Nuclear Reactions Coupled to Multi-dimensional Implicit Hydrodynamics

Philipp Edelmann
Max Planck Institute for Astrophysics (MPA), Garching, Germany

in collaboration with:
Fabian Miczek (MPA)
Friedrich Röpke, Alejandro Bolaños, Christian Klingenberg (Universität Würzburg)
Mach number $M = \frac{u}{c_{\text{sound}}}$ (low Mach number $M < 0.1$)

- stellar evolution is largely subsonic
- incompressible solution and sound waves decouple in low Mach number limit
- sound waves do not play a role in the evolution of the star
Mach number $M = \frac{u}{c_{\text{sound}}}$ (low Mach number $M < 0.1$)

▶ stellar evolution is largely subsonic
▶ incompressible solution and sound waves decouple in low Mach number limit
▶ sound waves do not play a role in the evolution of the star

situation in stellar evolution now (see also Raphael Hirschi’s talk)
▶ almost all stellar evolution simulations are performed in 1D
▶ need for modeling of intrinsically multi-dimensional phenomena (convection, shear instabilities, convective overshoot, etc.)
▶ treated using parametrized descriptions (e.g. mixing length theory)
Mach number $M = \frac{u}{c_{\text{sound}}}$ (low Mach number $M < 0.1$)

- stellar evolution is largely subsonic
- incompressible solution and sound waves decouple in low Mach number limit
- sound waves do not play a role in the evolution of the star

situation in stellar evolution now (see also Raphael Hirschi’s talk)

- almost all stellar evolution simulations are performed in 1D
- need for modeling of intrinsically multi-dimensional phenomena (convection, shear instabilities, convective overshoot, etc.)
- treated using parametrized descriptions (e.g. mixing length theory)

our aim

$\Rightarrow$ detailed, **multi-dimensional** simulations of critical phases required
Problems in Numerical Simulations

- Analytically, the Euler equations reduce to the incompressible equations in the limit $M \rightarrow 0$.
- Standard compressible numerical schemes have a different asymptotic behavior.

Employing standard Godunov-type compressible schemes causes:
- Artificial creation of sound waves.
- Excessive dissipation of kinetic energy in the low Mach number limit.
- But, the Euler equations do not include any viscosity terms $\Rightarrow$ ideally no dissipation.
Gresho Vortex

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

Mach number
Gresho Vortex with a Standard Compressible Code

$M = 0.1$

$M = 0.01$

$M = 0.001$

(F. Miczek)

Philipp Edelmann (MPA)

Nuclear Reactions Coupled to Multi-dimensional Implicit Hydrodynamics
Approaches to Low-Mach Number Simulations

change the underlying equations

1. Boussinesq approximation
   - assume only small deviations from hydrostatic background
   - spatially constant reference density
     - only thin atmospheric layers possible ($\ll$ pressure scale height)

2. Anelastic equations
   - time-independent, but spatially varying, hydrostatic background state
   - difficult to generalize to general equation of state and source terms
   - sound waves impossible, only valid in the low Mach number limit
Our Approach

- solve the compressible Euler equations with a Godunov-type finite volume scheme
- Roe’s approximate Riemann solver
- preconditioning matrix to ensure correct asymptotic behavior in the low Mach number limit

Advantages
- no simplifications in the basic equations
- all hydrodynamical effects modeled by the Euler equations are included
- applicable for all Mach numbers
Our Approach

- solve the compressible Euler equations with a Godunov-type finite volume scheme
- Roe’s approximate Riemann solver
- preconditioning matrix to ensure correct asymptotic behavior in the low Mach number limit

Advantages

- no simplifications in the basic equations
- all hydrodynamical effects modeled by the Euler equations are included
- applicable for all Mach numbers
LHC: Low Mach Number Hydro Code

- 1-, 2-, 3-D hydrodynamics
- implicit and explicit time stepping (up to 5\(^{th}\) order)
- 2\(^{nd}\) order spatial accuracy (no dimensional splitting)
- spatial and temporal discretization separate (method of lines)
- general structured meshes
- general equation of state
- radiation in the diffusion limit
- parallelized using MPI and/or OpenMP
- nuclear reaction network (operator-split and non-split)
Temporal Discretization

- **explicit schemes**
  - formula for the new time step can be written in an explicit form depending on information from the last time step only
  - evaluation of new time step simple and quick
  - numerical stability limits time step by CFL condition: 
    \[ \Delta t \leq \text{CFL} \cdot \frac{\Delta x}{c+|u|} \quad (\text{CFL} \approx 1) \]

- **implicit schemes**
  - new time step is the solution of an implicit equation
  - system of non-linear equations must be solved for every time step
  - no stability constraint
  - time step is typically chosen to resolve convective motions: 
    \[ \Delta t \approx \Delta x |u| \] (low Mach number case)
  - implicit time step are larger by a factor of 
    \[ (\Delta t)_{\text{imp}} = (\Delta t)_{\text{exp}} \approx c + |u| \approx M^{-1} \]
  - low Mach number preconditioner puts further constraints on CFL condition
Temporal Discretization

- **explicit schemes**
  - formula for the new time step can be written in an explicit form depending on information from the last time step only
  - evaluation of new time step simple and quick
  - numerical stability limits time step by CFL condition:
    \[ \Delta t \leq \frac{\Delta x}{c + |u|} \text{ (CFL} \approx 1) \]

- **implicit schemes**
  - new time step is the solution of an implicit equation
  - system of non-linear equations must be solved for every time step
  - no stability constraint
  - time step is typically chosen to resolve convective motions:
    \[ \Delta t \approx \frac{\Delta x}{|u|} \]
Temporal Discretization

- **explicit schemes**
  - formula for the new time step can be written in an explicit form depending on information from the last time step only
  - evaluation of new time step simple and quick
  - numerical stability limits time step by CFL condition: 
    \[ \Delta t \leq \text{CFL} \cdot \frac{\Delta x}{c + |u|} \]  
    (CFL \approx 1)

- **implicit schemes**
  - new time step is the solution of an implicit equation
  - system of non-linear equations must be solved for every time step
  - no stability constraint
  - time step is typically chosen to resolve convective motions: 
    \[ \Delta t \approx \frac{\Delta x}{|u|} \]

**low Mach number case**

- implicit time step are larger by a factor of 
  \[ \frac{(\Delta t)_{\text{imp}}}{(\Delta t)_{\text{exp}}} \approx \frac{c + |u|}{|u|} \approx M^{-1} \]
- low Mach number preconditioner puts further constraints on CFL condition
Gresho Vortex (revisited)

LHC with flux preconditioning

$M = 0.1$

$M = 0.01$

$M = 0.001$

(F. Miczek)
Efficiency Compared to Explicit

- implicit time steps are much larger
- but a single step is much more expensive

Test: simulation of the vortex problem at different Mach numbers

- comparison of computational time to reach the same physical time
- $512 \times 512$ grid
- speedup increases with larger grid sizes

<table>
<thead>
<tr>
<th>$M$</th>
<th>$10^{-1}$</th>
<th>$10^{-2}$</th>
<th>$10^{-3}$</th>
<th>$10^{-4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>speedup</td>
<td>0.7</td>
<td>4.0</td>
<td>39.8</td>
<td>389.5</td>
</tr>
</tbody>
</table>
nuclear reactions are a source term in the equations for conservation of species and energy
rate of change determined by rate equations (non-linear ODEs)
nuclear reactions are a source term in the equations for conservation of species and energy
rate of change determined by rate equations (non-linear ODEs)

Simplest Approach
operator splitting (alternating hydro and reaction steps)
Coupling Nuclear Reactions

- Nuclear reactions are a source term in the equations for conservation of species and energy.
- Rate of change determined by rate equations (non-linear ODEs).

**Simplest Approach**

- Operator splitting (alternating hydro and reaction steps).

**Extensions**

- Consider change of thermodynamic state during reaction step.
  Thermodynamics have to be imposed (e.g., constant $\rho$).
- Distribute energy release and composition change over hydro step.
Coupling Nuclear Reactions

- Nuclear reactions are a source term in the equations for conservation of species and energy.
- Rate of change determined by rate equations (non-linear ODEs).

**Simplest Approach**

- Operator splitting (alternating hydro and reaction steps).

**Extensions**

- Consider change of thermodynamic state during reaction step.
  - Thermodynamics have to be imposed (e.g. constant $\rho$).
- Distribute energy release and composition change over hydro step.

**Non-split Calculation**

- Add source terms directly to “right” side of hydro equations.
- Integration of reaction network together with the hydro equations.
Active vs. Passive Scalars

- composition is coupled to Euler equations through equation of state
- in principle: additional equation for every composition variable to be solved simultaneously with the Euler equations
- in practice: only a minor effect in many cases (e.g. ionized, ideal gas)
Active vs. Passive Scalars

- composition is coupled to Euler equations through equation of state
- in principle: additional equation for every composition variable to be solved simultaneously with the Euler equations
- in practice: only a minor effect in many cases (e.g. ionized, ideal gas)

Two Possibilities

**Passive Scalars**
composition is simply advected with the fluid flow
feedback with hydrodynamics only after the time step

**Active Scalars**
composition \( (\rho X_i) \) treated as additional variables
solve the whole system simultaneously
Non-split Treatment

- involved species must be active scalars
- active scalars are very expensive → do not use more than a few
- does not resolve processes below the chosen time step but finds consistent state
- provides a benchmark of splitting errors to justify the use of operator-splitting
Implementation in LHC

- nuclear reaction network YANN originally developed by Rüdiger Pakmor for SN Ia hydro simulations
- takes arbitrary REACLIB files as input
- electron screening
- Bader–Deuflhard scheme (adaptive time step) used in the operator-split case
- exactly the same functions for computing rates and derivatives in the split and non-split case
Test Problem

- test problem from Almgren et al. (2008)
- white dwarf model atmosphere
- initial composition: 30% $^{12}$C, 70% $^{16}$O
- one reaction rate: $^{12}$C + $^{12}$C $\rightarrow ^{24}$Mg
- high temperature bubbles
Philipp Edelmann (MPA) Nuclear Reactions Coupled to Multi-dimensional Implicit Hydrodynamics
Work in Progress

no flux preconditioning

flux preconditioning

active scalars (non-split)
passive scalars (operator split) 

active scalars (non-split)
Conclusions and Outlook

- conventional compressible hydro schemes exhibit unphysical behavior in the low Mach number case
- flux preconditioning can remedy this problem
- implicit time stepping in large multi-dimensional problems is efficient for low Mach numbers
- a nuclear reaction network has been integrated into the LHC
- systems of very few reaction rates can be solved in non-split fashion together with hydrodynamics
Conclusions and Outlook

- conventional compressible hydro schemes exhibit unphysical behavior in the low Mach number case
- flux preconditioning can remedy this problem
- implicit time stepping in large multi-dimensional problems is efficient for low Mach numbers
- a nuclear reaction network has been integrated into the LHC
- systems of very few reaction rates can be solved in non-split fashion together with hydrodynamics

Astrophysical Applications in multiple dimensions

- mixing in stellar interiors (e.g. convective overshoot)
- shear instabilities
- late stellar evolution phases (Si burning)
- classical novae