Mach-uniform time-stepping methods: The regularized Störmer-Verlet approach

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Outline

1. Euler equations for compressible fluid dynamics; Mach number $M = v_{ref}/c_s$; reversibility
2. incompressible limit ($M \to 0$); Lighthill radiation for small M
3. Regularization approach to Mach-uniform algorithms
4. Semi-Lagrangian Störmer-Verlet time-stepping
5. Numerical example

Outline

1 Euler equations

2 Lighthill radiation

3 Mach-uniform algorithms

4 Semi-Lagrangian Störmer-Verlet

5 Numerical example

Conservation form of Euler equations

Conservation of mass, momentum and energy leads (in dimensionless variables) to

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ (\rho \mathbf{v})_t + \nabla \cdot ((\rho \mathbf{v}) \circ \mathbf{v}) + M^{-2} \nabla p &= 0, \\ e_t + \nabla \cdot ((e + p)\mathbf{v}) &= 0 \end{aligned}$$

with energy density

$$e = \frac{M^2}{2\rho} \|\mathbf{v}\|^2 + \rho \varepsilon,$$

thermodynamic relation (ideal gas)

$$p = (\gamma - 1)\rho\varepsilon = R\rho T,$$

and Mach number

$$M = v_{ref}/c_s.$$

Incompressibility

The limit $M \to 0$ is easier to discuss in primitive variables $(\rho, \mathbf{v}, p)$:

$$\begin{aligned} \mathbf{v}_t + (\mathbf{v}\cdot\nabla)\mathbf{v} + \rho^{-1} M^{-2} \nabla p &= 0, \\ p_t + \mathbf{v}\cdot\nabla p + \gamma p \nabla\cdot\mathbf{v} &= 0 \end{aligned}$$

The boundedness of time-derivatives implies that

$$p(x,t) = p_0 + M^2 p_2(x,t;M)$$

and

$$\nabla\cdot\mathbf{v}_0 = 0,$$

where

$$\mathbf{v}(x,t) = \mathbf{v}_0(x,t) + M\,\mathbf{v}_1(x,t;M).$$

Reversibility and linearization

The Euler equations are reversible, i.e., the Euler equations are invariant under the involution

$$\mathbf{v} \mapsto -\mathbf{v}, \qquad t \mapsto -t.$$

Linearization about a motionless reference state leads to the acoustic wave equation

$$p_{tt} = \frac{\gamma p_0}{\rho_0 M^2} \nabla^2 p.$$

Here we have assumed, for simplicity, that ρ_0 and, hence, T_0 are constant.

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Lighthill equation

Recall that $p = p_0 + M^2 p_2$. We write

$$p_2 = p_{inc} + p',$$

where p_{inc} satisfies

$$\nabla \cdot \mathbf{v}_t = \nabla \cdot \left[(\mathbf{v} \cdot \nabla)\mathbf{v} + \rho^{-1} \nabla p_{inc} \right] = 0,$$

and

$$p'_{tt} - \frac{\gamma p_0}{\rho_0 M^2} \nabla^2 p' = S(x,t)$$

is the Lighthill equation [Lighthill, 1952] with source term S determined from the incompressible Euler equations.

Resonant interaction and wave generation

The Lighthill equation

$$p'_{tt} - \frac{\gamma p_0}{\rho_0 M^2} \nabla^2 p' = S(x,t)$$

allows for resonant interaction of slow vortical (incompressible) motion with sound waves of sufficiently large scales

$$l_{sound}/l_{ref} \sim M^{-1}.$$

The wave generation due to S is weak but of fixed power q in M.

This effect prevents the existence of a slow manifold to all orders in M.

Related problems

Related problems are discussed in the context of

- gravity waves in general relativity [Einstein, 1918]
- acoustic combustion instabilities; multiple length-scale analysis [Klein, 1995; Weinan E, 1992]
- inertia-gravity waves in atmospheric fluid dynamics
  - Numerical results lead to an exponent of $q = 4$ for the rotating shallow-water equations and unstable shear flow [Ford, 1994; McIntyre, 1998; Ford, McIntyre & Norton, 1999]).
  - simplified model: coupled ODE/PDE system [Lorenz, 1986; Vanneste, 2005]. Here an exponent of $q = 2$ appears.

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Existing approaches

It is desirable to have numerical algorithms that work for all Mach numbers $M < 1$.

A number of alternative approaches have been proposed:

- semi-implicit [Kwizak & Robert, 1971] and pressure correction methods [Harlow & Amsden, 1968], (2-TL non-reversible, 3-TL reversible, instabilities require numerical damping)
- fully (2-TL) implicit time-stepping methods [Coté et al, 1998] (iterative with typically 2 iterations, more expensive),
- scaling and preconditioning methods [Chorin, 1967; Browning & Kreiss, 1986; Darmofal & van Leer, 1998] (corrupt dynamics even on slow time-scales).

Regularization approach

The basic idea came out of a careful study of semi-implicit methods [Dubal, Frank, Reich, Staniforth, Wood, 2005-07]. We replace the Euler equations by

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ (\rho \mathbf{v})_t + \nabla \cdot ((\rho \mathbf{v}) \circ \mathbf{v}) + M^{-2} \nabla \widehat{p} &= 0, \\ e_t + \nabla \cdot ((e + \widehat{p}) \mathbf{v}) &= 0 \end{aligned}$$

The equations need to be closed by an appropriate relation between the thermodynamic pressure

$$p = RT\rho$$

(ideal gas) and its regularization $\widehat{p}$.

Regularized pressure equation

We define the divergence $\delta = \nabla \cdot \mathbf{v}$ and its "time derivative"

$$\delta^{(1)} = -\nabla \cdot \left[(\mathbf{v} \cdot \nabla)\mathbf{v} + \frac{1}{\rho M^2} \nabla p \right],$$

which is obtained from the Euler momentum equation.

Then we introduce the elliptic equation

$$\left[1 - \alpha^2 \frac{\gamma p}{\rho M^2} \nabla^2 \right] (\widehat{p} - p) = -\alpha^2 \gamma p \; \delta^{(1)}$$

in $\widehat{p}$. The parameter α is tunable.

Note that (i) $p = \widehat{p}$ for incompressible flows $\delta = \delta^{(1)} = 0$ and (ii) the regularized Euler equations are still reversible.

Properties of regularized equations

Linear stability: Linearization about motionless stationary state yields

$$|\omega| \le \frac{1}{\alpha}$$

for all frequencies $\omega(k)$ and wave numbers k.

Filtering: We obtain $\widehat{p} \approx p$ for $M \sim 1$. For $M \to 0$ recall that $p_2 = p_{inc} + p'$ and the regularization reduces to

$$\left[1 - \alpha^2 \frac{\gamma p}{\rho M^2} \nabla^2\right] \widehat{p'} \approx p'.$$

Hence we have either

(i) $\widehat{p'} \approx 0$ for $l_{sound}/l_{ref} = \mathcal{O}(M^0)$ (incompressible regime)

or

(ii) $\widehat{p'} \approx p'$ for $l_{sound}/l_{ref} = \mathcal{O}(M^{-1})$ (Lighthill regime).

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The basic idea

Ideal fluid dynamics may be viewed as the motion of a continuum of “particles” with positions $\mathbf{x}(\mathbf{a},t)$. Hence the Euler equations are equivalent to (Lagrangian formulation)

$$\frac{D\mathbf{u}}{Dt} = \mathbf{F} := -\frac{1}{\rho M^2}\nabla p, \qquad \frac{D\mathbf{x}}{Dt} = \mathbf{u}.$$

Formally apply Störmer-Verlet to the regularized formulation to yield:

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \widehat{\mathbf{F}}^{n+1/2}, \quad \mathbf{x}^{n+1/2} = \mathbf{x}^{n-1/2} + \Delta t \mathbf{u}^n$$

with

$$\widehat{\mathbf{F}} = -\frac{1}{\rho M^2}\nabla \widehat{p}.$$

Linear stability requires $\alpha \geq \Delta t/2$.

The semi-Lagrangian (SL) aspect

The continuum of particles is replaced by a set of grid-points $\mathbf{x}_\beta$. The SL method consists of two parts:

- Computation of departure points $\mathbf{x}_\beta^d$ (not necessarily grid points) such that

$$\mathbf{x}_\beta = \mathbf{x}_\beta^d + \Delta t\, \mathbf{u}^{n+1/2}(\mathbf{x}_\beta^d).$$

  Linear interpolation is used for finding $\mathbf{u}^{n+1/2}(\mathbf{x}_\beta^d)$.

- Advection equation

$$\frac{D\Theta}{Dt} = 0$$

  is then implementated numerically using

$$\Theta_\beta^{n+1} = \Theta^n(\mathbf{x}_\beta^d).$$

  Cubic interpolation is used for $\Theta^n(\mathbf{x}_\beta^d)$.

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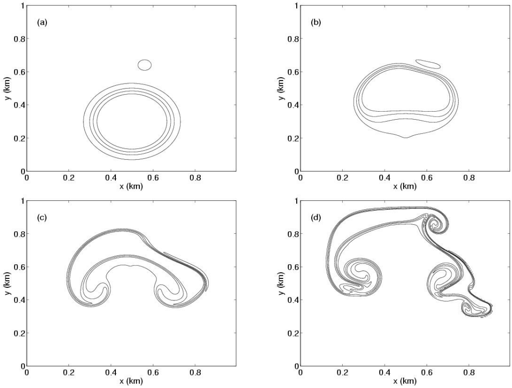
Robert's warm and cold bubble experiment



Step size Δt is about 100 x larger than what CFL condition would dictate for an explicit method. But a small $\Delta x = \Delta y = 5$ m is required to capture nonlinear advection.

Summary

- Generalization to strongly stratified flows (gravitation) non-trivial but feasible, algorithms applicable to both hydrostatic and non-hydrostatic flow regimes (Dubal, Wood, Staniforth, Reich [2007]; Hundertmark & Reich [2007]).
- If necessary, unresolved small-amplitude acoustic waves in p' can be accounted for by dissipation-fluctuation terms in the regularization $p \mapsto \widehat{p}$ (see Staniforth & Wood [2006] for dissipation).
- Combination with conservative spatial discretization techniques (conservative SL method of Cotter et al. [2007].
- Similar ideas can be used in molecular dynamics to treat the stiff bonded interactions of water, for example.