TVD-cased split-explicit methods for compressible flow

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OVERVIEW

- Atmospheric processes
- Multirate Infinitesimal Step approach
- Order conditions for MIS-RK methods
- Stability analysis for linear acoustics
- Optimized methods
  - Genetic optimization
  - TVD based methods
- Tests on the Euler equations

ATMOSPHERIC PROCESSES

- Model: Euler equations for inviscid compressible flow
- Atmospheric models contain slow modes (advection) and fast modes (gravity and sound wave)
- CFL number for sound waves is very restrictive
- Pure advection allows larger stepsizes

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

- Strategies: filtering, semi-implicit, split-explicit/multirate
  - Large timesteps for slow processes
  - small timesteps for fast processes
- Starting point: Linear acoustics ($U \lessapprox c_S/10$)

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

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CLASSIC RUNGE-KUTTA METHODS

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

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

$$y_{n+1} = Y_{n,s+1} \qquad \text{(final update=additional stage)}$$

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

$$\begin{aligned} \text{Start at } y_n: &\quad Z_{ni}(0) = y_n \\ \text{Solve ODE}: &\quad Z'_{ni}(\tau) = \sum_j a_{ij} f(Y_{nj}) \\ \text{Integrate over } [0,h]: &\quad Y_{ni} = Z_{ni}(h). \end{aligned}$$

PARTITIONED METHODS

$$y' = f(y) + g(y)$$

- In each RK-stage we solve an ODE with fixed f-evaluations

$$\begin{aligned} \text{Start at } y_n: \quad & Z_{ni}(0) = y_n \\ \text{Solve ODE}: \quad & Z'_{ni}(\tau) = \sum_j a_{ij} f(Y_{nj}) + c_i g(Z_{ni}(\tau)) \\ \text{Integrate over } [0,h]: \quad & Y_{ni} = Z_{ni}(h). \end{aligned}$$

NOTE: For $g = 0$ we obtain an RK-method!

- Split-explicit RK3-method (Wicker/Skamarock 01) uses finite number of steps of forward-backward Euler:

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

GENERALISED 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 based on preceeding stages

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

- Multirate Infinitesimal Step approach (MIS):
  Use exact integration to analyse order and stability.
  Computation: apply finite number of small steps of a simpler method.
  Small step size is determined such that accuracy/stability is preserved.

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MIS-RK METHODS

- The complete method is given by

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

- $g = 0 \Rightarrow$ underlying RK method

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

ORDER CONDITIONS for MIS-RK

Business as usual $\Rightarrow$ Taylor expansion.
Things become complicated: $Z_{ni}(\tau, h)$ is a function of τ and h!
$G(Y_{ni})^{(k)} := \frac{\partial^k}{\partial h^k}\Big|_{h=0} G(Y_{ni})$, $G(Z_{ni})^{(k,l)} := \frac{\partial^{k+l}}{\partial \tau^k \partial h^l}\Big|_{\tau=h=0} G(Z_{ni})$

- 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 recursions for derivatives of Z_{ni}:

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

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ORDER CONDITIONS FOR ORDER 3

- 4 classic conditions

$$b^T 1\!\!1 = 1, b^T c = 1/2, b^T c^2 = 1/3, b^T Ac = 1/6$$

- 5 additional conditions

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

with $\tilde{c} := \boldsymbol{\alpha} c$, $R := (I - \boldsymbol{\alpha} - \boldsymbol{\gamma})^{-1}$ and $\tilde{b} = e_{s+1}^T RD$.

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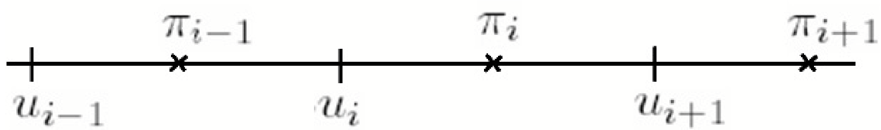
STABILITY: LINEAR ACOUSTICS

- Linear acoustics equation (linearised isentropic Euler equations)

$$u_t + U u_x = - c_s \pi_x$$
$$\pi_t + U \pi_x = - c_s u_x$$

U = constant background velocity, c_s = speed of sound, π = Exner pressure

- spatial discretisation on staggered grid (C-grid):
  - Advection → upwind
  - Sound waves → symmetric



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

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STABILITY ANALYSIS

- Amplification depends on Courant-numbers $C_A = U\Delta t/\Delta x$, $C_S = c_s \Delta t/\Delta x$ and wave numbers k (waves e^{ikx})

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

- Stability: scan amplification matrix $S(C_A, C_s, k)$ over all wave numbers k

$$R(C_A, C_S) := \max_k \varrho(S(C_A, C_S, k)) \leq 1.$$

- Numerical computation: Replace exact integration of $Z'_{ni} = c + g(Z_{ni})$ by small time steps.
  NOTE: Even then C_S is computed with respect to the large time step!

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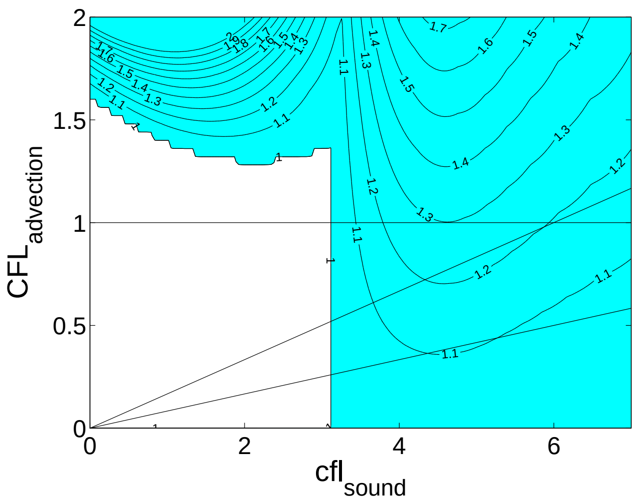
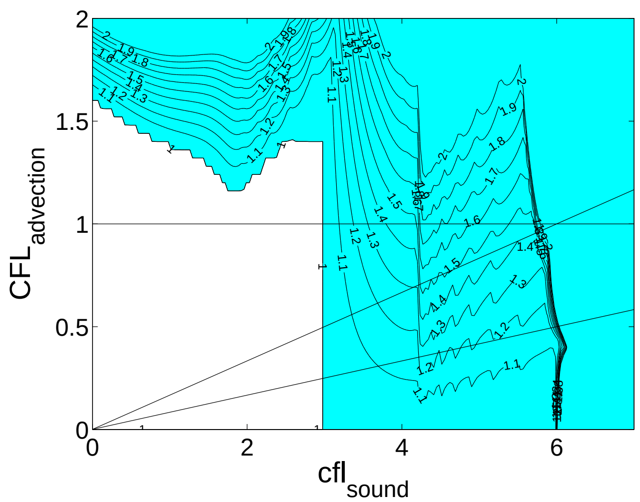
STABILITY REGIONS

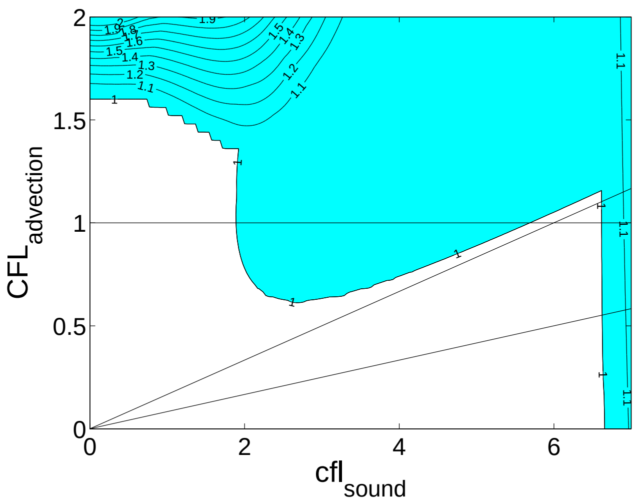
RK3, exact integration.



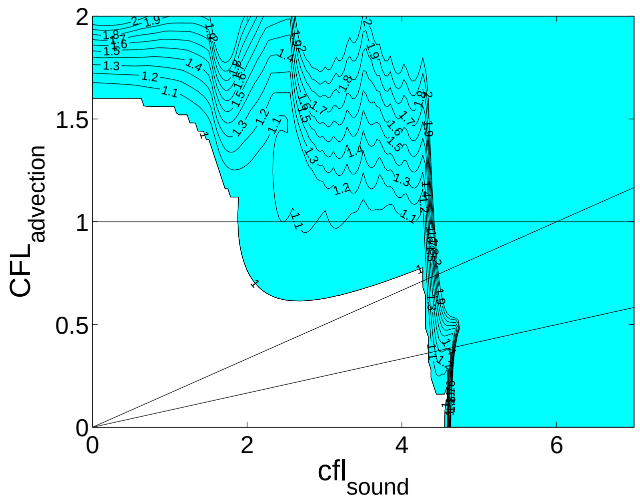
RK3, forward-backward Euler ($n_s = [2, 3, 6]$).



MIS3B, exact integration.



MIS3Ba, forward-backward Euler ($n_s = [2, 3, 4]$).



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OPTIMIZED METHODS

Design criteria:

- Computational cost: Total length of fast process integration intervals $D = \sum_i d_i$.
- Accuracy: Classical order 3 (4 conditions)
- Accuracy: Order 2 for partitioned systems
- Stability: We assume $C_A/C_S \leq \mu = 1/6$.
- Stability: The size $C_{S,max}$ of the stability triangle

$$(C_A, C_S) \in T[(0,0), (0, C_{S,max}), (\mu C_{S,max}, C_{S,max})]$$

- Stability: The maximum tracer CFL number $C_{A,\max}$.
- The fast integration procedure is Störmer-Verlet.

APPROACH I: GENETIC OPTIMIZATION

Objective function: combines good stability properties with small integration interval D

$$\widehat{\varphi} := \max(0, 30 - C_{S,max}), \quad \varphi := \begin{cases} \widehat{\varphi} & \text{if } \widehat{\varphi} > 0 \\ -1/\sum d_i & \text{if } \widehat{\varphi} = 0 \end{cases}$$

Genetic optimization $\Rightarrow$ order 2, good stability

- Deterministic optimization steps allow to construct 3rd order methods
- The small step integration procedure (Störmer-Verlet) is used to analyse stability
- The number of small steps is determined from $C_{S,max}$
- A 3-stage method is constructed, classsical order 3
- A 4-stage method is constructed, full order 3

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APPROACH II: TVD BASED METHODS

- We fix the underlying RK method to be 3rd order TVD.

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

Gottlieb/Shu

TVD radius=1

0			
2/3	2/3		
2/3	2/9	4/9	
	1/4	3/16	9/16

Knoth/W.

TVD radius=3/4

- Method 1 has $c_2 = 1 \Rightarrow d_2 = 1 \Rightarrow D$ is large.
- Use method 2 as underlying method

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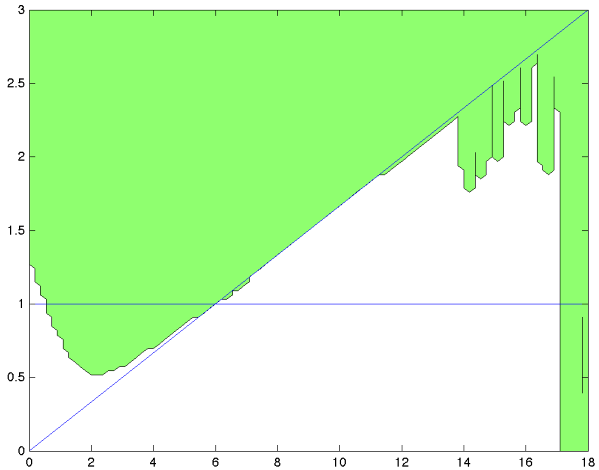
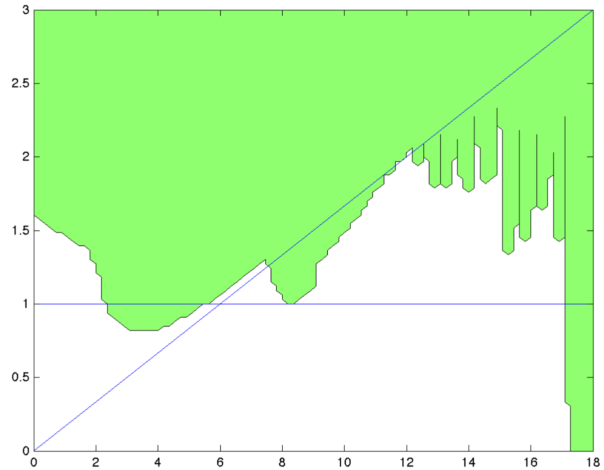
OPTIMIZATION

- Constraint: Stable on the boundary of the stability triangle.
- Objective functions:
  1. $\phi = -C_{S,max}$ where $C_{S,max}$ is a parameter.
  2. $\phi = D$ where $C_{S,max}$ is fixed.
  3. $\phi = -C_{S,max}/D$ where $C_{S,max}$ is a parameter.
- Cycle between (1) and (2) as preprocessing, use (3) for final optimization.
- Result: Methods with $D = 1.1$.

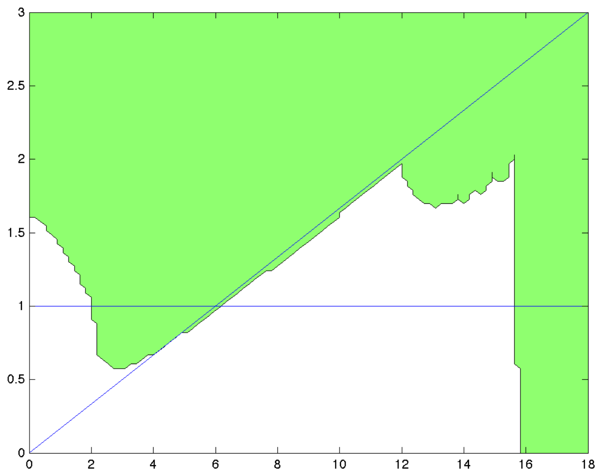
STABILITY PROPERTIES



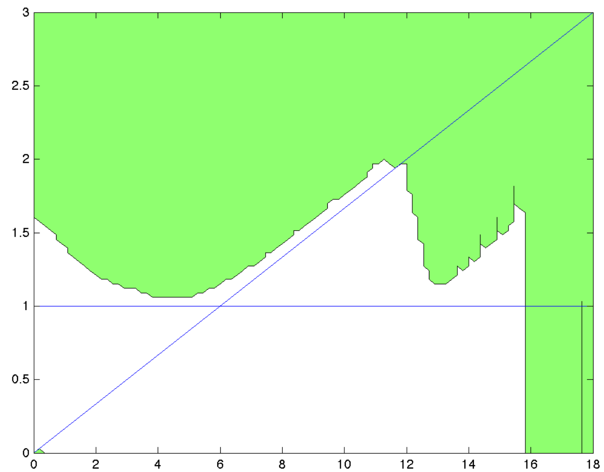
genetic, $s = 3$



genetic, $s = 4$



TVD A



TVD B

EULER EQUATIONS (2D)

- Conservation form with entropy as thermodynamic quantity

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

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho w \\ \rho\theta \end{bmatrix}, \quad F(Q) = \begin{bmatrix} u\rho \\ \rho u^2 + p \\ u\rho w \\ u\rho\theta \end{bmatrix}, \quad G(Q) = \begin{bmatrix} w\rho \\ w\rho u \\ \rho w^2 + p \\ w\rho\theta \end{bmatrix}.$$

- S denotes the gravity source terms.
- diagnostic equation: Pressure $p = p(\rho\theta) = p_0 \left(\frac{R\rho\theta}{p_0}\right)^\gamma$
- Red terms are "sound" terms, spatial discretization $\Rightarrow$

$$y' = B(y, y) = C(y)y + f(y) + g(y)$$

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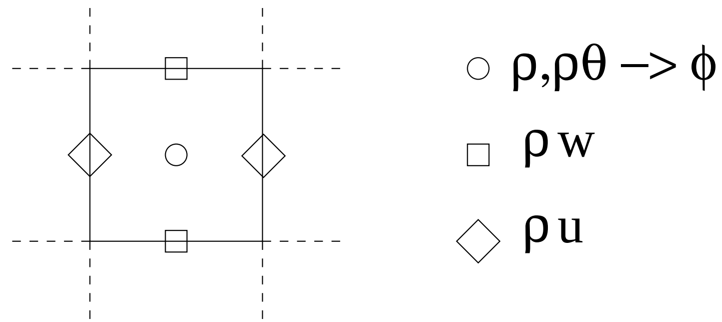
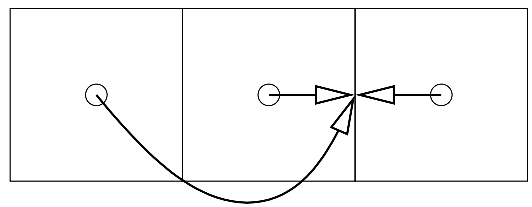
FINITE VOLUMES IN SPACE

- Staggered grid (Arakawa C-grid)





From Cell to Face: upwind

- shift $\rho u, \rho w \to \rho u_{L/R}, \rho w_{U/D}$: 6 cell-centered quantities $\rho\phi_{ij}$
- Advection: interpolate $\phi = \rho\phi/\rho$ to faces by 3rd order upwind, update in flux form (cheap fast terms $\rho u, \rho w$ at interface)

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

- Inertia $\rho u_{i+1/2,j}$ on faces: average advection over $\rho u_{L,i,j}$, $\rho u_{R,i+1,j}$
  pressure gradient $(p(\rho\theta_{i+1,j}) - p(\rho\theta_{i,j}))/\Delta x$ is fast term
  same for ρw, where gravitational force $-g\rho$ is fast term

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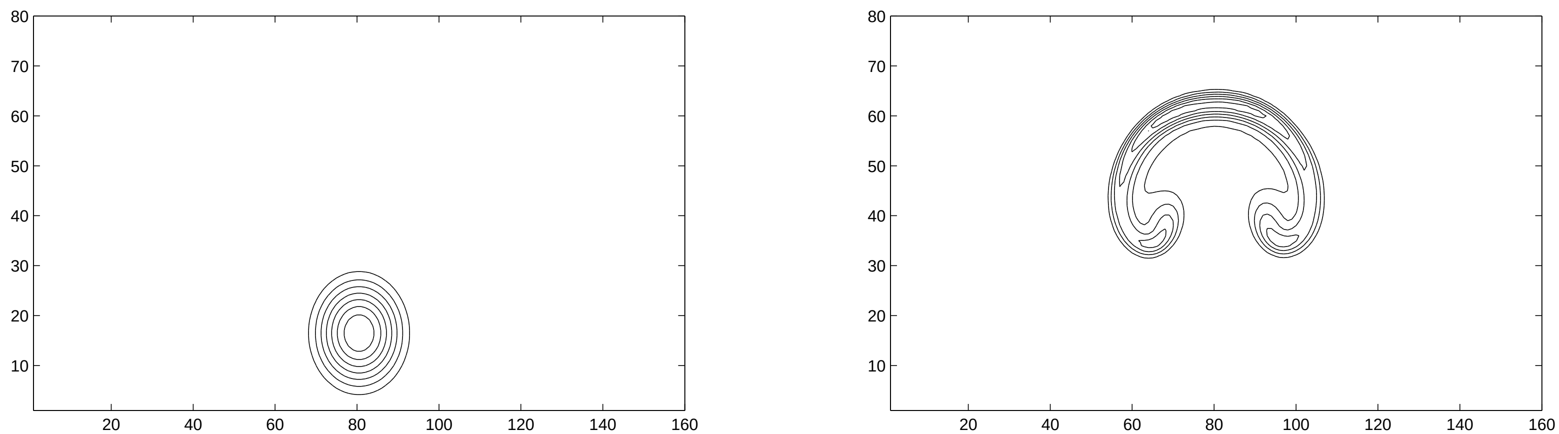
BUBBLE BENCHMARK

- Euler equations, rising bubble with advection
  - Domain $20km \times 10km$, Grid dx = dy = 125 m;
  - Final time = 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	MIS2	MIS4	TVDA
Macro Time Step in s	0.9	5.0	4.0	4.1

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SUMMARY

- MIS approach to analyse and develop time integration schemes for the invisvid compressible Euler equations
- Optimization with included small step integration procedure
- Two approaches: Genetic + TVD
- Optimized methods improve the stability bound by a factor of $4 - 5$.
- Excellent stability/accuracy for nonlinear Euler equations
- Open question: Can we have methods with $D = 1$, $D < 1$?

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