MAX-PLANCK-INSTITUT
FÜR ASTROPHYSIK

THE ROYAL SOCIETY

Physics-based preconditioning of sound waves

A Jacobian-free Newton-Krylov method for implicit multi-D hydrodynamics

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Workshop on Newton-Krylov methods

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Outline

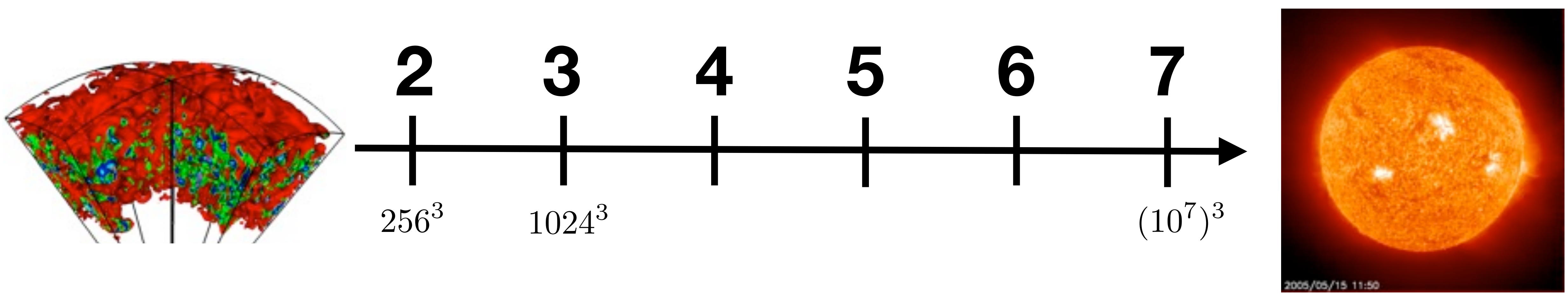
- **Introduction**
- Newton-Krylov solvers
- Conclusion

Flows in stellar interiors

Important physical characteristics guiding modelling

- ***Large stratification***: density decreases by orders of magnitude throughout the interior
- ***Low-Mach*** flow in the interior (CZ: 10^{-4}-10^{-3}, RZ much smaller), but ***transonic*** (~1) transition toward the surface
- Extreme parameter regime: e.g. Ra ~ 10^{15}, Pr $\lesssim 10^{-6}$, Re = LV/ν > 10^{10}
- ***Highly turbulent flow*** ⟶ $\frac{R}{\eta} \sim \mathrm{Re}^{\frac{3}{4}} \sim 10^{7.5}$

➜ We will not be able to model all scales of the flow



Credit: SOHO

Physical model
Compressible hydrodynamics

- We discard low-mach approaches (e.g. anelastic approximation)

  ➡ Modelling low-to-moderate Mach number flows in consistent background stratification

- Gas dynamics equations
  - Thermal diffusion (τ≫1) and external gravity
  - General equation-of-state (EOS)
- We do not consider (yet):
  - Rotation, multi-fluid, magnetic field
- In practice: no explicit viscosity !
  - **Implicit Large Eddy Simulation**: conservative, monotonicity-preserving schemes mimic a physical viscosity

Physical model

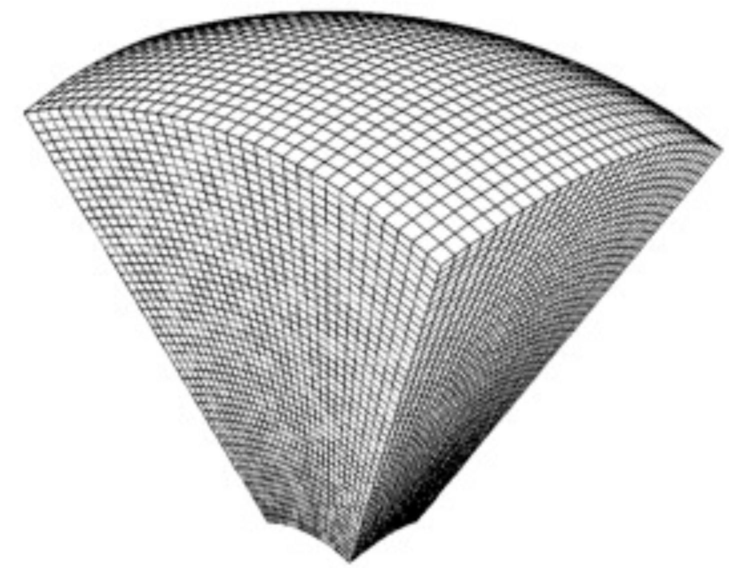
$$\partial_t \rho = -\vec{\nabla} \cdot (\rho \vec{u})$$
$$\partial_t (\rho e) = -\vec{\nabla} \cdot (\rho e \vec{u}) - p \vec{\nabla} \cdot \vec{u} + q_{\mathrm{visc}} + \vec{\nabla} \cdot (\chi \vec{\nabla} T)$$
$$\partial_t (\rho \vec{u}) = -\vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u}) - \vec{\nabla} p + \rho \vec{g} + \vec{\nabla} \cdot \bar{\bar{\tau}}_{\mathrm{visc}}$$

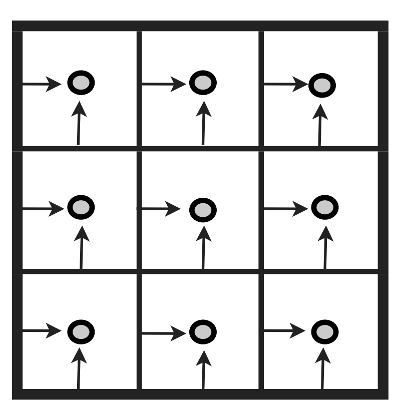
Photons conductivity: $\chi = \dfrac{4acT^3}{3\kappa\rho}$

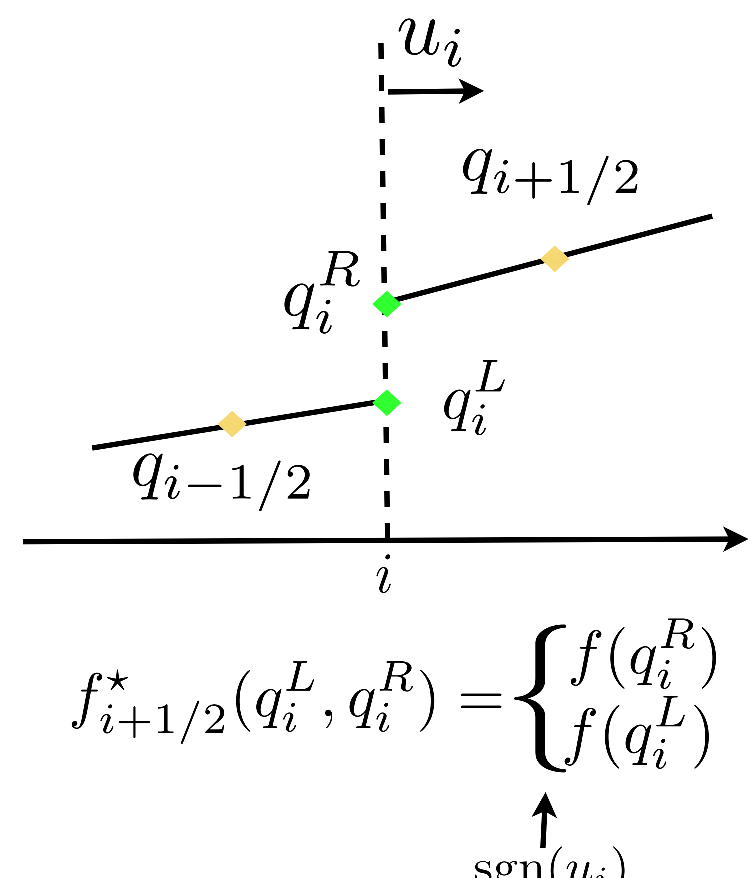
EOS: $P, T = f(\rho, e)$

Spatial discretization

- Geometry:
  - Spherical coordinates (wedges) in 2D/3D
- Spatial method
  - Finite volumes on a staggered grid
  - Advection: upwind method
    “High-order donor cell” (2[d] order in space)
  - Diffusion: 2[d] order central differences







Time integration of the equations

Difficulties

- Semi-discretised system: $\dfrac{dU}{dt} = R(U)$
- We have:
  - **Stiff sound waves**: $\tau_{\rm sound} \ll \tau_{\rm phys}$
  - **Stiff diffusion**: $\chi_r = \dfrac{k_r}{\rho c_p} = \dfrac{4acT^3}{3\kappa c_p \rho^2}$ can become very large

  ➡ **Severely restrict the time step when using explicit methods (CFL condition)**

  $$\frac{du(t)}{dt} = f(u(t)) \longrightarrow \quad u^{n+1} = u^n + \Delta t f(u^n)$$

  ➡ **Motivation for a fully implicit method**

  $$\frac{du(t)}{dt} = f(u(t)) \longrightarrow \quad u^{n+1} = u^n + \Delta t f(u^{n+1})$$ **unconditionally stable (A-stability)**
- Time step choice is based on accuracy considerations !

➡ ***MUSIC***: **MU**ltidimensional **S**tellar **I**mplicit **C**ode
(see Viallet, Baraffe, Walder, A&A, 2011, 2013)

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MUSIC

Implicit strategy: Newton-Krylov method

- Fully-implicit scheme: 2[d] order Crank-Nicholson
  - **Difficulty**: need to solve a large system of nonlinear equations $F(U^{n+1})=0$
  - 2D: $512^2 \rightarrow$ ***N* ~ 10⁶**, 3D: $256^3 \rightarrow$ ***N* ~ 84x10⁶**
  - **Challenge:** achieve *efficiency* and *scalability*

Implicit integration using Crank-Nicholson

$$\frac{dU}{dt} = R(U) \longrightarrow$$

$$F(U^{n+1}) = U^{n+1} - U^n - \frac{\Delta t}{2}\Big(R(U^{n+1}) + R(U^n)\Big) = 0$$

- Strategy: Newton-Raphson method
  - Initial guess: $U^{(0)} = U^n$
  - Linearization: $J^{(k)}\delta U^{(k)} = -F(U^{(k)})$ with $J^{(k)} \approx \frac{\partial F}{\partial U}(U^{(k)})$
  - Update: $U^{(k+1)} = U^{(k)} + \delta U^{(k)}$
  - Convergence: $\max \frac{\delta U^{(k)}}{U^{(k)}} < \epsilon \Rightarrow U^{n+1} = U^{(k+1)}$

Most expensive step !

1. Build matrix J (optional !)

2. Solve sparse linear system Ax=b

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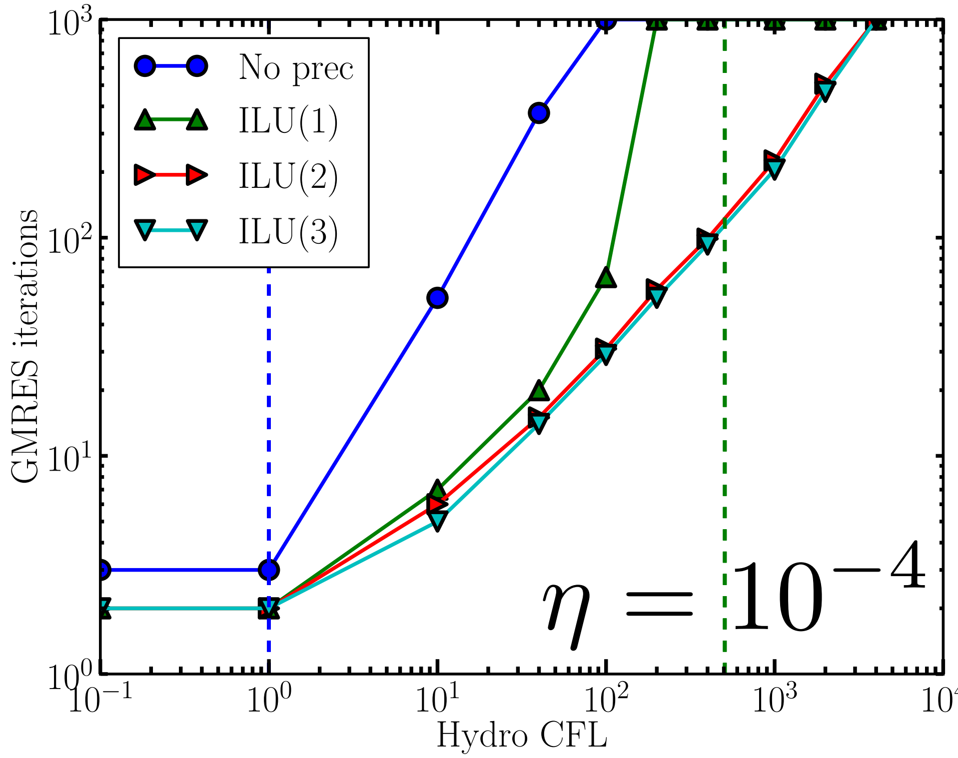
Newton-Krylov method

- "*Inexact strategy*" for $J^{(k)}\delta U^{(k)} = -F(U^{(k)})$ which is solved with GMRES iterations (Generalized Minimum Residual Method)
  - At iteration *p*, construct an approximation of the solution in the Krylov space $\mathcal{K}_p = \mathrm{span}(F, JF, J^2F, \ldots, J^{p-1}F)$
  - Accuracy can be tuned: reduce $||J\delta U + F||_2$ by a factor η (typically loose tolerance η = 10^{-1} - 10^{-2})
- Hope: a solution can be found for *p*≪*N* (e.g. *p* ≲ 30-40)
  - Stiffness spoils the convergence of the Krylov solver
  - **Preconditioning is necessary**: e.g. incomplete LU factorization of *J* (note: requires the computation of the matrix *J*)



Preconditioning

$$(JM^{-1})M\delta U = -F$$

Finite differences for *J*

$$\frac{\partial F_i}{\partial U_j} \approx \frac{F(U_j + \Delta U_j) - F(U_j)}{\Delta U_j}$$

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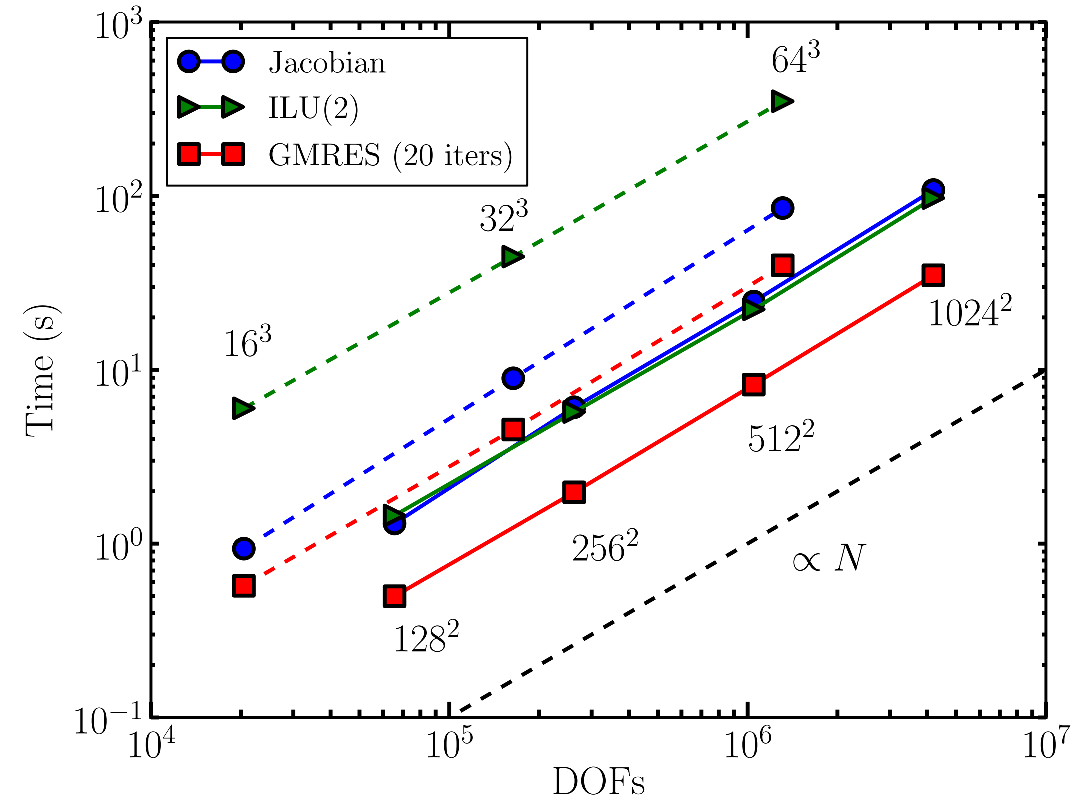
Fully implicit 3D computations

- Bottlenecks for fully-implicit 3D computations:

  1. Computation/storage of the Jacobian matrix
     2D: ~ 50 evaluations of *F*, 3D: ~ 100 evaluations of *F*

  2. Incomplete LU factorization: inefficiency + cost



1. Use *Jacobian-free Newton-Krylov* methods
   (see review by Knoll & Keyes, JCP, 2004)

   - Krylov methods do not need the Jacobian matrix, only its action on a vector

Jacobian-free approach

$$J\mathbf{v} = \frac{F(\mathbf{u} + \delta\mathbf{v}) - F(\mathbf{u})}{\delta}$$

2. Physics-based preconditioning
   (see e.g. Knoll et al, JSC, 25, 112, 2005, Park et al, JCP, 228, 2009)

   - Origin of the problem: change of the mathematical character of acoustic fluctuations at large wave-CFL numbers

MUSIC - 3D strategy

Jacobian-Free Newton-Krylov with physics-based preconditioning

- Semi-implicit scheme for hydrodynamics
  - Target the terms inducing sound-waves
- Solve equations for *V* = (*p*,*e*,*u*)
  - Use implicit Euler for specific terms and explicit Euler for advection
  - Use Picard linearization for implicit terms
  - Approximate $u^{n+1} = u^n - \Delta t \frac{1}{\rho^n} \partial_x p^{n+1}$
- Semi-implicit scheme is linear
  - Strategy: solve parabolic equation for δ*P*, then get δ*e* and δ*u*
  - Associated matrix with the "δ-form" of the scheme

"δ-form"

$$\tilde{J}_V \delta V = -\tilde{F}_V$$

$$\partial_t p + u \partial_x p = -\Gamma_1 p \partial_x u$$
$$\partial_t e + u \partial_x e = -\frac{p}{\rho} \partial_x u$$
$$\partial_t u + u \partial_x u = -\frac{1}{\rho} \partial_x p$$

$$\frac{\delta p}{\Delta t} + \Gamma_1 p^n \partial_x u^{n+1} = - u \partial_x p \big|^n$$
$$\frac{\delta e}{\Delta t} + \frac{p^n}{\rho^n} \partial_x u^{n+1} = - u \partial_x e \big|^n$$
$$\frac{\delta u}{\Delta t} + \frac{1}{\rho^n} \partial_x p^{n+1} = - u \partial_x u \big|^n$$

$$\frac{\delta p}{\Delta t} - a^2 \Delta t \partial_x^2 p^{n+1} = - u \partial_x p \big|^n - \Gamma_1 p^n \partial_x u^n$$
$$\frac{\delta e}{\Delta t} - \Delta t \frac{p^n}{(\rho^n)^2} \partial_x^2 p^{n+1} = - u \partial_x e \big|^n - \frac{p^n}{\rho^n} \partial_x u^n$$
$$\frac{\delta u}{\Delta t} + \frac{1}{\rho^n} \partial_x p^{n+1} = - u \partial_x u \big|^n$$

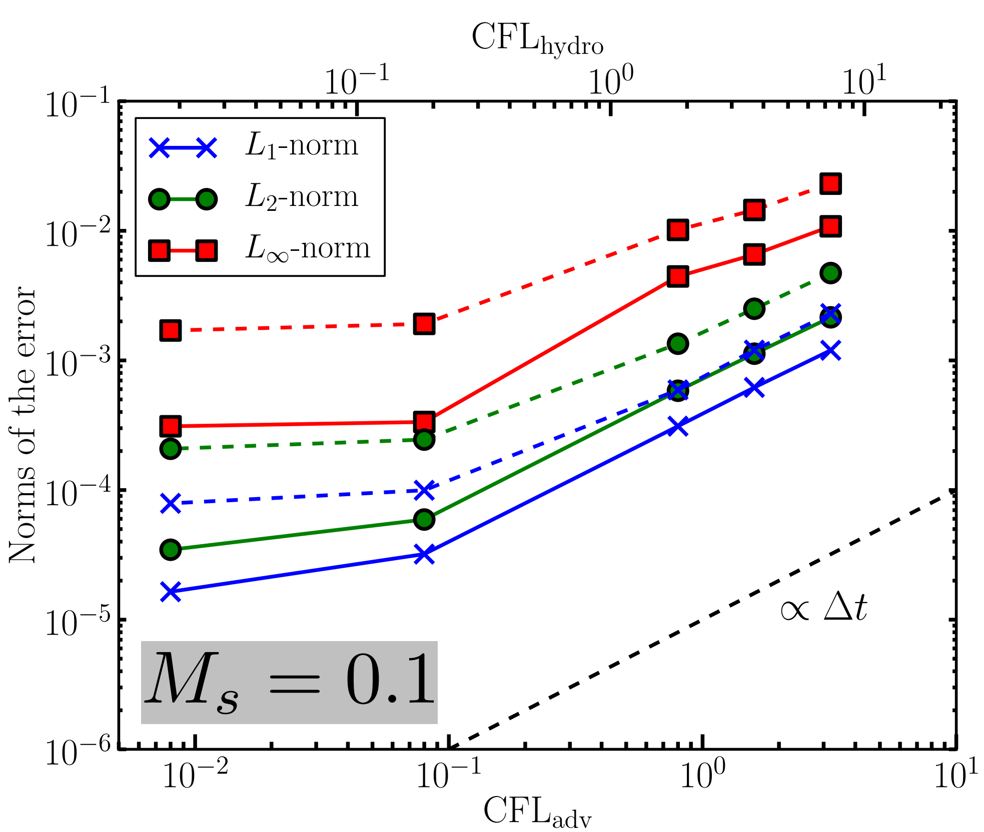
MUSIC - 3D strategy

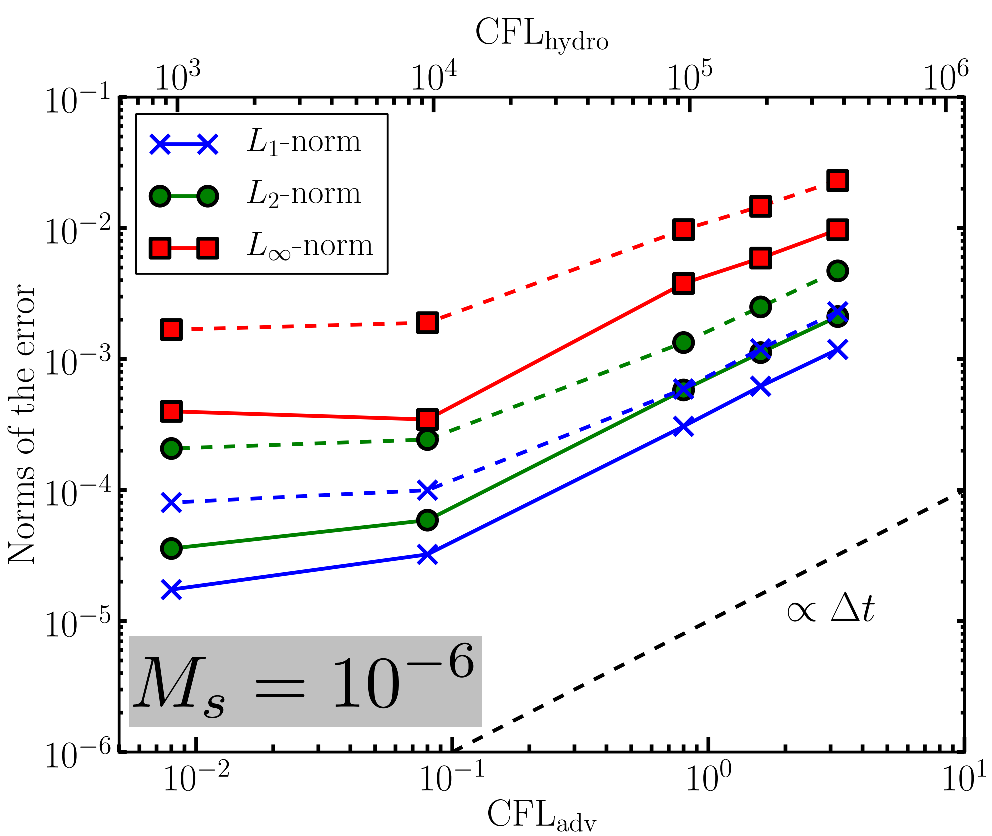
Jacobian-Free Newton-Krylov with physics-based preconditioning

- Test of the semi-implicit scheme
    - Advection of an isotropic vortex in 2D
- Scheme is not prone to a wave-CFL condition
    - But advection limits the time step ($\mathrm{CFL_{adv}} \lesssim 0.2$)

$$\mathrm{CFL_{hydro}} = \max\left(\frac{|u| + c_s}{\Delta x}\right)\Delta t$$

$$\mathrm{CFL_{adv}} = \max\left(\frac{|u|}{\Delta x}\right)\Delta t$$



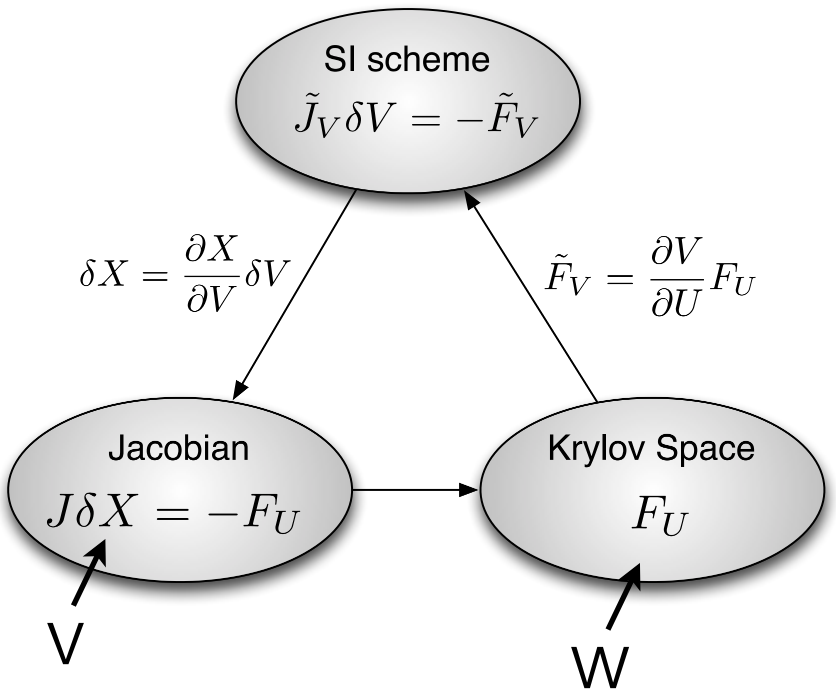


MUSIC - 3D strategy

Jacobian-Free Newton-Krylov with physics-based preconditioning

- Three sets of variables:
  - "Conservative" variables *U = (ρ, ρe, ρu)*
  - "Independent" variables *X = (ρ, e, u)*
  - "Primitive" variables *V = (p, e, u)*
- Right-Preconditioning of $J\delta X = -F_U(X)$ with matrix *M*
  - Search-space: $\mathcal{K}_p = \mathrm{span}(F, (JM^{-1})F, \ldots, (JM^{-1})^{p-1}F)$
- GMRES algorithm: for a given Krylov vector *w*, compute $(JM^{-1})w$
  1. Solve *Mv = w* for *v* (**Preconditioning step**)
  2. Compute *Jv* using a Jacobian-free approach
- PBP: interpret *Mv=w* as a SI step in δ-*form*

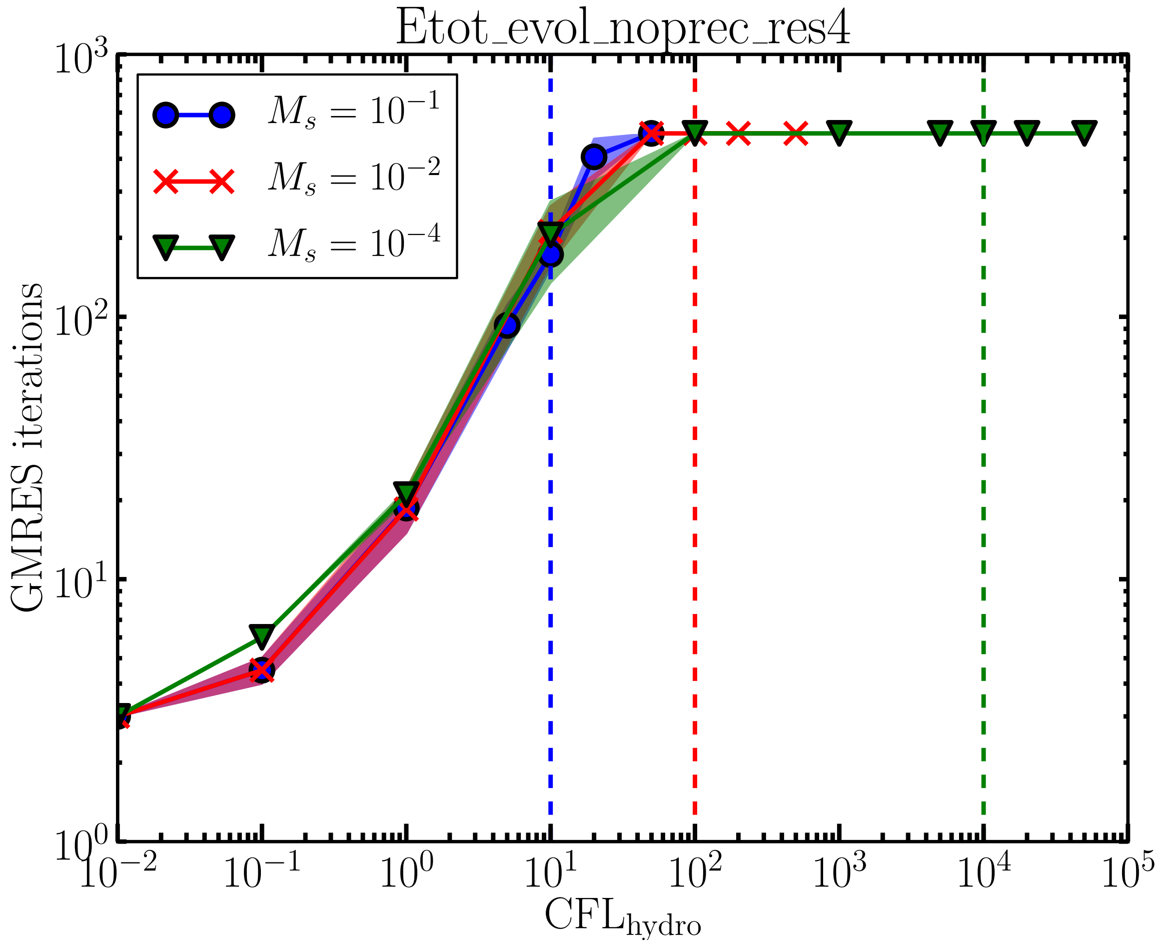
$$(JM^{-1})\delta X' = -F_U(X)$$
$$M\delta X = \delta X'$$

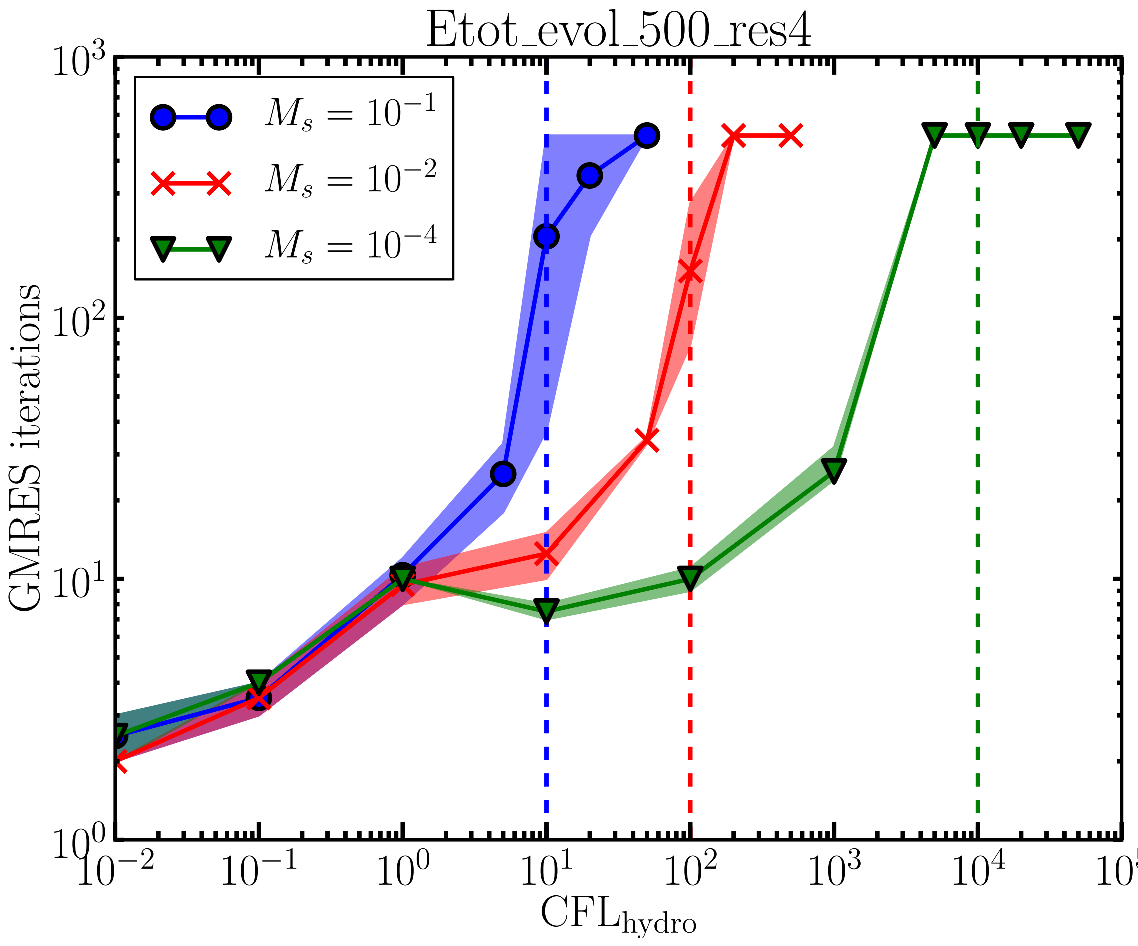


MUSIC - 3D strategy

Jacobian-Free Newton-Krylov with physics-based preconditioning

- Preliminary results on a 3D test: Taylor-Green vortex
  - Number iterations required to decrease the linear residual by a factor of $\eta = 10^{-4}$





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- **Conclusion**

Conclusion

- Jacobian-Free Newton-Krylov method for hydrodynamics
  - Stiffness spoils the convergence of the Krylov solver
- The preconditioner is the most important ingredient !
  - If you know any linear method that yields an approximate solution of your (nonlinear) problem, embedding it within a JFNK method will give you the accuracy
- Unlike algebraic preconditioning, physics-based preconditioning cures the stiffness at the level of the physical model
  - Pro: obtain maximum efficiency
  - Contra: problem dependent
- Free lunch: semi-implicit schemes also provide a better initial guess for NR
- Additional physics can be included in the preconditioner
  - Thermal diffusion: results in two coupled parabolic equations for p and e

END