

Numerical analyses of explicit time-stepping methods for use in atmospheric forecasting models

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With thanks to: Alan Gadian (Leeds); Nigel Wood, Andrew Staniforth (UK Met Office); Hilary Weller (Reading)

Talk outline

- Some background
- Motivation for analyses
- Description of analysis framework
- Outline schemes for analysis
- Present some results of numerical and empirical analyses
- Conclusions and future work

GUNG-HO! (aka UM* dynamical core project)

G	lobally
U	niform
N	ext
G	eneration
H	ighly
O	ptimized

UK Met Office; Science & Technology Facilities Centre;
Universities: Bath, Exeter, Imperial, Leeds, Manchester, Reading

Objective:

To research, design and develop a new dynamical core suitable for operational, global and regional, weather and climate simulation on massively parallel computers of the size envisaged over the coming 20 years.

Outline:

Phase 1 (2011-2013): exploration of alternative methods to address identified barriers to good performance on massively parallel computers in current UM:

- quasi-uniform horizontal grids
- conservative transport schemes
- time-stepping methods
- 2D testing

Phase 2 (2013 -2016): selected methods from Phase 1 will be combined with exploration of the vertical aspects and extended into a 3D model for extensive testing

Motivation for re-examining time-stepping

Problem:

Atmospheric (dry) dynamical equations: compressible, non-hydrostatic

- => include very wide range of wave frequencies:
acoustic, gravity, advection, Coriolis
- => inherently *stiff* system

And ... stiffness is compounded in the numerical model:

Aim for future (2020) global model forecasts is for
horizontal grid-spacing of $\Delta x \sim 1$ km

while nature of dynamics *already* requires

variable vertical grid-spacing of $\Delta z \sim 10$ m (near surface)
to $\Delta z \sim 1$ km (near top)

Currently ...

Current UM uses 3D semi-implicit time-stepping:

- handles fastest waves with implicit method
 - ⇒ no stability constraints associated with fastest waves
 - ⇒ achieve (very time-constrained) forecasts with long time-step

BUT requires solution of a 3D Helmholtz problem

⇒ requires (multiple) global communications each time-step

-> Q: looking to future (2020+) massively parallel architectures, can solvers be relied on to provide good scalability?

工合 GUNG-HO: Rob Scheichl, Bath University

Alternatively: consider explicit-based methods (no global communications)

How can explicit methods help?

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1D semi-implicit
⇒ tridiagonal problem
No inter-processor comms

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Explicit

=> accept stability constraint
assoc. with fastest horizontal
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Workshop, 25 June 2012



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Horizontally-explicit vertically-implicit
“HEVI” approach

variable vertical grid spacing of $\Delta z \sim 10\text{ m}$ (near surface)

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Analysis framework – exact system:

- Consider the 3D linear equation set (incl. important processes – advection, Earth's rotation, pressure-gradient force, gravity and acoustic waves):

$$\begin{aligned}u_t + Uu_x + Vu_y + Wu_z - fv + \Phi_x &= 0, \\v_t + Uv_x + Vv_y + Wv_z + fu + \Phi_y &= 0, \\w_t + Uw_x + Vw_y + Ww_z + \Phi_z &= 0, \\\Phi_t + U\Phi_x + V\Phi_y + W\Phi_z + c_g^2(u_x + v_y) + c_a^2w_z &= 0,\end{aligned}$$

- Can consider coupled equations to be represented by the single equation:

$$F_t + i\tilde{\omega}F = 0$$

- Enhance the problem to reflect the high (K_V) and low (K_H) frequency contributions:

$$\frac{\partial F}{\partial t} + iK_H F + iK_V F = 0$$

- Exact system has solution $F(t) = F_0 e^{-i(K_H + K_V)t}$

which yields amplification factor, $A_0 = F(t + \Delta t)/F(t)$: $A_0 = e^{-i(K_H + K_V)\Delta t}$

with amplitude $|A_0| = 1$ and phase $\theta_0 = -(K_H + K_V)\Delta t$,

and group velocity $d\omega/dk = -d(K_H + K_V)/dk$

Analysis framework – discrete system:

- For the discrete system, construct amplification factors from

$$F^{n+1} = AF^n \quad \text{where} \quad A = |A| e^{i\theta} = |A| (\cos \theta + i \sin \theta)$$

Hence, can extract numerical amplitude and phase by

$$|A| = \{\Re(A)^2 + \Im(A)^2\}^{1/2}$$
$$\theta = \arctan \left(\frac{\Im(A)}{\Re(A)} \right).$$

Stability: $|A| > 1 \Leftrightarrow$ amplifying = unstable

$|A| < 1 \Leftrightarrow$ damping = stable

Phase: $\theta_{\text{num}} > \theta_{\text{exact}} \Leftrightarrow$ accelerating

$\theta_{\text{num}} < \theta_{\text{exact}} \Leftrightarrow$ decelerating

Group velocity: re-write as $A = e^{\tilde{K}_\Im \Delta t} e^{-i\tilde{K}_\Re \Delta t}$, then $\tilde{\omega} = -\tilde{K}_\Re$ and

$$\frac{d\tilde{\omega}/dk}{d\omega/dk} = \frac{d\theta/dK}{d\theta_0/dK}$$

For “good” behaviour, require that *direction* (sign) is always correct

Analysis framework - comparison:

- Compare exact and discrete systems

1. Examine performance over small Courant numbers

$$\text{i.e. } |K_H \Delta t|, |K_V \Delta t| < 2$$

Looking for stability and accuracy (not too damping, good phase)

2. Examine performance over large (vertical) Courant numbers

$$\text{i.e. } 0 < |K_V \Delta t| < O(100)$$

reflecting range of Δz , e.g. $\frac{\Delta x}{100} \lesssim \Delta z \lesssim \Delta x$ ($\Delta x \sim 1$ km)

Looking for stability and “good” behaviour (group velocity)

3. Consider errors accumulated over multiple steps:

$$\Delta t_{\text{implicit}} / \Delta t_{\text{explicit}} = O(10)$$

Hence, over $M=O(10)$ steps, fair comparison with SI is

$$|A_{\text{implicit}}| \text{ versus } |A_{\text{explicit}}|^M \\ \theta_{\text{implicit}} \text{ versus } M\theta_{\text{explicit}}$$

“Control” scheme: CN(ϵ)

Current UM semi-implicit scheme:

In simplest sense, equivalent to off-centered Crank-Nicholson, “CN(ϵ)”,

$$F^{n+1} = F^n - iK\Delta t \left\{ \frac{(1-\epsilon)}{2} F^n + \frac{(1+\epsilon)}{2} F^{n+1} \right\}$$

with off-centering parameter: $\epsilon = 0.1$

Analysis reveals the amplification factor $A = \frac{1 - \frac{1-\epsilon}{2}iK\Delta t}{1 + \frac{1+\epsilon}{2}iK\Delta t}$

which has amplitude $|A|^2 = 1 - \frac{\epsilon(K\Delta t)^2}{1 + \left(\frac{1+\epsilon}{2}\right)^2 (K\Delta t)^2}$

which is always stable for $\epsilon > 0$;

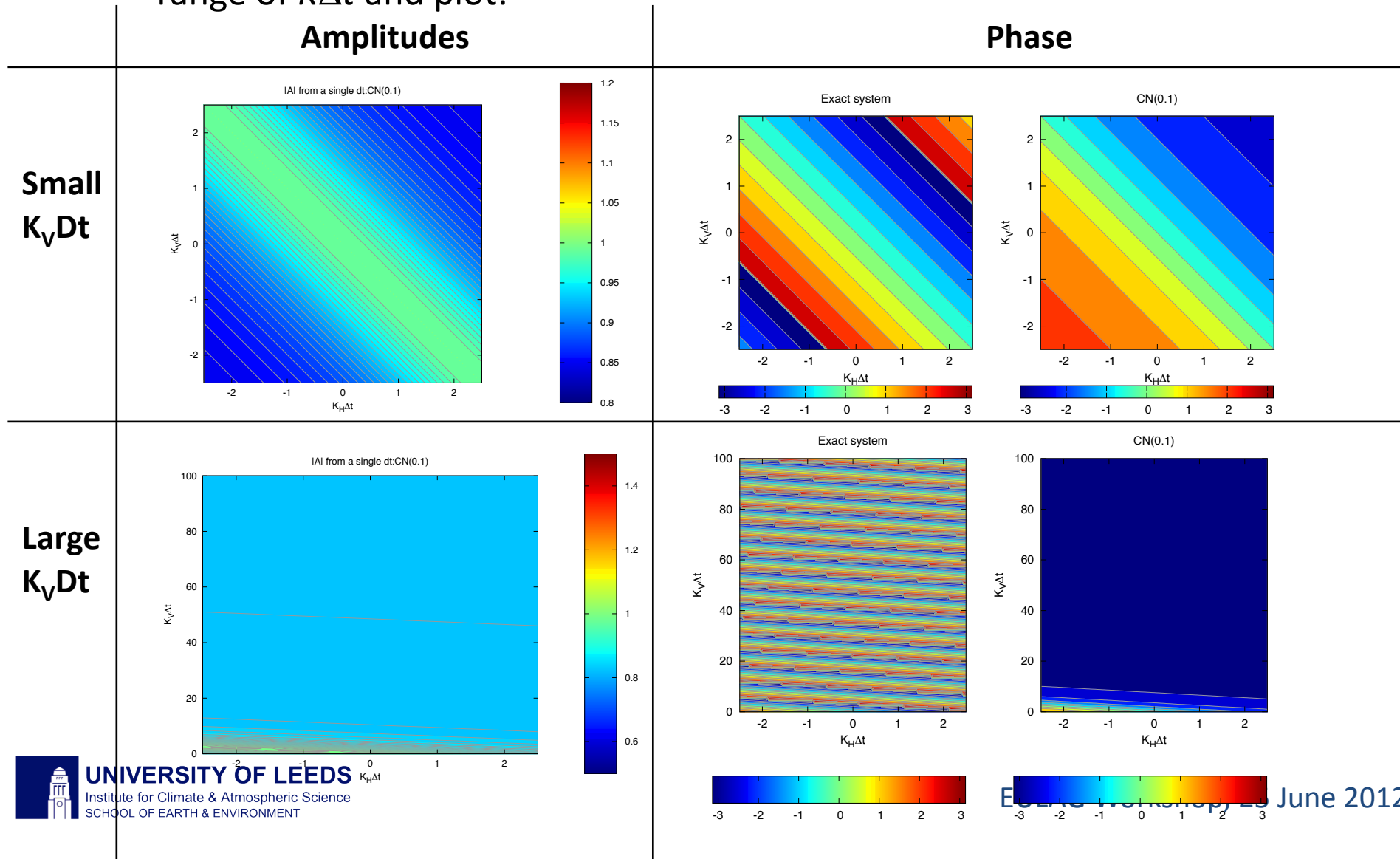
and phase $\theta \approx -K\Delta t \left(1 - \frac{1+3\epsilon^2}{12} (K\Delta t)^2 \right)$

which is always decelerating for $|\epsilon| > 0$.

“Control” scheme: CN(0.1)

Alternative (graphical) approach for considering scheme characteristics

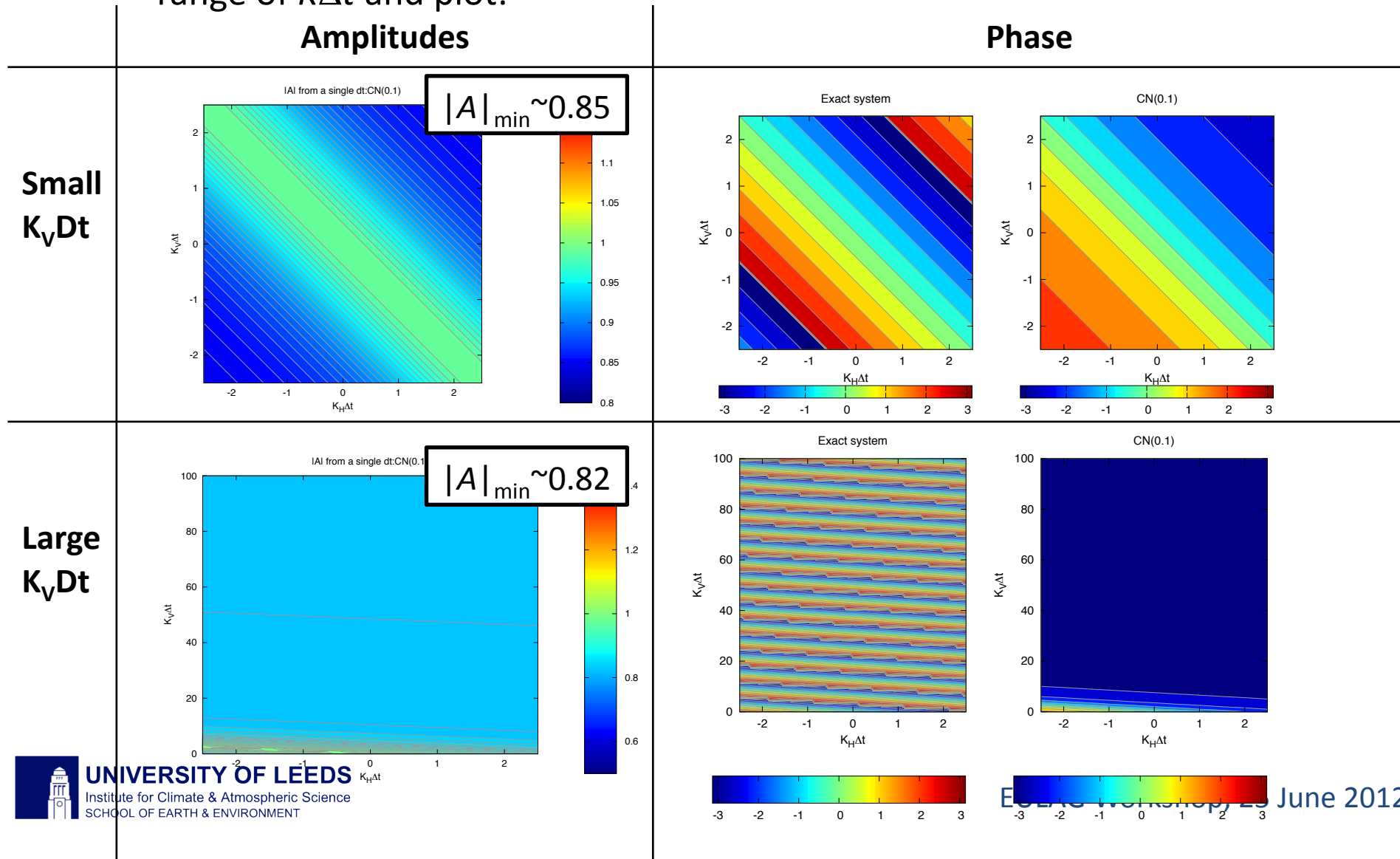
Generate the amplification factors empirically (e.g. Matlab), computing for range of $K\Delta t$ and plot:



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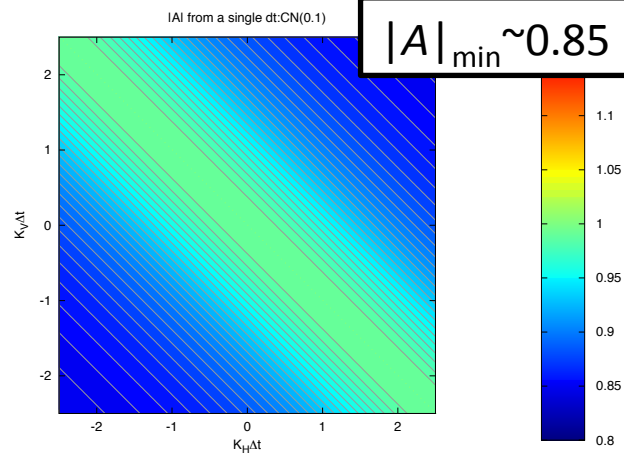
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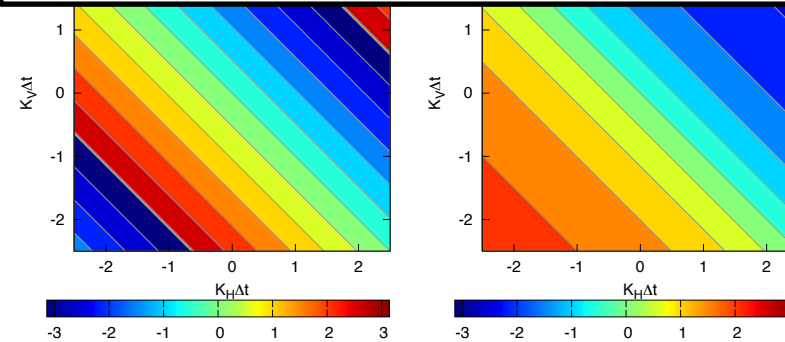
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Amplitudes

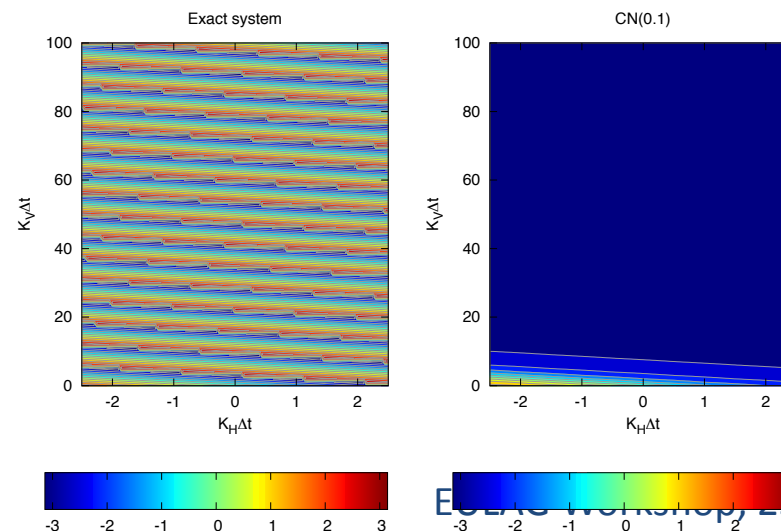
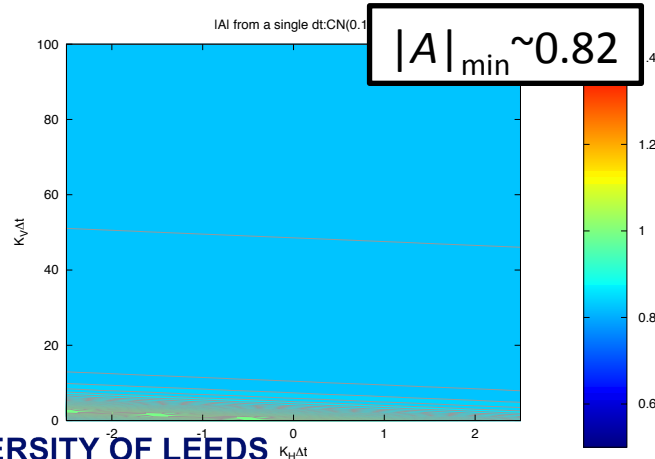
Small $K_V\Delta t$



Phase: for any given $K\Delta t$, numerical scheme yields smaller (magnitude) phase, i.e. rotates more slowly around the unit circle, than exact \Rightarrow always decelerating



Large $K_V\Delta t$



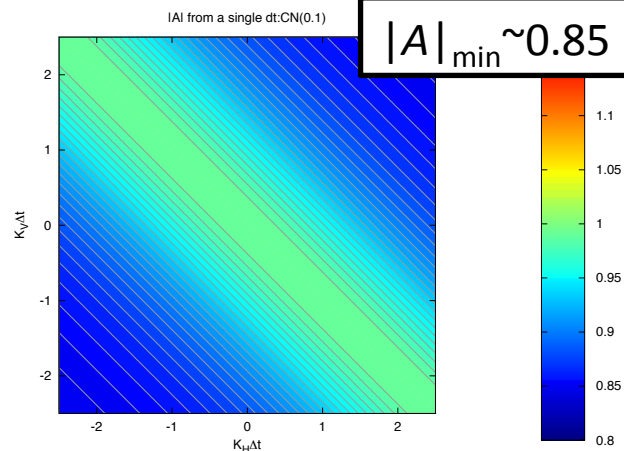
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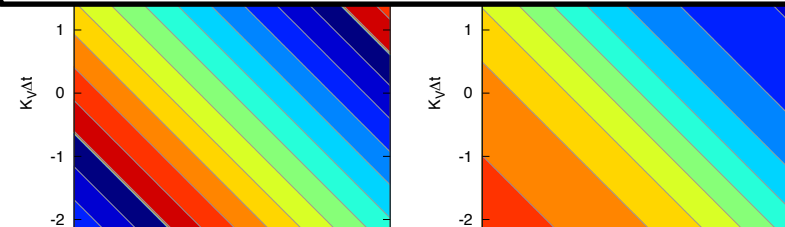
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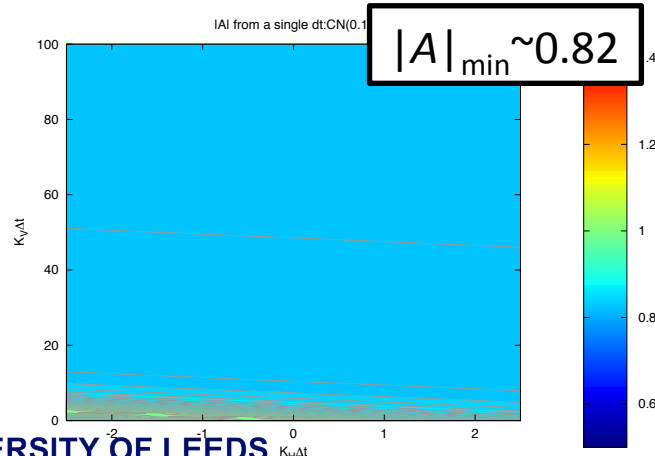
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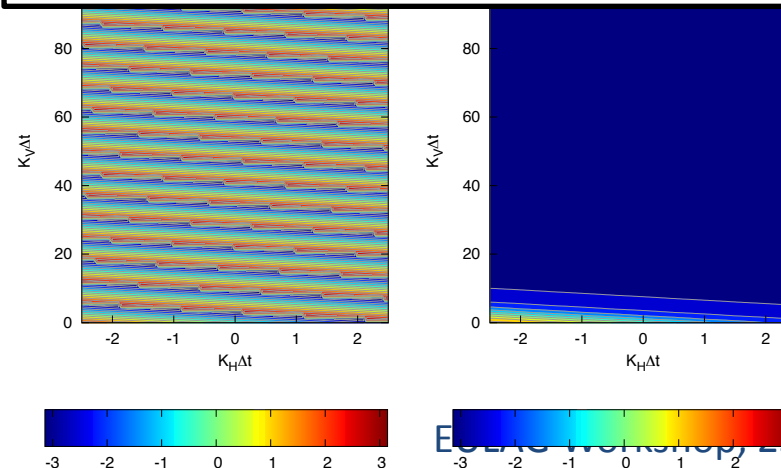
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Large $K_V \Delta t$



Group velocity: $d\omega/dk \sim d\theta/dK$
For “good” behaviour, signs must agree \Rightarrow requires that sign of *gradients* must agree



Potential new schemes:

- Initially, considered multi-step (e.g. leapfrog) schemes, but suffer computational (parasitic) modes
- Currently, focusing on single-step, multi-stage (Runge-Kutta) schemes
- Runge-Kutta (RK) IMEX schemes can be efficiently & usefully described by double Butcher tableau, e.g.

3rd-order RK (RK3) combined with CN(ε) presented

in full:

$$\begin{aligned} F^{(1)} &= F^n \\ F^{(2)} &= F^n - \frac{1}{3}iK_H\Delta t F^{(1)} \\ F^{(3)} &= F^n - \frac{1}{2}iK_H\Delta t F^{(2)} \\ F^* &= F^n - iK_H\Delta t F^{(3)} \\ F^{n+1} &= F^* - iK_V\Delta t \left\{ \frac{(1-\epsilon)}{2}F^* + \frac{(1+\epsilon)}{2}F^{n+1} \right\} \end{aligned}$$

and as double Butcher tableau:

Explicit tableau	Implicit tableau
$ \begin{array}{c ccc} 0 & 0 & & \\ 1/3 & 1/3 & 0 & \\ 1/2 & 0 & 1/2 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{array} $	$ \begin{array}{c cccc} 0 & 0 & & & \\ 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & (1-\epsilon)/2 \end{array} $
$ \begin{array}{c ccc} & 0 & 0 & 1 \\ & 0 & 0 & 1 \end{array} $	$ \begin{array}{c cccc} & 0 & 0 & 0 & (1+\epsilon)/2 \\ & 0 & 0 & 0 & (1+\epsilon)/2 \end{array} $

Potential new schemes:

RK IMEX combinations based on:

- 2nd-order RK (RK2)
- 3rd-order RK (RK3)
- from literature: SSP (strong stability preserving),
DIRK (diagonally implicit RK)

Identify them as

- fully “split”
- unsplit

0	0					0	0								
1/3	1/3	0				0	0	0							
1/2	0	1/2	0			0	0	0	0						
1	0	0	1	0		0	0	0	0			0			
1	0	0	1	0	0	1	0	0	0	(1 - ε) / 2	(1 + ε) / 2				
	0	0	1	0	0		0	0	0	(1 - ε) / 2	(1 + ε) / 2				

RK3-based schemes (fully split)

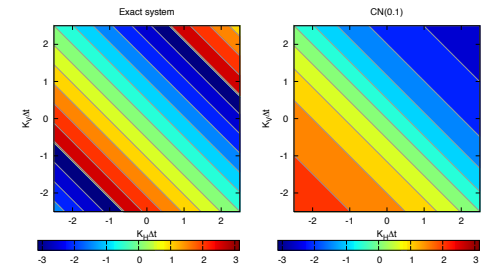
RK3-CN(0)

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

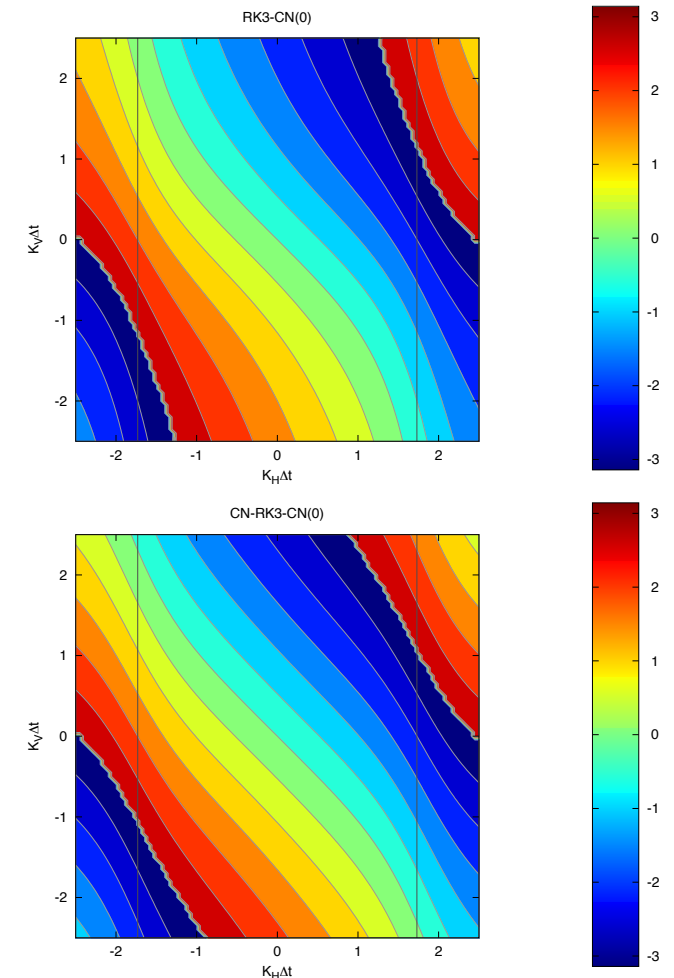
CN(0)-RK3-CN(0) yields better phase representation for small Courant numbers

CN(0)-RK3-CN(0)

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



Phase (small Courant numbers)



RK2-based schemes (unsplit)

ENDG-2

2-iteration Heun-CN + initial stage

0	0	0	0	0
δ_H	δ_H	0	0	0
1	$\frac{1}{2}$	$\frac{1}{2}$	0	0
1	$\frac{1}{2}$	0	$\frac{1}{2}$	0
	$\frac{1}{2}$	0	$\frac{1}{2}$	0

0	0	0	0	0
δ_V	$\delta_V \frac{(1-\alpha)}{2}$	$\delta_V \frac{(1+\alpha)}{2}$	0	0
1	$\frac{1}{2}$	0	$\frac{1}{2}$	0
1	$\frac{1}{2}$	0	0	$\frac{1}{2}$
	$\frac{1}{2}$	0	0	$\frac{1}{2}$

Initial stage: α = off-centering parameter
 $\delta_H, \delta_V = 0, 1$

For pure explicit initial stage:

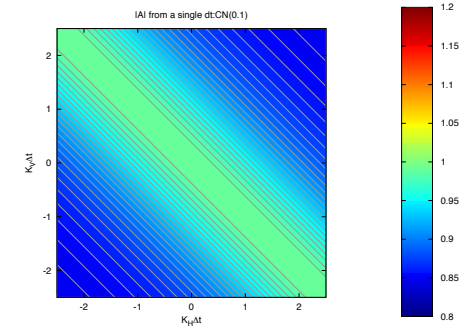
- stability conditional (only) on $K_H \Delta t$

For implicit initial stage:

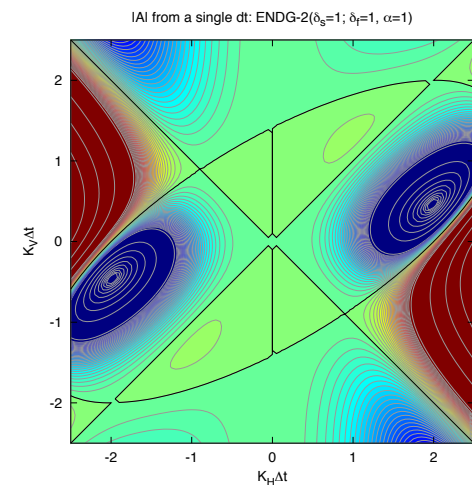
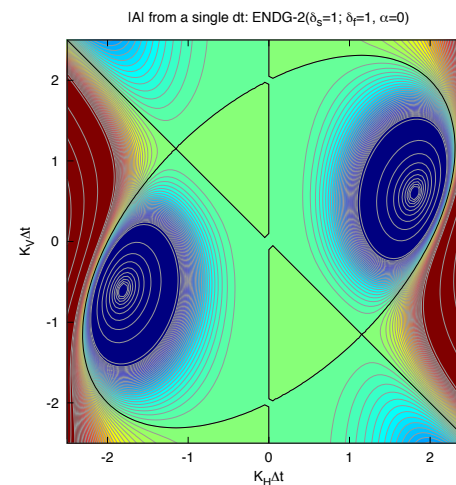
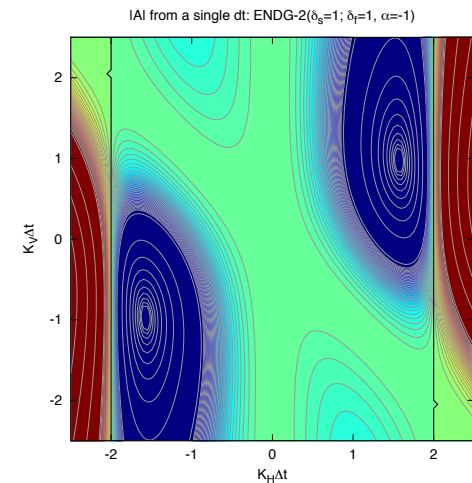
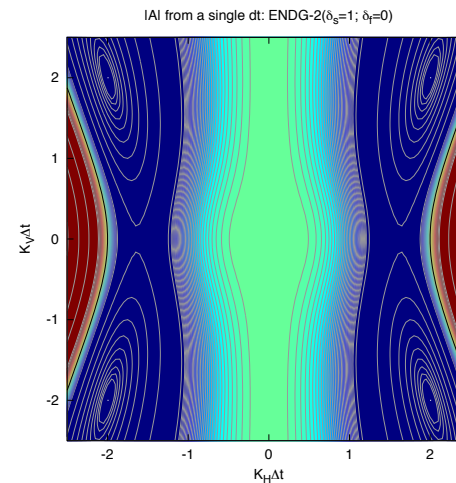
- regions of instability extending to $K_H \Delta t = 0$

Not shown here: for large $K_V \Delta t$, all have

$$|A| \rightarrow 1$$



Amplitudes (small Courant numbers)



RK2-based schemes (unsplit)

ENDG-4

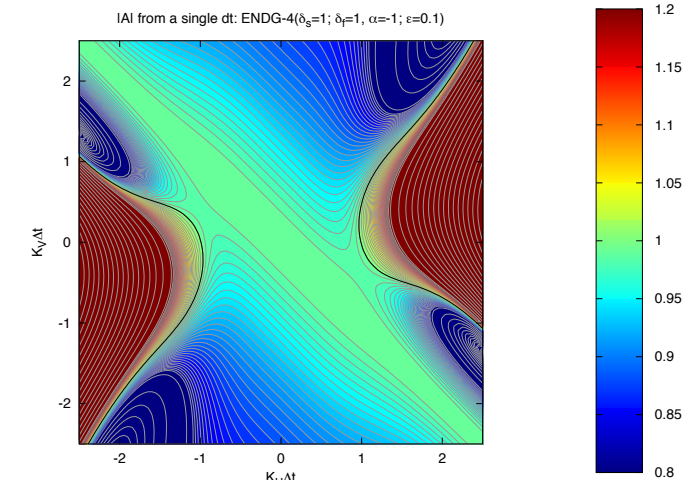
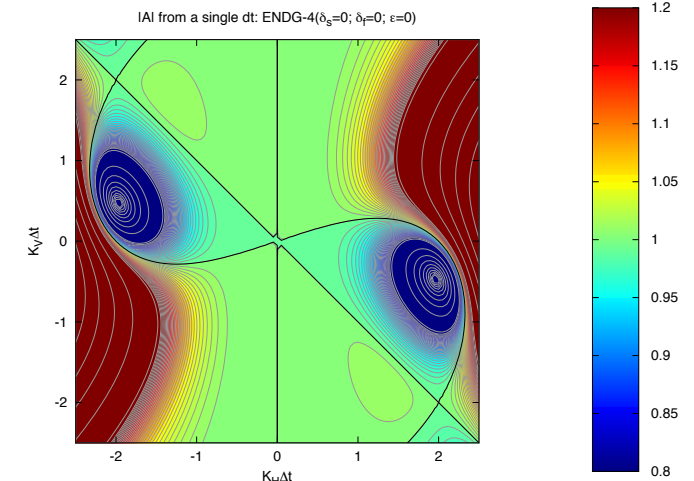
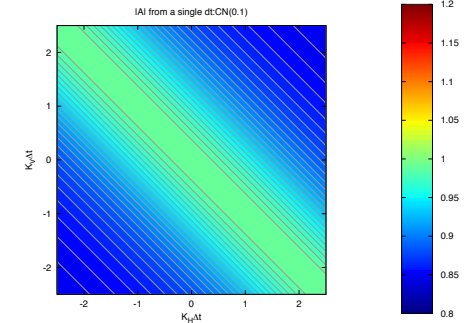
4-iteration Heun-CN + initial stage

0	0	0	0	0	0	0	0	0	0	0	0	0	0
δ_H	δ_H	0	0	0	0	0	δ_V	$\delta_V \frac{1-\alpha}{2}$	$\delta_V \frac{1+\alpha}{2}$	0	0	0	0
1	$\frac{1-\epsilon}{2}$	$\frac{1+\epsilon}{2}$	0	0	0	0	1	$\frac{1-\epsilon}{2}$	0	$\frac{1+\epsilon}{2}$	0	0	0
1	$\frac{1-\epsilon}{2}$	0	$\frac{1+\epsilon}{2}$	0	0	0	1	$\frac{1-\epsilon}{2}$	0	0	$\frac{1+\epsilon}{2}$	0	0
1	$\frac{1-\epsilon}{2}$	0	0	$\frac{1+\epsilon}{2}$	0	0	1	$\frac{1-\epsilon}{2}$	0	0	0	$\frac{1+\epsilon}{2}$	0
1	$\frac{1-\epsilon}{2}$	0	0	0	$\frac{1+\epsilon}{2}$	0	1	$\frac{1-\epsilon}{2}$	0	0	0	0	$\frac{1+\epsilon}{2}$
	$\frac{1-\epsilon}{2}$	0	0	0	$\frac{1+\epsilon}{2}$	0		$\frac{1-\epsilon}{2}$	0	0	0	0	$\frac{1+\epsilon}{2}$

Yields some weird and whacky stability constraints!

- “best”-looking combination from pure explicit initial stage and small off-centering in later stages

Amplitudes (small Courant numbers)



SSP-RK schemes (partially-split)

Pareschi & Russo (2005, J. Sci. Comp.)

Amplitudes (small Courant numbers)

SSP2(2,2,2)

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array} \quad \begin{array}{c|cc} \gamma & \gamma & 0 \\ 1-\gamma & 1-2\gamma & \gamma \\ \hline & 1/2 & 1/2 \end{array}$$

SSP2(3,3,2)

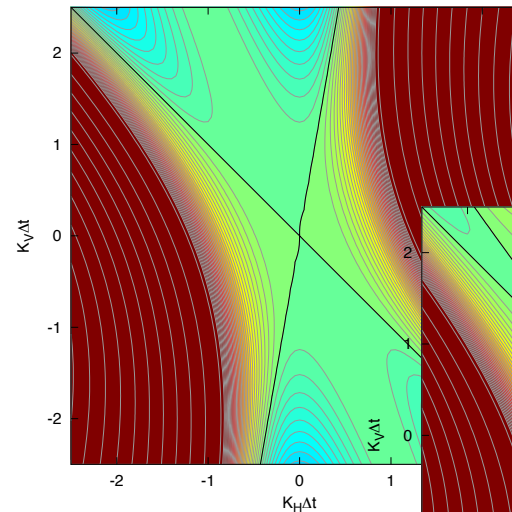
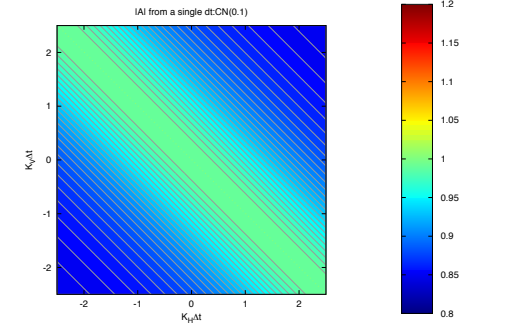
$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & 1/2 & 1/2 & 0 \\ \hline & 1/3 & 1/3 & 1/3 \end{array} \quad \begin{array}{c|ccc} 1/5 & 1/5 & 0 & 0 \\ 3/10 & 1/10 & 1/5 & 0 \\ 1 & 1/3 & 1/3 & 1/3 \\ \hline & 1/3 & 1/3 & 1/3 \end{array}$$

SSP3(3,3,2)

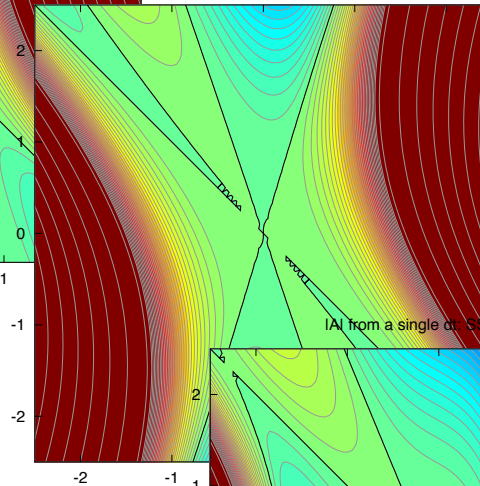
$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1/2 & 1/4 & 1/4 & 0 \\ \hline & 1/6 & 1/6 & 2/3 \end{array} \quad \begin{array}{c|cccc} \gamma & \gamma & 0 & 0 \\ 1-\gamma & 1-2\gamma & \gamma & 0 \\ 1/2 & 1/2-\gamma & 0 & \gamma \\ \hline & 1/6 & 1/6 & 2/3 \end{array}$$

SSP (RK2 & RK3) schemes all indicate some instability for small $K_H\Delta t$

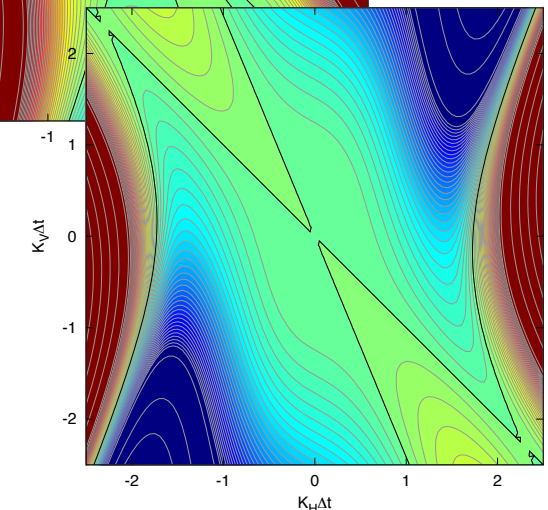
$$\gamma = 1 - \frac{1}{\sqrt{2}}$$



|A| from a single dt: SSP2(3,3,2)



|A| from a single dt: SSP3(3,3,2)



EULAG Workshop, 25 June 2012

Conclusions & Future work

Simple 1D analyses have

- identified good candidate schemes, e.g. CN-RK3-CN
- highlighted potential concerns (instabilities/poor behaviour) of some established schemes, e.g. (not shown here) leapfrog-CN($\varepsilon > 0$) instability (demonstrated in Durran & Blossey, 2012)

BUT experience suggests:

- fully split schemes (e.g. CN-RK3-CN) introduce errors due to the splitting
- from recent testing, some RK IMEX schemes are more stable in practice than indicated by 1D analyses

➔ Next steps:

- Extend analyses to
 - 1D coupled (atmospheric) system
 - 2D coupled system
- Perform numerical testing of some RK IMEX schemes (H. Weller, Reading)

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Thanks for your attention!