels: completely split;
- final stage: implicit.



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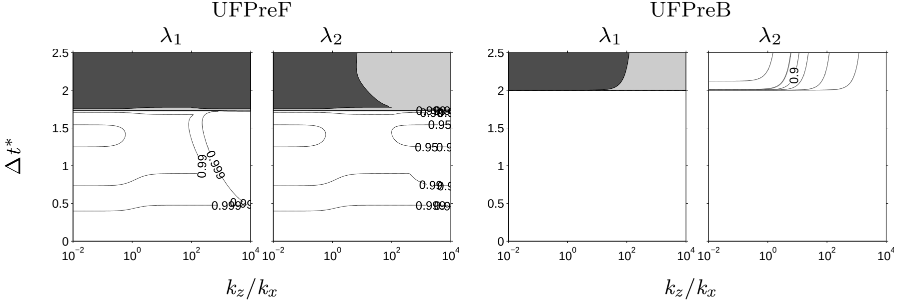
0	0	0				
1	0	1	0			
1/2	0	1/4	1/4	0		
1	0	1/6	1/6	2/3	0	
1	0	1/6	1/6	2/3	0	0
	0	1/6	1/6	2/3	0	0

0	0					
1/2	1/2	0				
1/2	1/2	0	0			
1/2	1/2	0	0	0		
1/2	1/2	0	0	0	0	
1	1/2	0	0	0	0	1/2
	1/2	0	0	0	0	1/2

Amplitudes of the two acoustic modes:



Amplitudes of the non-divergent mode remain neutral in the stable region.

Example amplitude and phase errors: UJ3(1,3,2)

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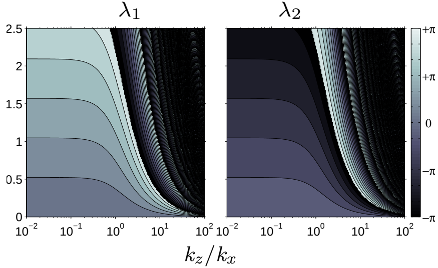
1	0	1/6	1/6	2/3	0	
1	0	1/6	1/6	2/3	0	0
	0	1/6	1/6	2/3	0	0

0	0					
1/2	1/2	0				
1/2	1/2	0	0			
1/2	1/2	0	0	0		
1/2	1/2	0	0	0	0	
1	1/2	0	0	0	0	1/2
	1/2	0	0	0	0	1/2

Phase of the two acoustic modes:

True phase:

- two acoustic modes: constant phase/group velocity wrt k_x or k_z;
- non-divergent mode: zero phase everywhere.



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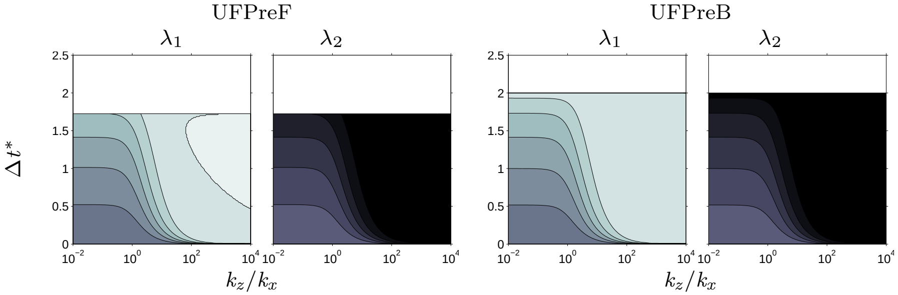
1/2	0	1/4	1/4	0		
1	0	1/6	1/6	2/3	0	
1	0	1/6	1/6	2/3	0	0
	0	1/6	1/6	2/3	0	0

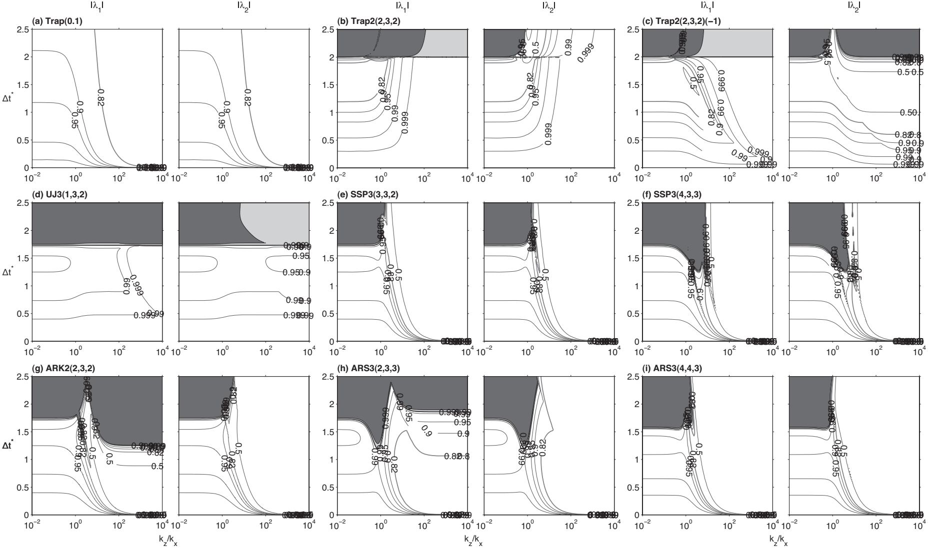
0	0					
1/2	1/2	0				
1/2	1/2	0	0			
1/2	1/2	0	0	0		
1/2	1/2	0	0	0	0	
1	1/2	0	0	0	0	1/2
	1/2	0	0	0	0	1/2

Phase of the two acoustic modes:



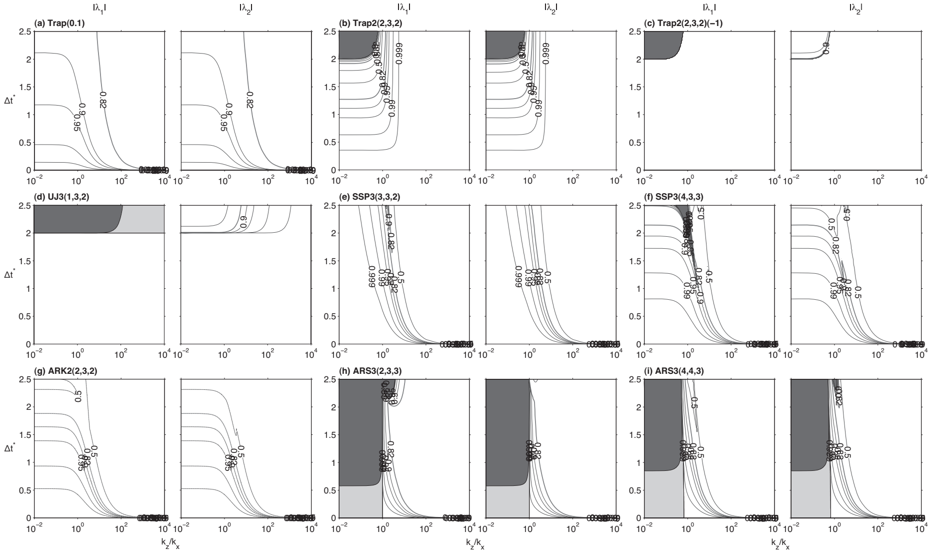
Phase of the non-divergent mode remains zero in the stable region.

Linear analyses: $|A|$ for acoustic modes (UFPreF)



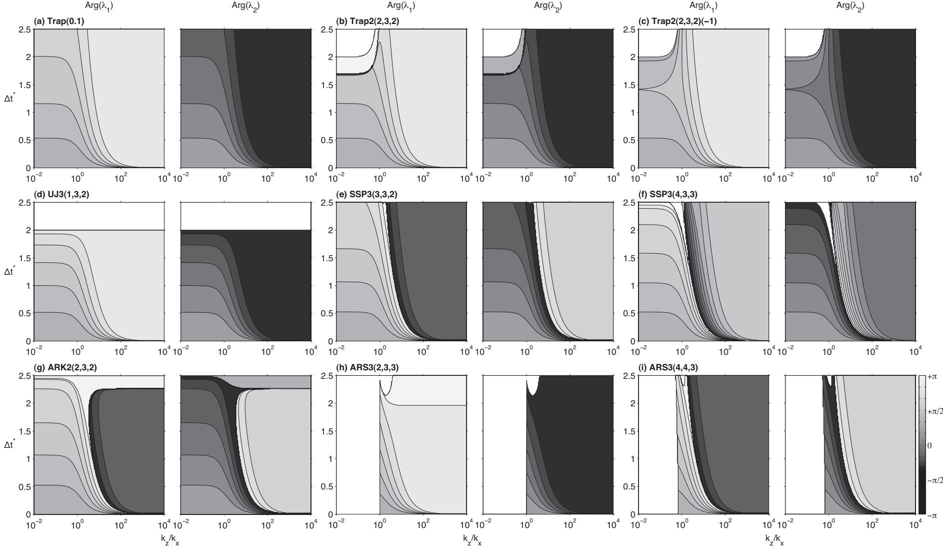
Good stability properties; some very strong damping; some asymmetry in acoustic modes

Linear analyses: $|A|$ for acoustic modes (UFPreB)



Generally, UFPreB $\Rightarrow$ greater stability than UFPreF, except "ARS" schemes

Linear analyses: θ for acoustic modes (UFPreB)



Good representation of phase for small Courant numbers; some evidence of group velocity reversal, but only close to limits of stability.

Numerical results (Weller et al., 2013)

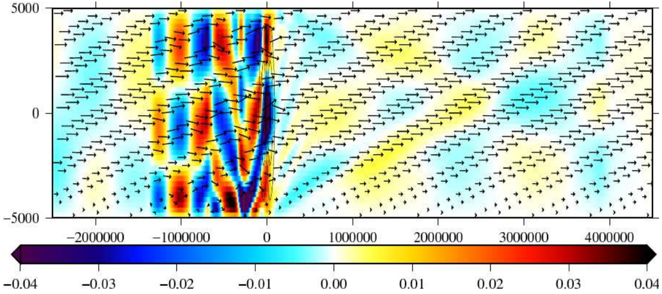
- Non-linear near-hydrostatic Boussinesq test (Durran & Blossey, 2012)
- Localized forcing ($\nabla \times \psi$) generating gravity waves in stratified shear flow

$$u_0(z) = 5 + z + 0.4(5 - z)(5 + z)\,\mathrm{m\,s}^{-1}$$

$$\psi(x,z,t) = \psi_0 \left(\frac{\pi x}{L_x}\right) \sin(\omega t) \exp\left[-\left(\frac{\pi x}{L_x}\right)^2 - \left(\frac{\pi z}{L_z}\right)^2\right] \mathrm{m}^2\,\mathrm{s}^{-1}$$

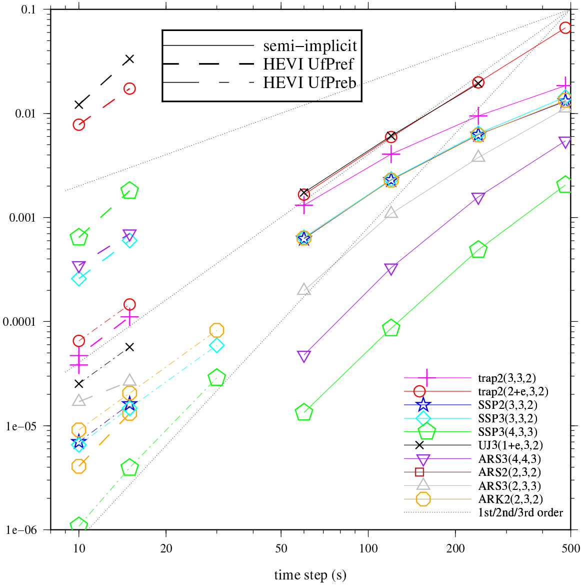
$$\omega = 1.25 \times 10^{-4}\,\mathrm{s}^{-1},\ L_x = 160\,\mathrm{km},\ L_z = 10\,\mathrm{km},\ \psi_0 = 10\,\mathrm{m}^2\,\mathrm{s}^{-1}$$

$$\Delta x = 10\,\mathrm{km},\ \Delta z = 250\,\mathrm{m}$$



a) Buoyancy (coloured), velocity vectors and forcing streamfunction

Numerical results: RMS buoyancy error (33.3h)



Indication of relative computational cost

	Number of RHS evaluations		Δt^*_{max}		$v/\Delta t^*_{\text{max}}$	
Scheme	Total (v)	Implicit (s)	UFPreF	UFPreB	UFPreF	UFPreB
Trap2(2,3,2)	3	2	2.00	2.00	1.5	1.5
UJ3(1,3,2)	4	1	1.73	2.00	2.31	2.00
SSP3(3,3,2)	4	3	1.70	2.48	2.35	1.61
SSP3(4,3,3)	5	4	0.89	1.39	5.62	3.60
ARK2(2,3,2)	3	2	1.25	>2.5	2.40	<1.20
ARS3(2,3,3)	3	2	1.19	0.00	2.52	∞
ARS3(4,4,3)	4	4	1.54	0.00	2.60	∞

- v and s: number of RHS computations (total and implicit respectively) required per Δt;
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RK IMEX schemes from the literature have been analysed and demonstrate:

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- spurious reversal of group velocities can be avoided;
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- "Trap2(2,3,2)" and "UJ3(1,3,2)" — both already used in atmospheric models (Wood et al., 2013, QJRMS accepted; Ullrich & Jablonowski, 2012) — perform consistently well (linear analyses and numerical experiments);
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Horizontally-explicit vertically-implicit (HEVI) time-stepping methods for NWP and climate models

Sarah-Jane Lock

Thanks for your attention!