Split-explicit time integration methods in numerical weather prediction

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ASAM All Scale Atmospheric Model

MetStröm

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

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

- Apply multirate strategy
  - slow processes are integrated by large time steps
  - fast processes are integrated by small time steps where the slow (advective) tendencies are fixed
- The linearized, discretized, one-dimensional compressible Euler equations serve as the model equation set for examining the stability of the integration schemes

- Dry 2D Euler equations in conservative form:

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\frac{\partial \rho u}{\partial x} - \frac{\partial \rho w}{\partial z}\\
\frac{\partial \rho u}{\partial t} &= -\frac{\partial \rho uu}{\partial x} - \frac{\partial \rho wu}{\partial z} - \frac{\partial p}{\partial x}\\
\frac{\partial \rho w}{\partial t} &= -\frac{\partial \rho uw}{\partial x} - \frac{\partial \rho ww}{\partial z} - \frac{\partial p}{\partial z} - \rho g\\
\frac{\partial \rho \theta}{\partial t} &= -\frac{\partial \rho u\theta}{\partial x} - \frac{\partial \rho w\theta}{\partial z}
\end{aligned}
$$

- Prognostic variables are density ρ and the products of density with winds u, w and potential temperature θ. Pressure p is a diagnostic variable from the equation of state

$$
p = \left(\frac{R\rho\theta}{p_0^{\kappa}}\right)^{\frac{1}{1-\kappa}},
$$

with $\kappa = \frac{R}{c_p}$, R gas constant for dry air, c_p the heat capacity of dry air at constant pressure and p_0 the pressure at ground, g is the acceleration of gravity.

- Test equations for linear stability analysis
- The approximate, quasi-Boussinesq linearized equations

$$\begin{aligned} u_t &= -c_s p_x - U u_x \\ w_t &= -c_s p_z - U w_x - N\theta \\ \theta_t &= -Nw - U u_x \\ p_t &= -c_s(u_x + w_z) - U p_x \end{aligned}$$

where $c_s >> U$.

- One dimensional acoustic advection system

$$\begin{aligned} u_t &= -c_s p_x - U u_x \\ p_t &= -c_s u_x - U p_x \end{aligned}$$

- Time integration methods for

$$\dot{y} = f(y) + g(y) \qquad \text{with} \quad y(0) = y_0$$

- where f represents the energetically relevant slow mode (advection, Rossby waves)
- and g the fast mode (sound waves, gravity waves).
- To integrate the fast system, the forward–backward or Stoermer-Verlet method is used. For a symplectic structure

$$\dot{u} = g_u(p)$$
$$\dot{p} = g_p(u)$$

  the FB scheme reads
-

$$u^{n+1} = u^n + \Delta\tau g_u(p^n)$$
$$p^{n+1} = v^n + \Delta\tau g_p(u^{n+1})$$

- FB is of second order and in connection with staggered central differences is stable for a CFL–condition

$$c_s \frac{\Delta\tau}{\Delta x} \leq 1.$$

- The approximate, quasi-Boussinesq linearized equations

$$\begin{aligned} u_t &= -c_s p_x - Uu_x \\ w_t &= -c_s p_z - Uw_x - N\theta \\ \theta_t &= -Nw - Uu_x \\ p_t &= -c_s(u_x + w_z) - Up_x \end{aligned}$$

- One dimensional acoustic advection system

$$\begin{aligned} u_t &= -c_s p_x - Uu_x \\ p_t &= -c_s u_x - Up_x \end{aligned}$$

- Splitting in the dry 2D Euler equation:

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= -\frac{\partial\rho u}{\partial x} - \frac{\partial\rho w}{\partial z}\\
\frac{\partial\rho u}{\partial t} &= -\frac{\partial\rho u u}{\partial x} - \frac{\partial\rho w u}{\partial z} - \frac{\partial p}{\partial x}\\
\frac{\partial\rho w}{\partial t} &= -\frac{\partial\rho u w}{\partial x} - \frac{\partial\rho w w}{\partial z} - \frac{\partial p}{\partial z} - \rho g\\
\frac{\partial\rho\theta}{\partial t} &= -\frac{\partial\rho u\theta}{\partial x} - \frac{\partial\rho w\theta}{\partial z}
\end{aligned}$$

- $$\dot{y} = F(y, y)$$

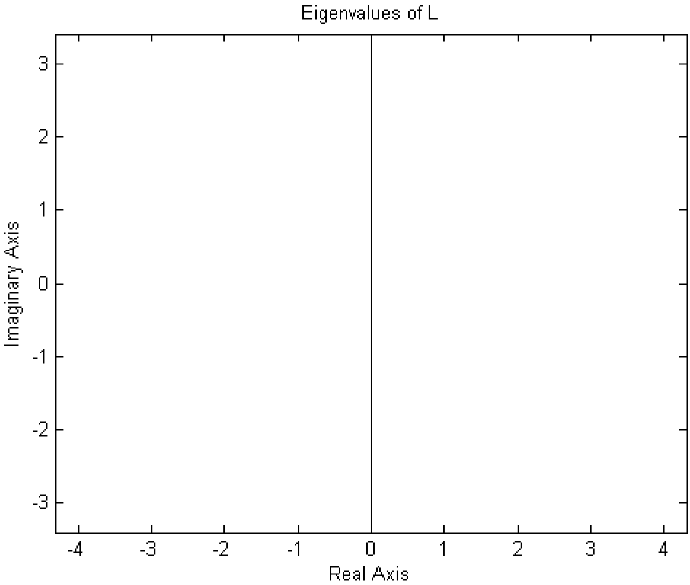
-

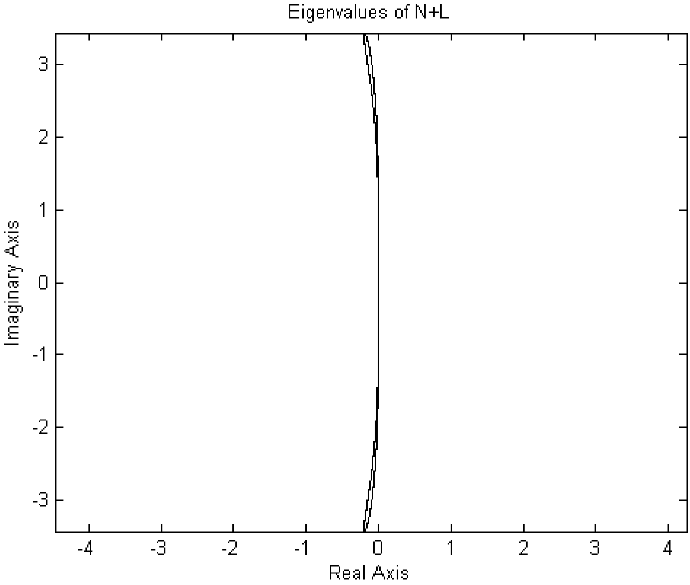
- Splitting in the dry "pressure linearized" 2D Euler equation:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u}{\partial x} - \frac{\partial \rho w}{\partial z}$$
$$\frac{\partial \rho u}{\partial t} = -\frac{\partial \rho u u}{\partial x} - \frac{\partial \rho w u}{\partial z} - \frac{\partial p}{\partial \rho\theta}\frac{\partial \rho\theta}{\partial x}$$
$$\frac{\partial \rho w}{\partial t} = -\frac{\partial \rho u w}{\partial x} - \frac{\partial \rho w w}{\partial z} - \frac{\partial p}{\partial \rho\theta}\frac{\partial \rho\theta}{\partial z} - \rho g$$
$$\frac{\partial \rho\theta}{\partial t} = -\frac{\partial \rho u\theta}{\partial x} - \frac{\partial \rho w\theta}{\partial z}$$

- $$\dot{y} = F(y) + A(y)y$$

- Discretize linear one-dimensional acoustic equation in space
- Advection: Third order upwinding, Acoustic: Central differences
- Apply Fourier decomposition
- We obtain a 2 by 2 linear ODE for each Fourier component $\dot{y} = Ly + Ny$


Eigenvalues of L
Imaginary Axis
Real Axis
3
2
1
0
-1
-2
-3
-4
-3
-2
-1
0
1
2
3
4


Eigenvalues of N+L
Imaginary Axis
Real Axis
3
2
1
0
-1
-2
-3
-4
-3
-2
-1
0
1
2
3
4

- Wicker and Skamarock (MWR 2002) used a three-stage Runge-Kutta method as slow integrator:

$$
\begin{aligned}
u^{n+1/3} &= u^n + \frac{\Delta t}{3} f_u(u^n) \\
p^{n+1/3} &= p^n + \frac{\Delta t}{3} f_p(p^n) \\
u^{n+1/2} &= u^n + \frac{\Delta t}{2} f_u(u^{n+1/3}) \\
p^{n+1/2} &= p^n + \frac{\Delta t}{2} f_p(p^{n+1/3}) \\
u^{n+1} &= u^n + \Delta t f_u(u^{n+1/2}) \\
p^{n+1} &= p^n + \Delta t f_p(p^{n+1/2})
\end{aligned}
$$

- Resulting splitting scheme:

$$
\begin{aligned}
& u = u^n, \qquad p = p^n \\
& \text{for } k = 1 : n_s/3 \\
& \qquad u = u + \Delta\tau g_u(p) + \Delta\tau f_u(u^n) \\
& \qquad p = p + \Delta\tau g_p(u) + \Delta\tau f_p(p^n) \\
& \text{end} \\
& u^{n+1/3} = u, \qquad p^{n+1/3} = p, \qquad u = u^n, \qquad p = p^n \\
& \text{for } k = 1 : n_s/2 \\
& \qquad u = u + \Delta\tau g_u(p) + \Delta\tau f_u(u^{n+1/3}) \\
& \qquad p = p + \Delta\tau g_p(u) + \Delta\tau f_p(p^{n+1/3}) \\
& \text{end} \\
& u^{n+1/2} = u, \qquad p^{n+1/2} = p, \qquad u = u^n, \qquad p = p^n \\
& \text{for } k = 1 : n_s \\
& \qquad u = u + \Delta\tau g_u(p) + \Delta\tau f_u(u^{n+1/2}) \\
& \qquad p = p + \Delta\tau g_p(u) + \Delta\tau f_p(p^{n+1/2}) \\
& \text{end} \\
& u^{n+1} = u, \qquad p^{n+1} = p
\end{aligned}
$$

- for $i = 1 : s+1$

  $y := y_0, \quad F := \sum \frac{a_{ij}}{c_i} f(y_j), \quad \Delta\tau := \frac{\Delta t}{n_s}$

  for $k = 1 : c_i n_s$

  $y := y + \Delta\tau g(y) + \Delta\tau F$

  end

  $y_i := y$

  end
- Underlying Runge–Kutta method:

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & a_{21} & & & \\
 & & & & \\
c_i & a_{i1} & \dots & a_{ii-1} & \\
c_s & a_{s1} & & & a_{ss-1} \\
\hline
1 & a_{s+11} & \dots & & a_{s+1s}
\end{array}
$$

- RK3 after L.J. Wicker and W.C. Skamarock: Time-Splitting Methods for Elastic Models Using Forward Time Schemes, MWR, 2002.

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

- Assume that we can solve the fast part of

$$\dot{y} = f(y) + g(y)$$

analytically

- Then a split Runge–Kutta method reads:

$$Z_{ni}(0) = y_n$$
$$\frac{\partial}{\partial \tau} Z_{ni}(\tau) = \frac{1}{c_i} \sum_{j=1}^{i-1} a_{ij} f(Y_{nj}) + g(Z_{ni}(\tau))$$
$$Y_{ni} = Z_{ni}(c_i h), \qquad y_{n+1} = Y_{n,s+1}$$

- For the nonlinear case

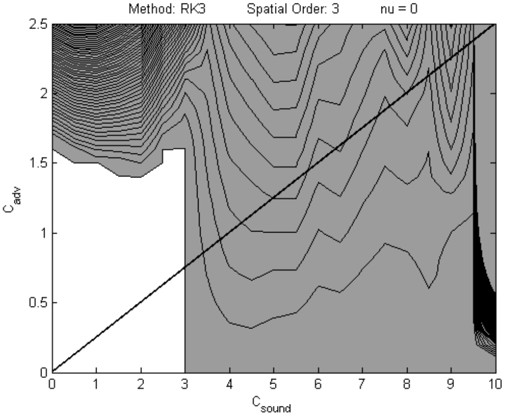
$$Z_{ni}(0) = y_n$$
$$\frac{\partial}{\partial \tau} Z_{ni}(\tau) = \frac{1}{c_i} \sum_{j=1}^{i-1} a_{ij} F(Y_{nj}, Z_{ni}(\tau))$$
$$Y_{ni} = Z_{ni}(c_i h), \qquad y_{n+1} = Y_{n,s+1}$$

- Application of a split-explicit Runge-Kutta method to the linear test equation $\dot{y} = Ly + Ny$ yields stability matrix $M \in \mathbb{C}^{2\times 2}$:

$$y^{n+1} = My^n$$

- M depends on:
  - wave number k
  - Number of small time steps n_s
  - CFL number for advection $U\frac{\Delta t}{\Delta x}$
  - CFL number for sound $c_s\frac{\Delta t}{\Delta x}$
- Spectral radius of M as a function of the two CFL numbers by $n_s = 10$ or $n_s = \text{inf}$.
- Line has slope $1/4$, below the line $U < \frac{c_s}{4} \approx 85\text{m/s} \approx 340\text{m/s}$.

- Stability plot for RK3, exact fast integration:



- Resulting CFL restrictions:

$$U\frac{\Delta t}{\Delta x} \leq 1.7 \qquad \rightarrow \qquad \Delta t \leq 6.8s$$

$$c_s\frac{n_s \Delta \tau}{\Delta x} \leq 3.1 \qquad \rightarrow \qquad \Delta t \leq 1.8s$$

- To enlarge stability there are the following possibilities
  - Introduce divergence damping, helps for some methods.
  - Use other integration methods for the fast part.
  - Look for other methods for the slow part.
-

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u}{\partial x} - \frac{\partial \rho w}{\partial z}$$
$$\frac{\partial \rho u}{\partial t} = -\frac{\partial \rho u u}{\partial x} - \frac{\partial \rho w u}{\partial z} - \frac{\partial p}{\partial x} + \nu \frac{\partial D}{\partial x}$$
$$\frac{\partial \rho w}{\partial t} = -\frac{\partial \rho u w}{\partial x} - \frac{\partial \rho w w}{\partial z} - \frac{\partial p}{\partial z} - \rho g + \nu \frac{\partial D}{\partial z}$$
$$\frac{\partial \rho \theta}{\partial t} = -\frac{\partial \rho u \theta}{\partial x} - \frac{\partial \rho w \theta}{\partial z}$$

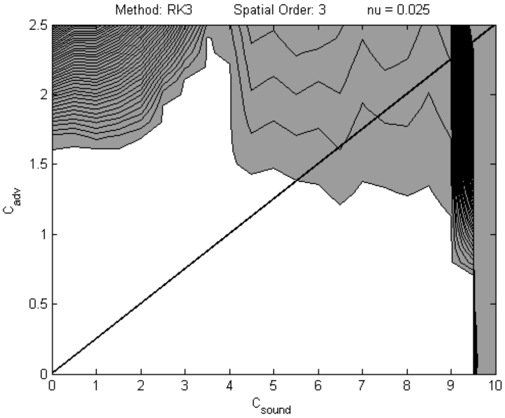
where the divergence D

$$D = \frac{\partial \rho u}{\partial x} + \frac{\partial \rho w}{\partial z}$$

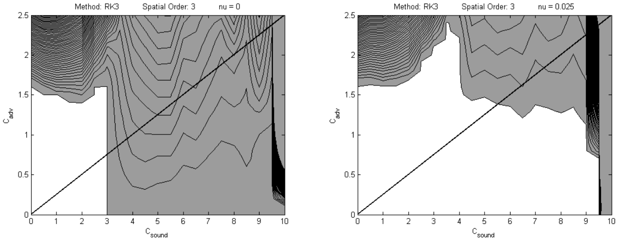
- The smoothing parameter ν is choosen in the FB-method for the fast part by

$$\alpha = 0.025 = \frac{\nu \Delta \tau}{\Delta x^2}$$

- Stability plot for RK3, FB fast integration, divergence damping:



- Comparison of stability plot for RK3



- Wensch et al. generalized the splitting Runge-Kutta ansatz:
- We generalise the exact integration procedure in two directions:
    - arbitrary starting points based on preceeding stages

$$Z_{ni}(0) = y_n + \sum_{j=1}^{i-1} \alpha_{ij}(Y_{nj} - y_n)$$

    - increments in the constant term F based on preceeding stages

$$\frac{\partial}{\partial \tau} Z_{ni}(\tau) = \frac{1}{\alpha_i}\left(\frac{1}{h}\sum_{j=1}^{i-1}\gamma_{ij}(Y_{nj} - y_n) + \sum_{j=1}^{i-1}\beta_{ij} f(Y_{nj})\right) + g(Z_{ni}(\tau))$$

- Jörg Wensch, Oswald Knoth, Alexander Galant: *Multirate infinitesimal step methods for atmospheric flow simulation*, BIT Numerical Mathematics, 2009, Volume 49, Number 2, 449-473

- Expand numerical solution in a Taylor series.
  Note: Z_{ni} is a function of τ and h.
- 3 different recursions for derivatives of Z_{ni}
- For order three 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
- No 3rd order method for $\alpha = \gamma = 0$ (classic splitting like RK3)
- We search for 3 stage 2rd order method
- And for a 4 stage 3rd order method
- Search is done by solving a large nonlinear optimization problem
- Constraints are order conditions and stability constraints
- Optimization goal: Small number of fast steps
- We found several methods

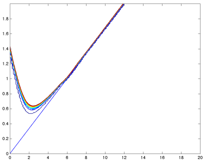
- Three stage second order method
- Length of small time step intervals: 1.18

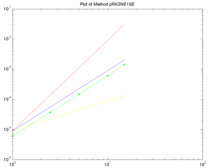
$$\beta = \begin{pmatrix} 0.126848494553D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ -0.784838278826D+00 & 0.137442675268D+01 & 0.000000000000D+00 \\ -0.456727081749D-01 & -0.875082271190D-02 & 0.524775788629D+00 \end{pmatrix}$$

$$\alpha = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.536946566710D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.480892968551D+00 & 0.500561163566D+00 \end{pmatrix}$$

$$\gamma = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.652465126004D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & -0.732769849457D-01 & 0.144902430420D+00 \end{pmatrix}$$

$$A = \begin{pmatrix} 0.126848494553D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ -0.633963196202D+00 & 0.137442675268D+01 & 0.000000000000D+00 \\ -0.403167397375D+00 & 0.878391608746D+00 & 0.524775788629D+00 \end{pmatrix}$$





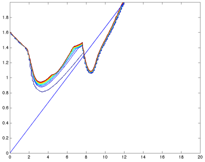
- Four stage third order method
- Length of small time step intervals: 1.43

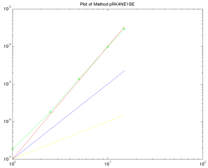
$$\beta = \begin{pmatrix} 0.136296478423D+00 & 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.280462398979D+00 & -0.160351333596D-01 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.904713355208D+00 & -0.104011183154D+01 & 0.652337563489D+00 & 0.000000000000D+00 \\ 0.671969845546D-01 & -0.365621862610D+00 & -0.154861470835D+00 & 0.970362444469D+00 \end{pmatrix}$$

$$\alpha = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.914092810304D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.114274417397D+01 & -0.295211246188D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.112965282231D+00 & 0.337369411296D+00 & 0.503747183119D+00 \end{pmatrix}$$

$$\gamma = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.678951983291D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & -0.138974164070D+01 & 0.503864576302D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & -0.375328608282D+00 & 0.320925021109D+00 & -0.158259688945D+00 \end{pmatrix}$$

$$A = \begin{pmatrix} 0.136296478423D+00 & 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.497588794316D+00 & -0.160351333596D-01 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.974872029275D+00 & -0.104345761551D+01 & 0.652337563489D+00 & 0.000000000000D+00 \\ 0.695803814606D+00 & -0.736679258484D+00 & 0.705129993298D-01 & 0.970362444469D+00 \end{pmatrix}$$





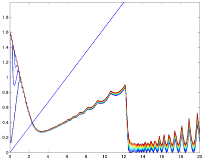
- Three stage first order method, after Osher/Shu, TVD scheme
- Implemented in COSMO
- Length of small time step intervals: 1.92

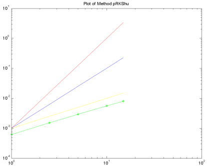
$$\beta = \begin{pmatrix} 0.100000000000D+01 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.250000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.666666666667D+00 \end{pmatrix}$$

$$\alpha = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.250000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.666666666667D+00 \end{pmatrix}$$

$$\gamma = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \end{pmatrix}$$

$$A = \begin{pmatrix} 0.100000000000D+01 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.250000000000D+00 & 0.250000000000D+00 & 0.000000000000D+00 \\ 0.166666666667D+00 & 0.166666666667D+00 & 0.666666666667D+00 \end{pmatrix}$$





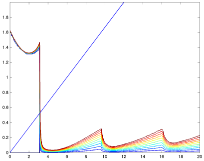
- Three stage second order method
- Implemented in WRF and COSMO with divergence damping
- Length of small time step intervals: 1.83

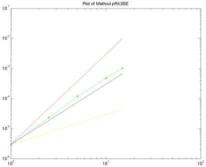
$$\beta = \begin{pmatrix} 0.333333333333D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.500000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.100000000000D+01 \end{pmatrix}$$

$$\alpha = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \end{pmatrix}$$

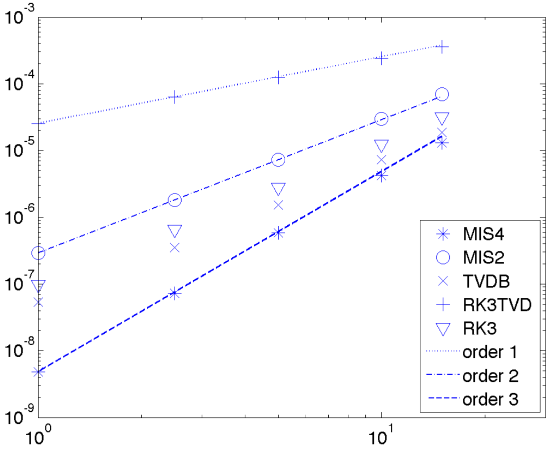
$$\gamma = \begin{pmatrix} 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.000000000000D+00 \end{pmatrix}$$

$$A = \begin{pmatrix} 0.333333333333D+00 & 0.000000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.500000000000D+00 & 0.000000000000D+00 \\ 0.000000000000D+00 & 0.000000000000D+00 & 0.100000000000D+01 \end{pmatrix}$$





- Order plots overview



- Application of the schemes to either pure long wave initial data, or multiscale initial data in a periodic domain $x \in [0, 1]$
- Relationship between pressure and momentum leads to a right running acoustic simple wave
- The pure long wave data is given by

  $$p(x, 0) = p_0(x - x_0) \quad \text{and} \quad m(x, 0) = p(x, 0)/c$$

  where

  $$p_0(x) = \exp(-(\frac{x}{\sigma_0})^2)$$

  and $x_0 = 0.75$ and $\sigma_0 = 0.1$.
- The multiscale initial data

  $$p(x, 0) = p_0(x - x_0) + p_1(x - 1) \quad \text{and} \quad m(x, 0) = p(x, 0)/c$$

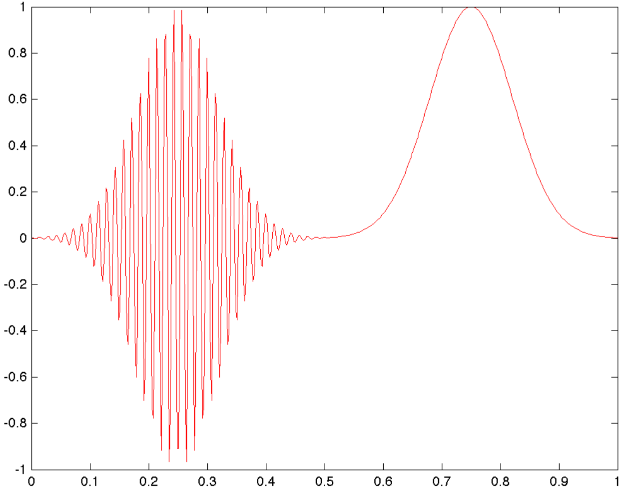
  and

  $$p_1(x) = p_0(x) * \cos(kx/\sigma_0)$$

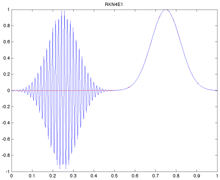
  with $x_1 = 0.25$ and $k = 7 \cdot 2\pi$.

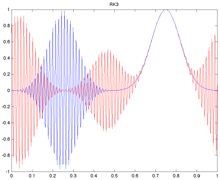
- One dimensional acoustic advection system, $U = 0$, $(f = 0)$

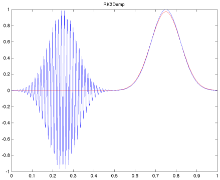
$$u_t = -c_s p_x - Uu_x$$
$$p_t = -c_s u_x - Up_x$$

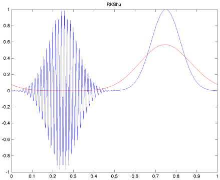


Test case of Klein

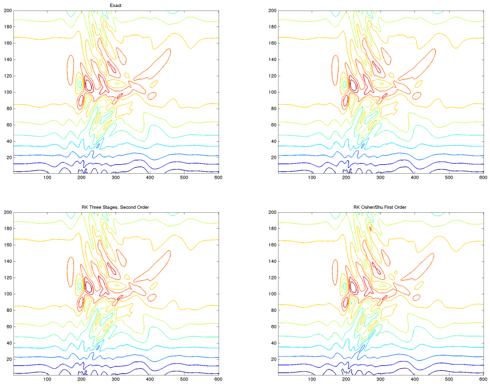




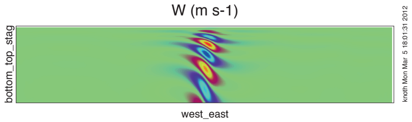




- Implicit-Explicit Multistep Methods for Fast-Wave Slow-Wave Problems, Dale R. Durran, Peter Blossey, Monthly Weather Review
- Highly nonlinear problem, used to perform order tests (see above)
- Implemented the discretization from the paper

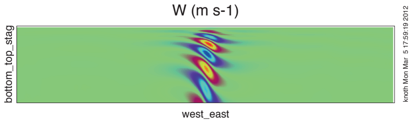


- Implemented in WRFV3 (thanks to Alexander Smalla)
- Switched on all divergence parameters, FB scheme in all three directions
- RKN4E1



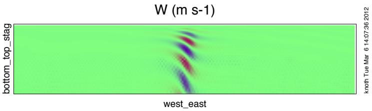
Range of W: -0.151088 to 0.154341 m s-1
Range of west_east: 0 to 200
Range of bottom_top_stag: 0 to 40
Current Time: 96
Current south_north: 0
Frame 97 in File wrfoutRKN4E1Hill

- RKN2E1



Range of W: -0.149748 to 0.152674 m s-1
Range of west_east: 0 to 200
Range of bottom_top_stag: 0 to 40
Current Time: 96
Current south_north: 0
Frame 97 in File wrfout_d01_0001-01-01_00:00:00

- RK3 without divergence damping is unstable



Range of W: -0.5 to 0.5 m s-1
Range of west_east: 0 to 200
Range of bottom_top_stag: 0 to 40
Current Time: 60
Current south_north: 0
Frame 61 in File wrfout_d01_0001-01-01_00:00:00

- Improved RUNGE-KUTTA like schemes are presented which have larger stability regions than RK3 in the absence of divergence damping
- 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 codes ASAM and WRF

Thanks for listening!