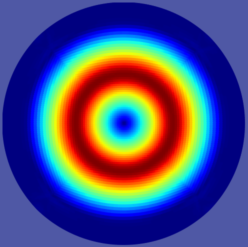

Efficient solution of large systems of non-linear PDEs in science
October 8, 2013

A Preconditioned Roe Scheme for All Mach Numbers

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Outline

Astrophysical Motivation

Mach number

$M = \frac{u}{c}$

sound speed in an ideal gas: $c = \sqrt{\gamma \frac{p}{\rho}} = \sqrt{\gamma R \frac{T}{\mu}} \propto \sqrt{\frac{T}{\mu}}$

- Flows in stellar interiors are poorly understood.
- 1D stellar evolution simulations use simple, physically motivated prescriptions of inherently multi-D phenomena (convective mixing, shear instabilities, ...).
- These flows involve very low Mach numbers and long time scales.

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We need simulation codes that...

- ...can resolve flows at low Mach number accurately.
- ...can simulate long time scales efficiently.

Euler Equations

$$\partial_t \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix} + \partial_x \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ u(\rho E + p) \end{pmatrix} + \partial_y \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v w \\ v(\rho E + p) \end{pmatrix} + \partial_z \begin{pmatrix} \rho w \\ \rho u w \\ \rho v w \\ \rho w^2 + p \\ w(\rho E + p) \end{pmatrix} = 0$$

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- introduce typical reference quantities: ρ_r, u_r, c_r, x_r, $\ldots$
- non-dimensionalize quantities: $\rho = \hat{\rho}\rho_\mathrm{r}$, $u = \hat{u}u_\mathrm{r}$, $\ldots$

Euler Equations

$$\partial_{\hat{t}} \begin{pmatrix} \hat{\rho} \\ \hat{\rho}\hat{u} \\ \hat{\rho}\hat{v} \\ \hat{\rho}\hat{w} \\ \hat{\rho}\hat{E} \end{pmatrix} + \partial_{\hat{x}} \begin{pmatrix} \hat{\rho}\hat{u} \\ \hat{\rho}\hat{u}^2 + \frac{1}{{M_r}^2}\hat{p} \\ \hat{\rho}\hat{u}\hat{v} \\ \hat{\rho}\hat{u}\hat{w} \\ \hat{u}(\hat{\rho}\hat{E} + \hat{p}) \end{pmatrix} + \partial_{\hat{y}} \begin{pmatrix} \hat{\rho}\hat{v} \\ \hat{\rho}\hat{u}\hat{v} \\ \hat{\rho}\hat{v}^2 + \frac{1}{{M_r}^2}\hat{p} \\ \hat{\rho}\hat{v}\hat{w} \\ \hat{v}(\hat{\rho}\hat{E} + \hat{p}) \end{pmatrix} + \partial_{\hat{z}} \begin{pmatrix} \hat{\rho}\hat{w} \\ \hat{\rho}\hat{u}\hat{w} \\ \hat{\rho}\hat{v}\hat{w} \\ \hat{\rho}\hat{w}^2 + \frac{1}{{M_r}^2}\hat{p} \\ \hat{w}(\hat{\rho}\hat{E} + \hat{p}) \end{pmatrix} = 0$$

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- asymptotic expansion in Mach number $M_r = \frac{u_r}{c_r}$
  i.e. $\hat{\rho} = \hat{\rho}^{(0)} + M_r\hat{\rho}^{(1)} + {M_r}^2\hat{\rho}^{(2)} + \cdots$

Euler Equations

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Two Decoupled Solution Spaces ($M_r \to 0$)

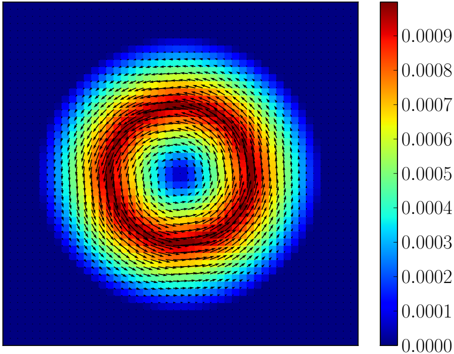
- sound waves governed by linear wave equation
- $\hat{p} = \hat{p}^{(0)} + M_r\hat{p}^{(1)}$

- incompressible Euler equations
- $\hat{p} = \hat{p}^{(0)} + M_r{}^2\hat{p}^{(2)}$

Gresho Vortex

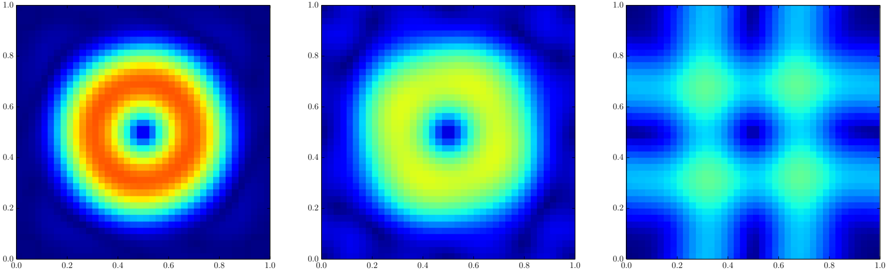
- rotating vortex
- dynamic pressure counteracts centrifugal force
- stationary solution to the incompressible Euler equations

Mach number



Standard Roe scheme
Mach number at $t = 2$

$M = 10^{-1}$ $M = 10^{-2}$ $M = 10^{-3}$



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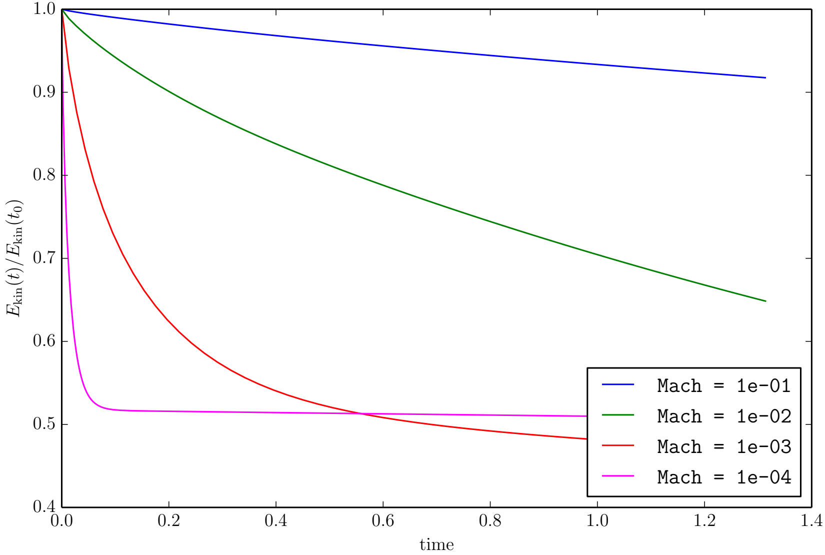

The Roe Scheme

$$\boldsymbol{F}_{i+1/2} = \frac{1}{2}\left(\boldsymbol{F}(\boldsymbol{U}^L_{i+1/2}) + \boldsymbol{F}(\boldsymbol{U}^R_{i+1/2}) - |A_{\text{roe}}|(\boldsymbol{U}^R_{i+1/2} - \boldsymbol{U}^L_{i+1/2})\right)$$

A_{roe}: flux Jacobian $\left(\dfrac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}}\right)$ evaluated at the Roe average state

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physical flux: $\boldsymbol{F}(\boldsymbol{U}^L_{i+1/2}) + \boldsymbol{F}(\boldsymbol{U}^R_{i+1/2})$

upwind term / numerical dissipation: $|A_{\text{roe}}|(\boldsymbol{U}^R_{i+1/2} - \boldsymbol{U}^L_{i+1/2})$

A_{roe}: flux Jacobian $\left(\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}}\right)$ evaluated at the Roe average state

Asymptotic Analysis

in primitive variables $\boldsymbol{V} = (\rho, u, v, w, p, X)^T$

$$\left(\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}}\right)_{\boldsymbol{V}} := \frac{\partial \boldsymbol{V}}{\partial \boldsymbol{U}} \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}} \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{V}}$$

$$\begin{pmatrix} q_n & \rho n_x & \rho n_y & \rho n_z & 0 & 0 \\ 0 & q_n & 0 & 0 & \frac{n_x}{\rho M_r^2} & 0 \\ 0 & 0 & q_n & 0 & \frac{n_y}{\rho M_r^2} & 0 \\ 0 & 0 & 0 & q_n & \frac{n_z}{\rho M_r^2} & 0 \\ 0 & \rho c^2 n_x & \rho c^2 n_y & \rho c^2 n_z & q_n & 0 \\ 0 & 0 & 0 & 0 & 0 & q_n \end{pmatrix}$$

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Roe matrix $|A_{\mathrm{roe}}|_{\boldsymbol{V}}$

$$\begin{pmatrix} \mathcal{O}(1) & \mathcal{O}(M_r) & \mathcal{O}(M_r) & \mathcal{O}(M_r) & \mathcal{O}(\frac{1}{M_r}) & 0 \\ 0 & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & 0 \\ 0 & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & 0 \\ 0 & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & \mathcal{O}(\frac{1}{M_r}) & 0 \\ 0 & \mathcal{O}(M_r) & \mathcal{O}(M_r) & \mathcal{O}(M_r) & \mathcal{O}(M_r) & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathcal{O}(1) \end{pmatrix}$$

Preconditioned Roe Scheme

modify the upwinding term to reduce artificial dissipation

$$\boldsymbol{F}_{i+1/2} = \frac{1}{2}\left(\boldsymbol{F}(\boldsymbol{U}^{L}_{i+1/2}) + \boldsymbol{F}(\boldsymbol{U}^{R}_{i+1/2}) - (P^{-1}|PA|)_{\text{roe}}(\boldsymbol{U}^{R}_{i+1/2} - \boldsymbol{U}^{L}_{i+1/2})\right)$$

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Preconditioner by Weiss & Smith (1995)

$$P_{\boldsymbol{V}} = \begin{pmatrix} 1 & 0 & 0 & 0 & \frac{\delta^2-1}{c^2} & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \delta^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\delta = \min(1, \max(M, M_{\text{cut}}))$$

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Asymptotic Behavior of $(P^{-1}|PA|)_{\boldsymbol{V}}$

$$\begin{pmatrix} \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r^2}) & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathcal{O}(1) \end{pmatrix}$$

A New Preconditioner

Preconditioner by Miczek (2013)

$$P_V = \begin{pmatrix} 1 & n_x \frac{\rho\delta M_r}{c} & n_y \frac{\rho\delta M_r}{c} & n_z \frac{\rho\delta M_r}{c} & 0 & 0 \\ 0 & 1 & 0 & 0 & -n_x \frac{\delta}{\rho c M_r} & 0 \\ 0 & 0 & 1 & 0 & -n_y \frac{\delta}{\rho c M_r} & 0 \\ 0 & 0 & 0 & 1 & -n_z \frac{\delta}{\rho c M_r} & 0 \\ 0 & n_x \rho c \delta M_r & n_y \rho c \delta M_r & n_z \rho c \delta M_r & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\delta = \frac{1}{\min(1, \max(M, M_{\text{cut}}))} - 1$$

A New Preconditioner – Asymptotic Behavior

$(P^{-1}|PA|)_{\boldsymbol{V}}$

$$\begin{pmatrix} \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r{}^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r{}^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(\frac{1}{M_r{}^2}) & 0 \\ 0 & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & \mathcal{O}(1) & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathcal{O}(1) \end{pmatrix}$$

$\left(\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}}\right)_{\boldsymbol{V}}$

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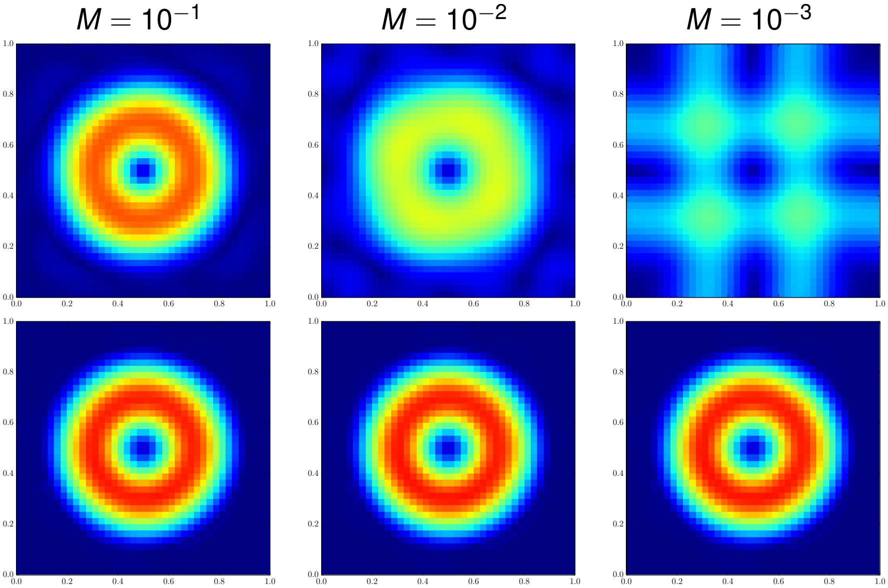
Gresho Vortex – Revisited



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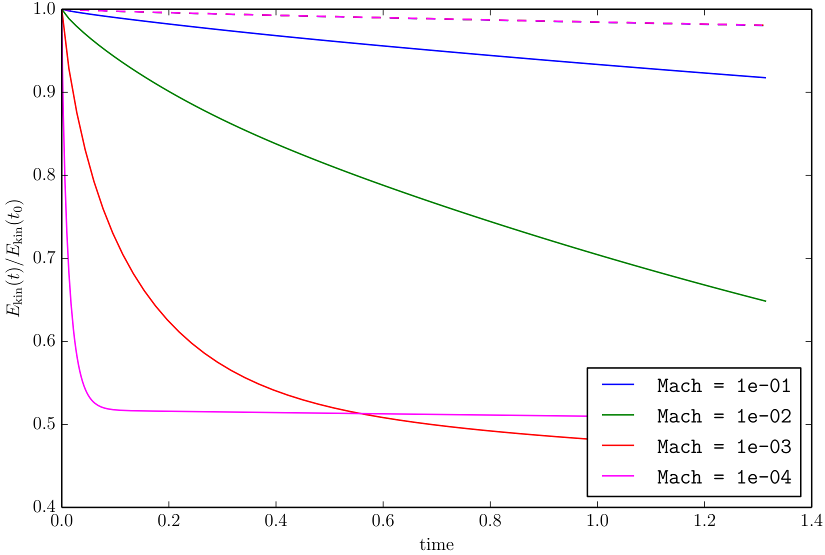

SLH (Seven League Hydro) Code

F. Miczek, F. K. Röpke, P. V. F. Edelmann

- solves the compressible Euler equations in 1-, 2-, 3-D
- explicit and implicit time integration
- flux preconditioning to ensure correct behavior at low Mach numbers
- other low Mach number schemes (e.g. AUSM$^+$-up)
- works for low and high Mach numbers on the same grid
- several solvers for the linear system:
  BiCGSTAB, GMRES, Multigrid, (direct)
- fully MPI-parallelized
- arbitrary curvilinear meshes
- radiation in the diffusion limit
- general equation of state
- general nuclear reaction network

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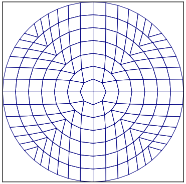

The Non-Linear System

- Discretize spatial terms first. (Method of Lines)

$$\frac{\partial \boldsymbol{U}}{\partial t} = \boldsymbol{R}(\boldsymbol{U})$$

- Explicit time step limited by sound speed (stability)
  $\Delta t_{\text{explicit}} \leq \text{CFL}\frac{\Delta x}{|u+c|} \overset{u \ll c}{\approx} \text{CFL}\frac{\Delta x}{c}$
- Implicit time step limit by fluid velocity (accuracy)
  $\Delta t_{\text{implicit}} \leq \text{CFL}\frac{\Delta x}{|u|}$
- Implicit time step larger by $1/M$

Example Backward Euler

$$\frac{\boldsymbol{U}^{n+1} - \boldsymbol{U}^{n}}{\Delta t} = \boldsymbol{R}(\boldsymbol{U}^{n+1})$$

$$0 = \Delta t \boldsymbol{R}(\boldsymbol{U}^{n+1}) - \boldsymbol{U}^{n+1} + \boldsymbol{U}^{n}$$

- non-linear system of $5 N_x N_y N_z$ equations
- solve with Newton–Rapshon
- sparse Jacobian with dense 5×5 blocks

Time Stepping

- implicit time stepping using Explicit first stage, Singly Diagonally Implicit Runge–Kutta schemes
  (ESDIRK23, ESDIRK34, ESDIRK46, ESDIRK58)
- subsequent solution of $N_{\text{stage}} - 1$ non-linear systems
- schemes offer an integrated error estimator
- lower limit in time step ensures it does not try to resolve sound waves
- pseudo time stepper to find steady states (e.g. hydrostatic equilibrium)

Non-Linear Solver

$$\boldsymbol{D}_{i,j,k}(\boldsymbol{U}) = \boldsymbol{R}_{i,j,k}(\boldsymbol{U}) + c_t \boldsymbol{U}_{i,j,k} + \boldsymbol{C}_{i,j,k} = 0$$

- Newton–Raphson: $\boldsymbol{U}^{k+1} = \boldsymbol{U}^{k} - \left(\lambda \frac{\partial \boldsymbol{D}^k}{\partial \boldsymbol{U}}\right)^{-1} \boldsymbol{D}^k$
- last RK stage as initial guess
- scaled norm as the convergence indicator:
  $\frac{\|(\boldsymbol{D})_q\|}{\|(\boldsymbol{C})_q\|} \quad q \in \{\rho, \rho u, \cdots\}$
- typical criterion for convergence $\approx 10^{-7}$
- monitor the dominant component to detect stalled convergence

Computation of the Jacobian

- automatic differentiation
  i.e. each quantity caries its derivatives w.r.t. every independent variable in addition to its value
- no additional calls to $\boldsymbol{F}$ (but the single call is more expensive)
- no need to chose a step ϵ (as for finite differences)
- some additional programming effort necessary

Computation of the Jacobian

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time to compute $\boldsymbol{F}$ with/without derivative

- Roe scheme: ≈ 4
- AUSM$^+$-up: ≈ 17

Iterative Linear Solvers

- size of matrix: $n \times n = (5N_xN_yN_z)^2$ ($n \approx 10^7$ for 128^3 grid)
- non-zero entries: $13 \times 5^2 \times N_xN_yN_z$
- density of Jacobian: $13/(N_xN_yN_z)$ ($\approx 6 \times 10^{-4}\,\%$ for 128^3 grid)
- no symmetry
- flexible linear solver framework to combine different solvers and preconditioners
- available methods: BiCGSTAB(ℓ), GMRES, Multigrid, ...
- available preconditioners: transformation to different variables, non-dimensionalization, inverse of the block-diagonal elements

Parallelization

- MPI
  - domain decomposition and ghost cells
  - each process computes its part of the Jacobian locally
  - linear solvers work on distributed matrices
- OpenMP
  - can be used in conjunction with MPI
  - important on modern HPC systems with many cores per node
  - reduces number of ghost cells per grid cell
  - special effort taken to ensure that a thread always work on the same slice of an array

Benchmark Overview (Miczek, 2013)

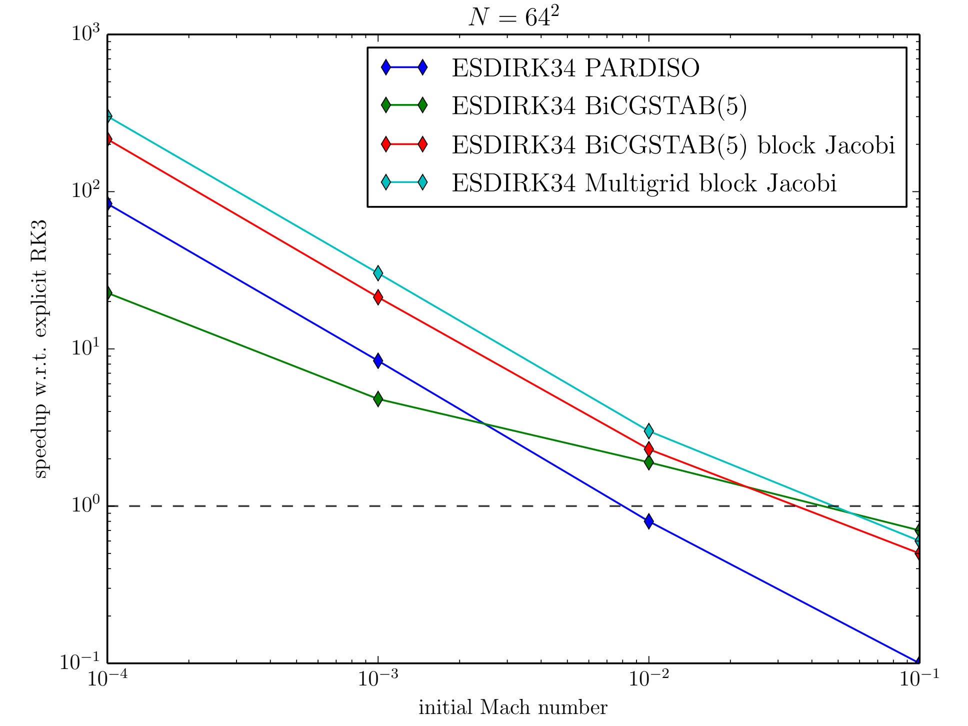
Gresho vortex, ESDIRK34, Roe-Lowmach scheme
advective CFL time step

Compared Solvers

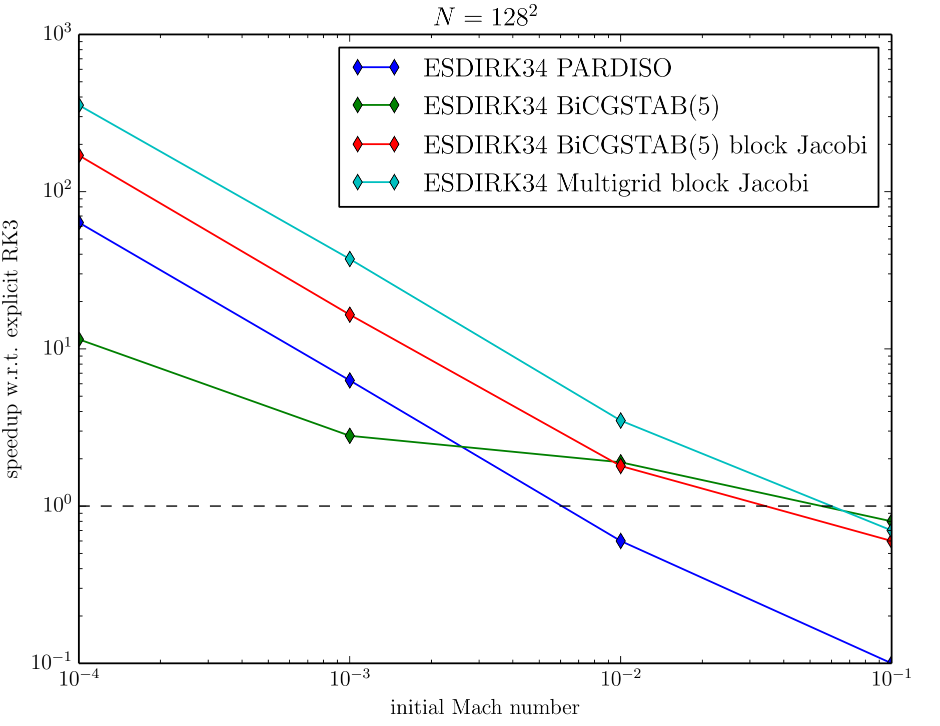
- direct solver PARDISO
- BiCGSTAB(5)
- BiCGSTAB(5) with block Jacobian preconditioning
- Multigrid with block Jacobian preconditioning and GMRES(20) and BiCGSTAB(5) smoothing

Measure of Performance

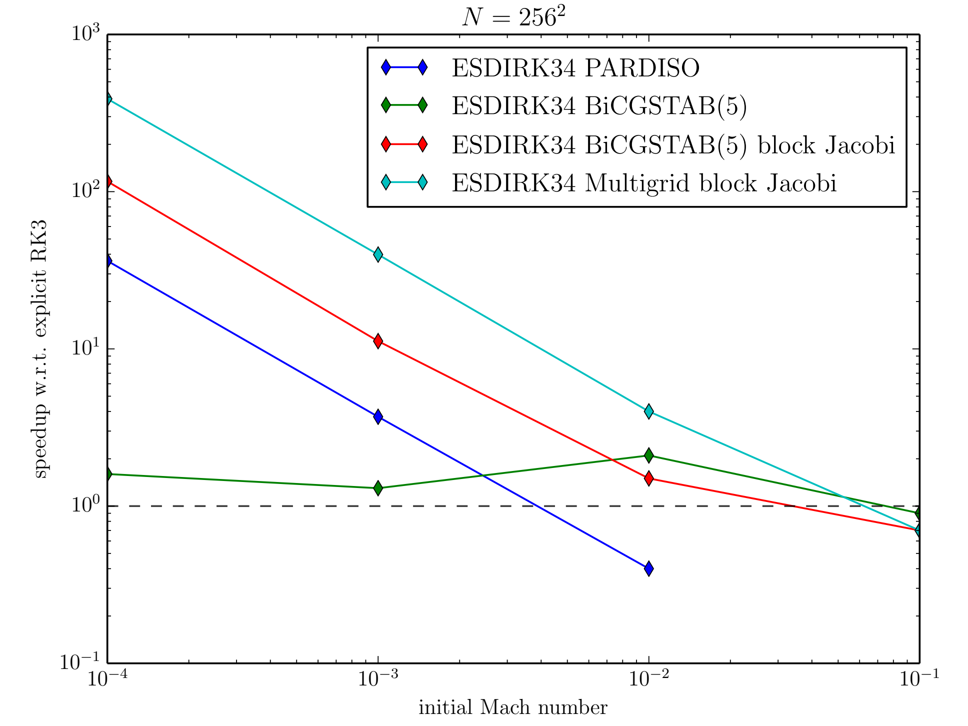
- speedup in computation time with respect to explicit RK3 for the same physical simulation time



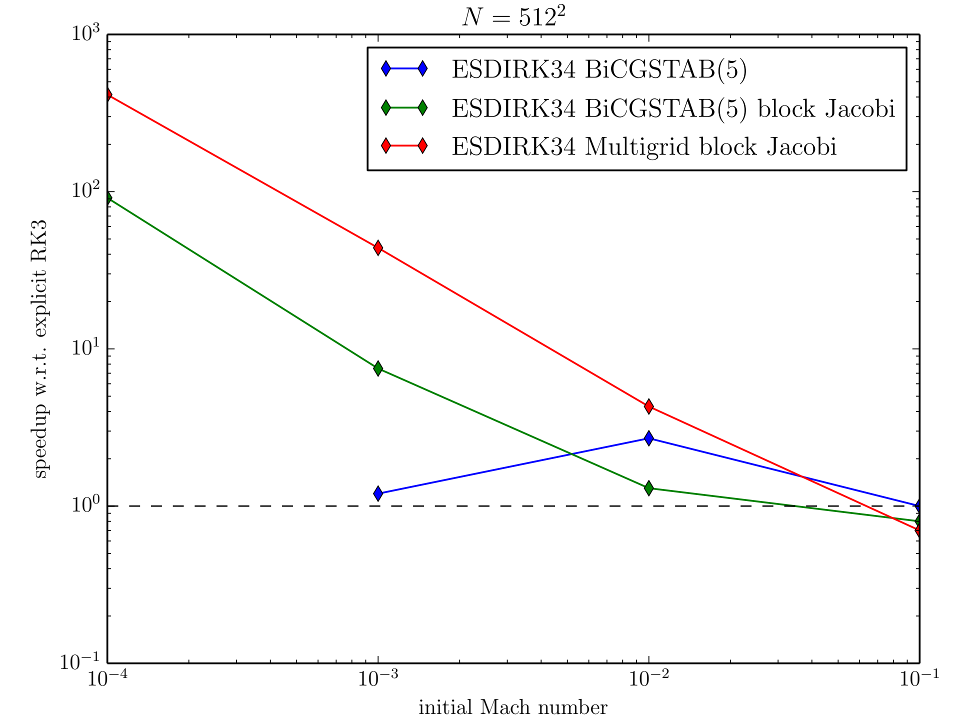
$N = 64^2$
ESDIRK34 PARDISO
ESDIRK34 BiCGSTAB(5)
ESDIRK34 BiCGSTAB(5) block Jacobi
ESDIRK34 Multigrid block Jacobi
speedup w.r.t. explicit RK3
initial Mach number
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-4}
10^{-3}
10^{-2}
10^{-1}



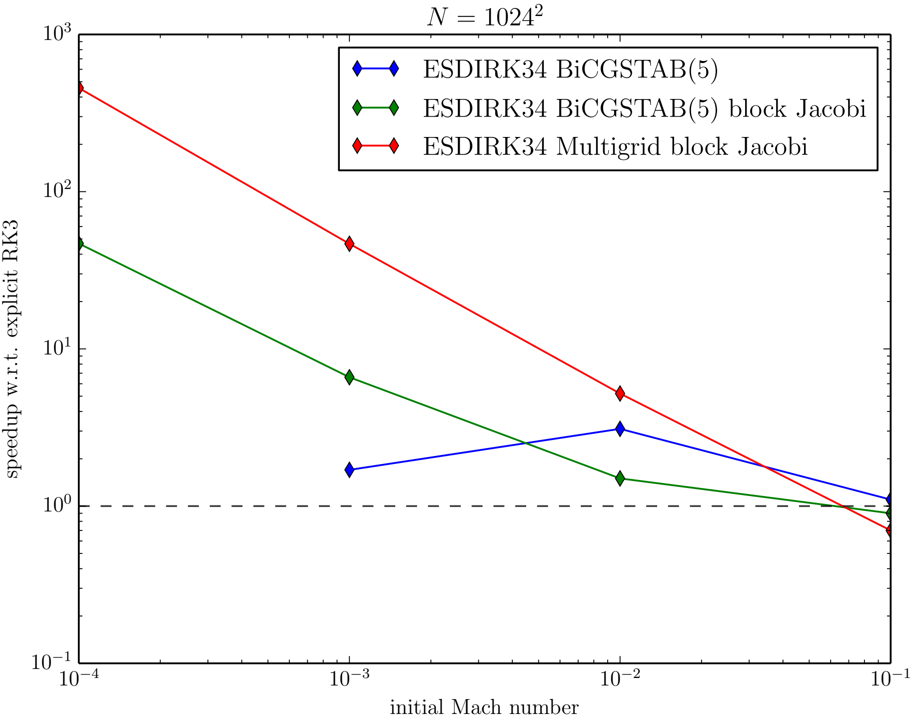
$N = 128^2$
ESDIRK34 PARDISO
ESDIRK34 BiCGSTAB(5)
ESDIRK34 BiCGSTAB(5) block Jacobi
ESDIRK34 Multigrid block Jacobi
speedup w.r.t. explicit RK3
initial Mach number
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-4}
10^{-3}
10^{-2}
10^{-1}



$N = 256^2$
ESDIRK34 PARDISO
ESDIRK34 BiCGSTAB(5)
ESDIRK34 BiCGSTAB(5) block Jacobi
ESDIRK34 Multigrid block Jacobi
speedup w.r.t. explicit RK3
initial Mach number
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{-4}
10^{-3}
10^{-2}
10^{-1}



$N = 512^2$
ESDIRK34 BiCGSTAB(5)
ESDIRK34 BiCGSTAB(5) block Jacobi
ESDIRK34 Multigrid block Jacobi
speedup w.r.t. explicit RK3
initial Mach number
10^3
10^2
10^1
10^0
10^{-1}
10^{-4}
10^{-3}
10^{-2}
10^{-1}


$N = 1024^2$
ESDIRK34 BiCGSTAB(5)
ESDIRK34 BiCGSTAB(5) block Jacobi
ESDIRK34 Multigrid block Jacobi
speedup w.r.t. explicit RK3
initial Mach number
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{-4}
10^{-3}
10^{-2}
10^{-1}

Conclusions

- Simulations of stellar interiors greatly benefit from implicit time stepping.
- Many traditional finite volume schemes show excessive dissipation at low Mach number flows.
- The Roe scheme can be modified to behave properly at low Mach numbers.
- Implicit time stepping is more efficient than explicit time stepping already at moderately low Mach numbers ($\approx 10^{-2}$).
- Multigrid and block Jacobian preconditioning well also for large systems.

References

Miczek, F. 2013, PhD thesis, Technische Universität München

Weiss, J. M. & Smith, W. A. 1995, AIAA Journal, 33, 2050