Time splitting methods for the compressible Euler equation using Runge-Kutta and peer methods

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OVERVIEW

- Multirate time integration for atmospheric dynamics
- Generalised split-explicit Runge-Kutta methods
- Split-explicit peer methods
- Order and Stability
- Relation to exponential integrators
- Application to nonlinear atmospheric dynamics

SPLITTING METHODS

- Motivation:
  - Atmospheric models contain slow (advection) and fast (gravity and sound wave) modes.
  - Metheorologically important: Medium and low frequencies
  - CFL-number of fast waves resticts time step
  - Pure advection allows larger stepsizes

$$CFL_{ADVECTION}/CFL_{SOUND} \leq 1/10$$

- Apply multirate strategy
  - slow processes are integrated by large time steps
  - fast processes are integrated by small time steps where the advective tendencies are fixed

CLASSICAL RUNGE-KUTTA METHODS

- Runge-Kutta method for integration of $y' = f(y)$ uses internal stages

$$Y_{ni} = y_n + h \sum_j a_{ij} f(Y_{nj})$$

- Stage is interpreted as the exact solution of $z' = c := \sum_j a_{ij} f(Y_{nj})$

$$\begin{aligned} Z_{ni}(0) &= y_n \\ Z'_{ni}(\tau) &= \sum_j a_{ij} f(Y_{nj}) \\ Y_{ni} &= Z_{ni}(h). \end{aligned}$$

RUNGE-KUTTA PARTITIONED METHODS

- Extend to a partitioned equation $y' = f(y) + g(y)$.
- In each stage compute $Z_{ni}(\tau)$ as solution of $Z'(\tau) = F + g(Z(\tau))$, where $F = \text{const}$ are the fixed slow tendencies

$$\begin{aligned} Z_{ni}(0) &= y_n \\ Z'_{ni}(\tau) &= \sum_j a_{ij} f(Y_{nj}) + c_i g(Z_{ni}(\tau)) \\ Y_{ni} &= Z_{ni}(h). \end{aligned}$$

- Split-explicit RK3-method (widely used in numerical weather prediction):

Coefficients $A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$, nodes $c = (0, 1/3, 1/2, 1)^T$

RUNGE-KUTTA PARTITIONED METHODS

- We generalise the exact integration procedure in two directions:
  - arbitrary starting points based on preceeding stages

$$Z_{ni}(0) = y_n + \sum_j \alpha_{ij}(Y_{nj} - y_n)$$

  - increments in the constant term F based on preceeding stages

$$Z'_{ni}(\tau) = \frac{1}{h}\sum_j \gamma_{ij}(Y_{nj} - y_n) + \sum_j \beta_{ij} f(Y_{nj}) + d_i g(Z_{ni}(\tau))$$

- In order to balance the processes f and g in each RHS we demand

$$d_i = \sum_j \beta_{ij}.$$

RUNGE-KUTTA PARTITIONED METHODS

- The complete method is given by

$$
\begin{aligned}
Z_{ni}(0) =& y_n + \sum_j \alpha_{ij}(Y_{nj} - y_n) \\
Z'_{ni}(\tau) =& \frac{1}{h} \sum_j \gamma_{ij}(Y_{nj} - y_n) + \sum_j \beta_{ij} f(Y_{nj}) + d_i g(Z_{ni}(\tau)) \\
Y_{ni} =& Z_{ni}(h) \\
y_{n+1} =& Y_{n,s+1}.
\end{aligned}
$$

- $g = 0 \Rightarrow$ underlying RK method

$$
\begin{aligned}
Y =& \mathbb{1} \otimes y_n + ((\boldsymbol{\alpha} + \Gamma) \otimes I)(Y - \mathbb{1} \otimes y_n) + h(\boldsymbol{\beta} \otimes I) f(Y) \\
Y =& \mathbb{1} \otimes y_n + h((I - \boldsymbol{\alpha} - \Gamma)^{-1} \boldsymbol{\beta} \otimes I) f(Y) \\
\Rightarrow A =& (I - \boldsymbol{\alpha} - \Gamma)^{-1} \boldsymbol{\beta} =: R\beta
\end{aligned}
$$

DERIVATION OF ORDER CONDITIONS

Expand numerical solution in a Taylor series.
Note: Z_{ni} is a function of τ and h. Define
$G(Y_{ni})^{(k)} := \frac{\partial^k}{\partial h^k}\Big|_{h=0} G(Y_{ni})$, $G(Z_{ni})^{(k,l)} := \frac{\partial^{k+l}}{\partial \tau^k \partial h^k}\Big|_{\tau=h=0} G(Z_{ni})$

- Recursion for derivatives of Y_{ni}:

$$Y_{ni} = Z_{ni}(h,h) \quad \Rightarrow \quad Y_{ni}^{(k)} = \sum_{l=0}^{k} \binom{k}{l} Z_{ni}^{(l,k-l)}.$$

- 3 different recursions for derivatives of Z_{ni}:

$$\begin{aligned}
Z_{ni}^{(0,l)} &= \sum_j \alpha_{ij} Y_{nj}^{(l)} \\
Z_{ni}^{(1,l)} &= \frac{1}{l+1} \sum_j \gamma_{ij} Y_{nj}^{(l+1)} + \sum_j \beta_{ij} f(Y_{nj})^{(l)} + d_i g(Z_{ni})^{(0,l)} \\
\Rightarrow \quad Z_{ni}^{(k,l)} &= d_i g(Z_{ni})^{(k-1,l)}, \quad k \geq 2.
\end{aligned}$$

ORDER CONDITIONS

- The recursion leads to following order conditions for 3rd order
  - four classical order conditions

$$b^T \mathbb{1} = 1, b^T c = 1/2, b^T c^2 = 1/3, b^T Ac = 1/6$$

  - and five additional order conditions

$$\begin{aligned}
\tilde{b}(c + \tilde{c}) &= 1 \\
\tilde{b}(I + \boldsymbol{\alpha})Ac &= 1/3 \\
3\tilde{b}(\boldsymbol{\alpha} + \Gamma/2)RD(c + \tilde{c}) + \tilde{b}^T D(c + 2\tilde{c}) &= 1 \\
b^T RD(c + \tilde{c}) &= 1/3 \\
\tilde{b}^T (c^2 + \tilde{c}^2 + c \cdot \tilde{c}) &= 1
\end{aligned}$$

where we use $\tilde{c} := \boldsymbol{\alpha} c$ and $\tilde{b} = e_{s+1}^T RD$.

CONSTRUCTION OF METHODS

- we search for a 3 stage 3rd order method
- 12 free parameters for 9 order conditions
- No 3rd order method for $\alpha = \Gamma = 0$ (classic splitting like RK3)
- Parametrization: Eliminate 8 order conditions
  4 free parameters and 1 complex nonlinear condition remain
- Exhaustive search of parameter space for methods with good stability properties
- We found several methods. Here: WKG
- Compare with conventional split–explicit methods (RK3) and exponential integrators (CF3)

PEER METHODS

- Peer method for integration of $y' = f(y)$ can be written compactly

$$Y_n = BY_{n-1} + hAF_{n-1} + hRF_n$$

with notations

$$Y_n := (Y_{ni})_{i=1}^s \in \mathbb{R}^{s\times n} \qquad \text{with} \qquad Y_{ni} \approx y(t_{ni}) = y(t_n + c_i h),$$
$$F_n := \Big(f(t_{ni}, Y_{ni})\Big)_{i=1}^s \in \mathbb{R}^{s\times n}$$

and $A, B, R \in \mathbb{R}^{s\times s}$ where R is a strictly lower triangular matrix

- Each stage is a linear multistep method
- Cyclic recurrence equals the stage number
- Each stage has maximal order, order theory from linear multistep methods
- Starting procedure necessary (like BDF)
- Various generalizations (parallel in time, linear implicit)

PEER PARTITIONED METHODS

- The i-th stage of a split-explicit peer method is given by:

$$Z(0) = \sum_{j=1}^{s} b_{ij} Y_{n-1,j} + \sum_{j=1}^{i-1} s_{ij} Y_{nj},$$

$$Z'(\tau) = \frac{1}{\alpha_i}\left(\sum_{j=1}^{s} a_{ij} F_{n-1,j} + \sum_{j=1}^{i-1} r_{ij} F_{nj}\right) + g(Z(\tau))$$

$$Y_{ni} = Z(\alpha_i h).$$

- New order conditions are derived in similar way
- More free parameters than for Runge-Kutta methods
- Free parameters are determined with respect to good stability properties for linear acoustics

PEER PARTITIONED METHODS

$$\mathbf{c} = \begin{pmatrix} -0.0899531627878552 & 0.4676428830697650 & 1 \end{pmatrix}^T$$

$$\boldsymbol{\alpha} = \begin{pmatrix} 0.0663272206869390 & 0.5550418090653672 & 0.8254622965775625 \end{pmatrix}^T$$

$$\mathbf{B} = \begin{pmatrix} -0.0967059983845656 & 0.4915598645202344 & 0.6051461338643311 \\ -0.0470929826281593 & 0.2169946581702936 & 0.5720815963722115 \\ -0.0891437312845480 & 0.1573830315884013 & 0.1973233392586685 \end{pmatrix}$$

$$\mathbf{S} = \begin{pmatrix} 0 & 0 & 0 \\ 0.2580167280856541 & 0 & 0 \\ 0.3269306113397434 & 0.4075067490977347 & 0 \end{pmatrix}$$

$$\mathbf{A} = \begin{pmatrix} 0.0721007322008575 & -0.1322804288331288 & 0.1265069173192104 \\ 0.0478238719665258 & -0.4831372398722279 & -0.1163332106046261 \\ 0.0325906971440313 & 0.0702440095890842 & 0.1286761505892647 \end{pmatrix}$$

$$\mathbf{R} = \begin{pmatrix} 0 & 0 & 0 \\ 1.1066883875756954 & 0 & 0 \\ -0.5020271673748957 & 1.0959786066300778 & 0 \end{pmatrix}$$

PEER PARTITIONED METHODS

It has the following properties where the indices of the Courant numbers denote the spatial order (the corresponding values for RK3 arranged behind for comparison):

$$C_3 = 1.72 \quad (1.73) \qquad\qquad C_5 = 1.47 \quad (1.44)$$

The moduli of the eigenvalues of $\mathbf{B} + \mathbf{S}$ must not exceed 1 for zero stability, they are:

$$\lambda_1 = 0.296 \qquad\qquad \lambda_2 = 0.386 \qquad\qquad \lambda_3 = 1$$

EXPONENTIAL INTEGRATION VIA FRAMES

- Frame: Vectorfield F where we can solve $y'(t) = F(y)$ with solution operator $y(t) = \exp(tF)y(0)$
  - $M = \mathbb{R}^n$, $F|_y = v \Rightarrow \exp(tF)y = y + tv$
  - $M = \mathbb{R}^{n\times n}$, $F|_Y = AY \Rightarrow \exp(tF)Y = \mathrm{Exp}(tA)\cdot Y$
- System of frames F_i: we can solve $y'(t) = \sum_j \alpha_j F_j(y)$
  - $n + n^2$ frames in $\mathbb{R}^n$: $y' = c + Ay$ where the frames are: $F_i(y) = e_i$ and $F_{ij}(y) = e_i y_j$ for $i, j = 1, \ldots, n$.
  - exact solution

$$y(t) = \mathrm{Exp}(hA)y(0) + h\phi(hA)c, \quad \text{where } \phi(z) := (e^z - 1)/z$$

- Solve $y'(t) = f(y) := g(y) + A(y)y$
  - Fixed Frame $f[p]$: $f[p](y) = g(p) + A(p)y \Rightarrow$ exact integration!
  - Note: y occurs twice on the RHS!

GENERALISED RK METHODS

- Internal stages of RK methods $Y_{ni} = y_n + h\sum_{j=1}^{i-1} a_{ij} f(Y_{nj})$
- This is the solution operator of

$$Y_{ni} = \mathrm{SOLUTION}(t = h, Y' = \sum_j a_{ij} f(Y_{nj}), Y(0) = y_n)$$

- Apply solution operator **exp** to frames

$$Y_{ni} = \exp(h \sum_j a_{ij} f[Y_{nj}]) y_n$$

- BUT: these methods have maximum order TWO (Munthe-Kaaas, 95/98)
- Higher order via commutators of vectorfields

COMMUTATOR FREE HIGH ORDER METHODS

- With multiple exponentials in the stages $\Rightarrow$ arbitrary order

$$Y_{ni} = \exp(h \sum_j a_{ij}^{(2)} f[Y_{nj}]) \exp(h \sum_j a_{ij}^{(1)} f[Y_{nj}]) y_n$$

- Exponentials are expansive $\Rightarrow$ reuse them

$$a_{ij}^{(1)} = a_{k(i)j}^{(1)} \Rightarrow Y_{ni} = \exp(h \sum_j a_{ij}^{(2)} f[Y_{nj}]) Y_{n,k(i)}$$

- Applied to

$$y' = g(y) + A(y)y \Rightarrow f[p](y) = g(p) + A(p)y$$

$$y' = g_1(y) + g_2(y) \Rightarrow f[p](y) = g_1(p) + g_2(y)$$

$$y' = g(y, y) \Rightarrow f[p](y) = g(p, y)$$

THE METHOD CF3

Butcher tableau of CF3 (Celledoni et.al. 03, Owren 06), method has order 3

$$
\begin{array}{c|ccc}
0 & & & \\
1/3 & 1/3 & & \\
2/3 & 0 & 2/3 & \\
\hline
1 & 1/3 & & \\
 & -1/12 & 0 & 3/4
\end{array}
$$

In our notation we have

$$
\boldsymbol{\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 \\ 0 & 2/3 & 0 & 0 \\ -1/12 & 0 & 3/4 & 0 \end{pmatrix}, \boldsymbol{\alpha} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \Gamma = 0.
$$

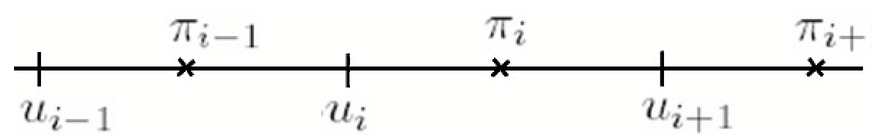
STABILITY: LINEAR ACOUSTICS

- Given

$$\begin{aligned} u_t + U u_x &= -\, c_s \pi_x \\ \pi_t + U \pi_x &= -\, c_s u_x \end{aligned}$$

where U is the mean advective velocity, c_s is the constant sound speed, and π is a normed perturbation Exner pressure.

- The spatial discretisation based on staggered grids (C-grid):
  - advection $\rightarrow$ upwind-differences.
  - sound waves $\rightarrow$ symmetric differences.



This leads to partitioned ODE:

$$\begin{aligned} u_i'(t) &= \{-\frac{U}{6\Delta x}[2u_{i+1} + 3u_i - 6u_{i-1} + u_{i-2}]\} + \{-\frac{c_s}{\Delta x}[\pi_i - \pi_{i-1}]\} \\ \pi_i'(t) &= \{-\frac{U}{6\Delta x}[2\pi_{i+1} + 3\pi_i - 6\pi_{i-1} + \pi_{i-2}]\} + \{-\frac{c_s}{\Delta x}[u_{i+1} - u_i]\} \end{aligned}$$

STABILITY ANALYSIS

- Stability: fixed Courant numbers $C_A = U\Delta t/\Delta x$, $C_S = c_s\Delta t/\Delta x$ variable wave number k (wave e^{ikx})

$$\begin{pmatrix} u \\ \pi \end{pmatrix}^{n+1} = S(C_A, C_S, k) \begin{pmatrix} u \\ \pi \end{pmatrix}^{n}$$

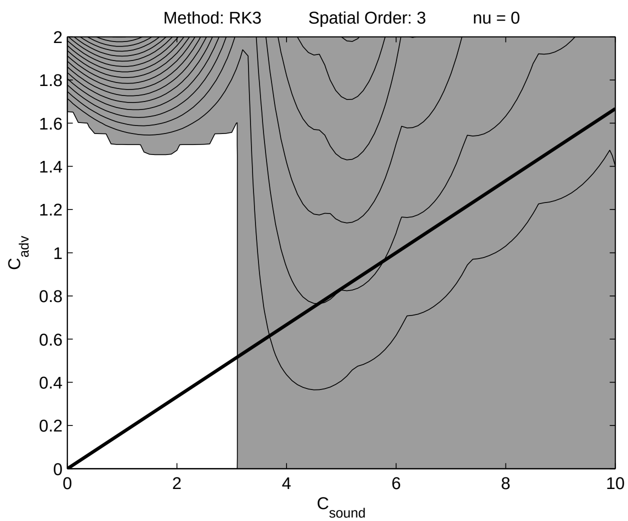
- The stability requires that the absolute values of eigenvalues of amplification matrix $S(C_A, C_s)$ must not exceed 1.
  We define:

$$R(C_A, C_S) := \max_k |(S(C_A, C_S, k))|.$$

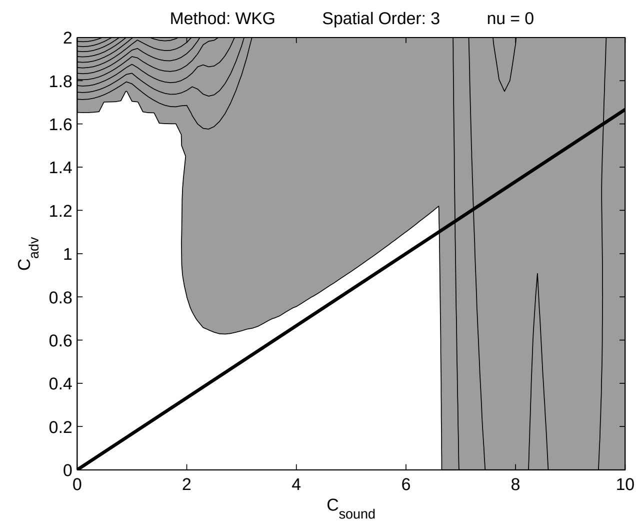
- Moreover, we discuss the case when a finite number of small time steps is applied, i.e. in each stage i of the methods we integrate the underlying equation $Z'_{ni} = c + g(Z_{ni})$ not exactly, but numerically with n_{si} small steps.

STABILITY REGIONS

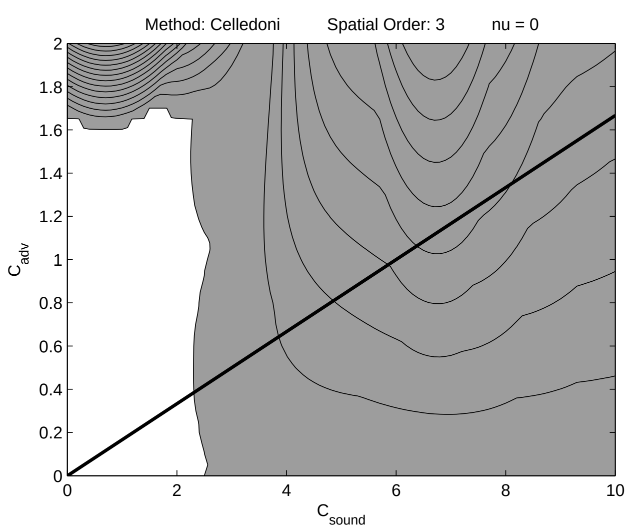
RK3, exact integration.



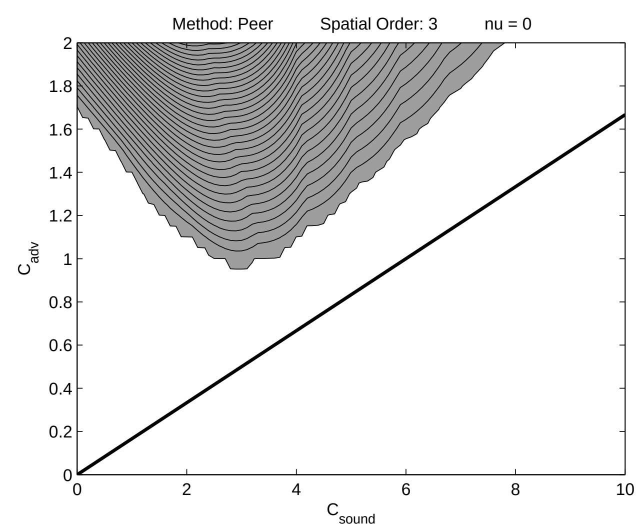
WKG, exact integration



CF3, exact integration.

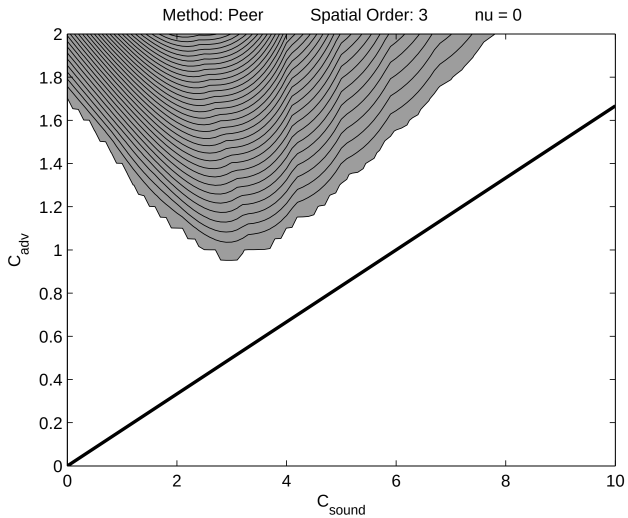


Peer, exact integration

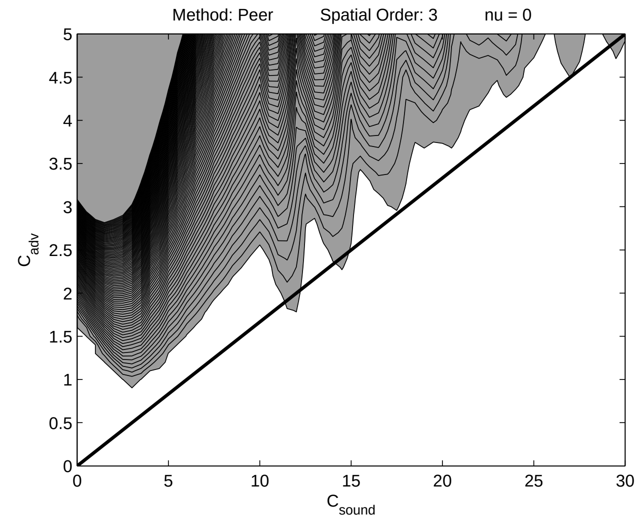


STABILITY REGIONS

Peer, exact integration, short interval.



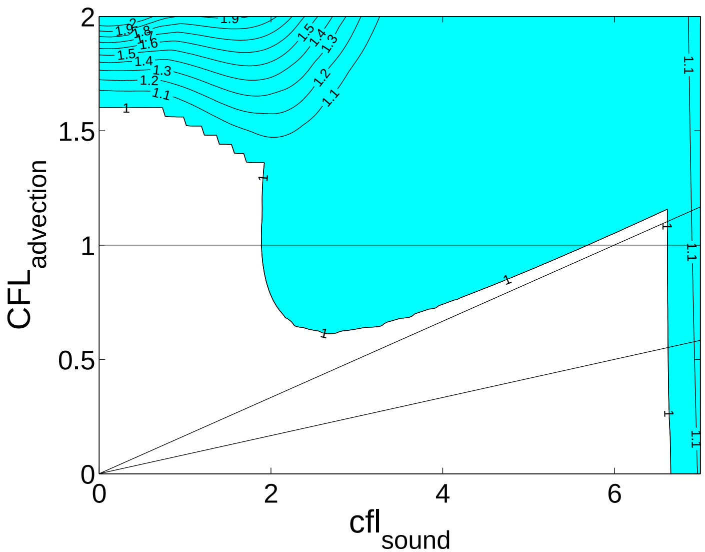
Peer, exact integration, large interval.



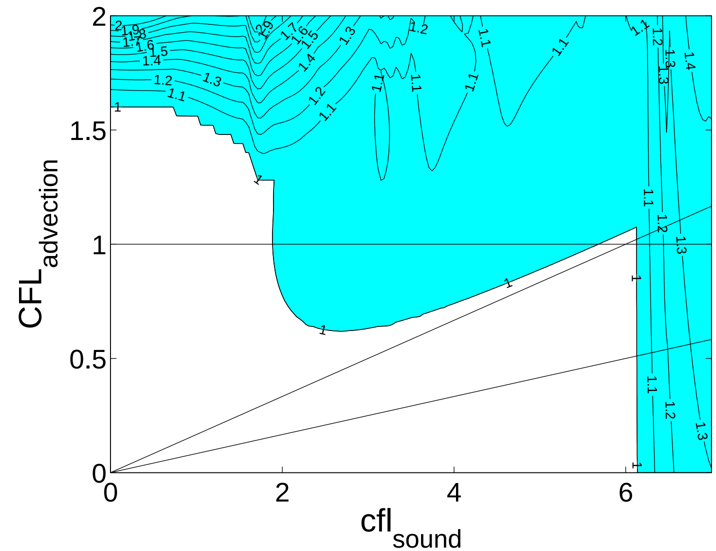
STABILITY REGIONS

- Exact integration versus forward-backward method

WKG exact integration.



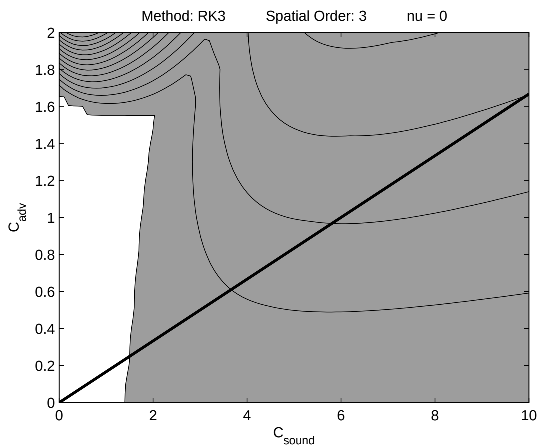
WKG, forward-backward Euler ($n_s = [4, 6, 8]$).



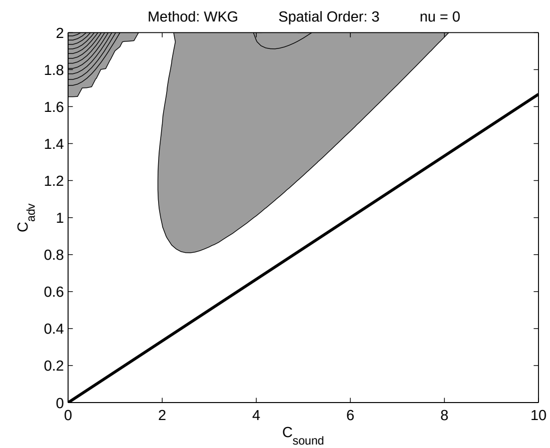
STABILITY REGIONS

- Exact integration versus linear implicit midpoint rule
- Small time step equals large time step

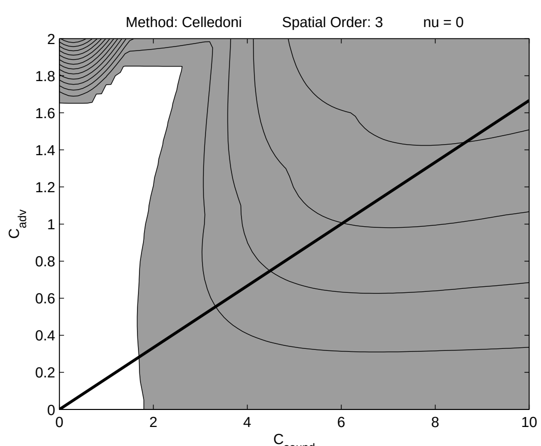
RK3, midpoint rule.



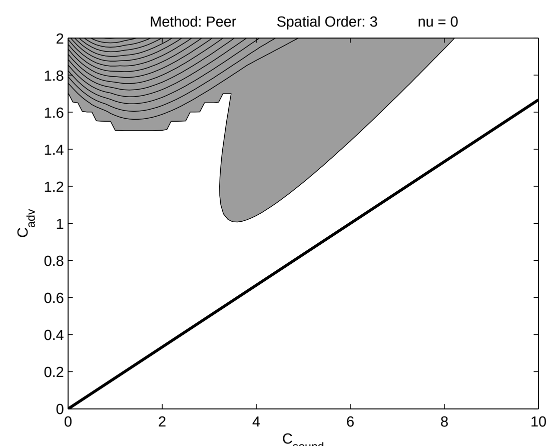
WKG, midpoint rule.



CF3, midpoint rule.



Peer, midpoint rule.



EULER EQUATIONS (2D)

- Conservation form with entropy as thermodynamic quantity

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial z} = Q$$

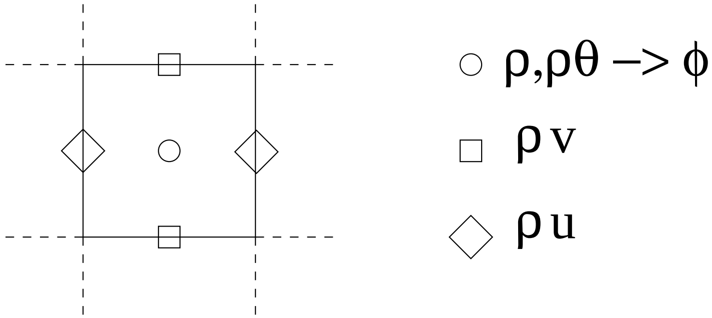
$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho w \\ \rho\theta \end{bmatrix}, \quad F(U) = \begin{bmatrix} \rho u \\ \rho uu + p \\ \rho wu \\ \rho u\theta \end{bmatrix}, \quad G(U) = \begin{bmatrix} \rho w \\ \rho uw \\ \rho ww + p \\ \rho w\theta \end{bmatrix}.$$

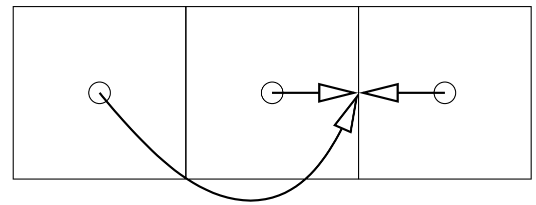
- Q denotes the gravity source terms.
- diagnostic equation: Pressure $p = p(\rho\theta)$

$$p = p_0 \left(\frac{R\rho\theta}{p_0} \right)^{\gamma}$$

Spatial Discretization: Finite Volumes

- Staggered grid (Arakawa C-grid)





From Cell to Face: upwind

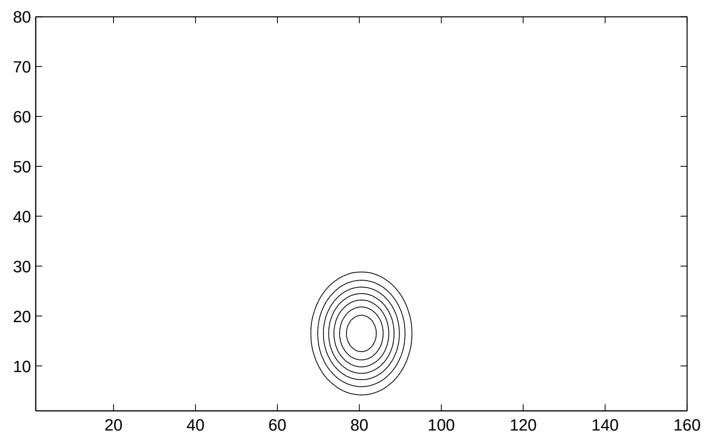
- For $\phi \in \{1, \theta, u, w\}$ we interpolate (upwind, 3rd order) from center to face

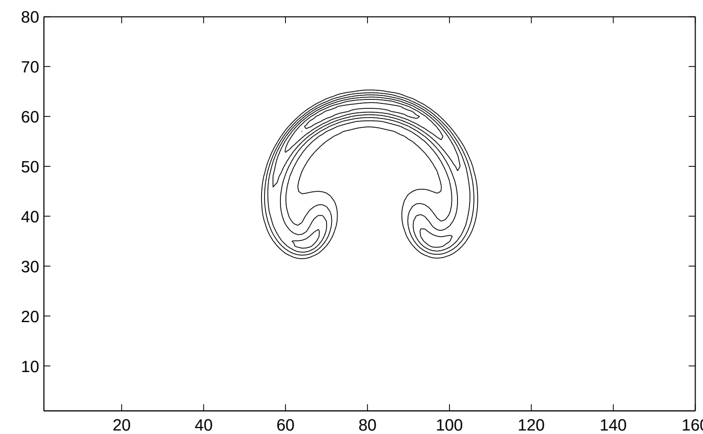
$$\frac{\partial}{\partial t}(\rho\phi)_{ik} = -\frac{1}{\Delta x}\left[(\rho u)_{i+1/2,k}\phi_{i+1/2,k} - (\rho u)_{i-1/2,k}\phi_{i-1/2,k}\right] - \frac{1}{\Delta z}\left[(\rho w)_{i,k+1/2}\phi_{i,k+1/2} - (\rho w)_{i,k-1/2}\phi_{i,k-1/2}\right]$$

  - ρu-update: shift to left/right cell center, then average update
  - Pressure gradient: symmetric difference

NONLINEAR TESTS

- Euler equations, rising bubble with advection
  - Domain $20km \times 10km$, Grid dx = dz = 125 m;
  - Final time = 1000s = 17 minutes
  - Initial state: $u = 20m/s, v = 0$, hydrostatic balance, $\theta = 300K$.
  - Thermal bubble with $\Delta\theta = +2K$, radius $2km$
  - Boundary conditions: periodic/no-flux





- Maximum step sizes

Method	RK3	CF3	WKG	Peer
Macro Time Step in s	0.9	0.5	1.6	5.0
Small time interval	1.83	1.67	1.62	1.44

SUMMARY

- Improved RUNGE-KUTTA like schemes are presented which have larger stability regions than RK3 in the absence of divergence damping
- Especially Peer methods are very promising
- Proposed idea can be applied in recursive way for including even faster processes like microphysics
- Order conditions are derived for third order methods in time
- Methods are included in the atmospheric code ASAM