

Simulating Variable Density Flows in the Low-Mach Number Limit with Incompact3D

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Introduction

Outline

- Introduction
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 - The Low Mach Number (LMN) approximation
- QuasIncompact3D: LMN in Incompact3D
 - Algorithm to solve LMN
 - Treatment of pressure equation
- Results
 - Scaling on ARCHER and MARCONI
 - 2D mixing layer
 - Non-Boussinesq gravity currents
- Conclusion

Introduction

What problem are we trying to solve?

- Incompact3D provides powerful capabilities for solving *incompressible* flows...
- or flows with small density variations ($\Delta\rho \lesssim 0.01\rho_0$)

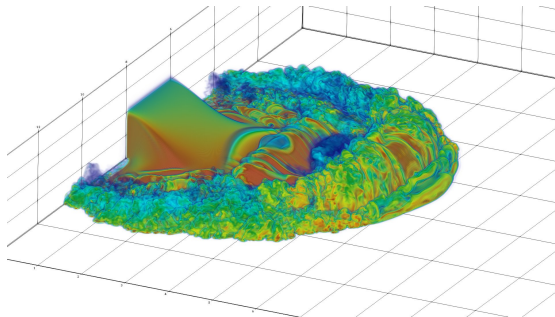


Figure: Gravity-driven flow simulated by Incompact3D¹

¹<https://twitter.com/incompact3d>

Introduction

The problem with compressible flow

- If density variations are significant, needs to be treated as *compressible* flow
- Flow velocity may still be low ($\gamma M^2 \ll 1$)
- Results in ill-conditioned equations, e.g.

$$\gamma M^2 \rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \frac{\gamma M^2}{Re} \nabla \cdot \boldsymbol{\tau}$$

- Numerically this leads to requirement for very small timesteps
 - Inefficient!

Introduction

The Low Mach Number Approximation

- Expand variables as power series using $\varepsilon = \gamma M^2$ as the small parameter and take lowest order terms (recall $\gamma M^2 \ll 1$)

$$\mathbf{u} = \mathbf{u}^{(0)} + \varepsilon \mathbf{u}^{(1)} + \varepsilon^2 \mathbf{u}^{(2)} + \dots$$

$$p^{(0)} = \rho^{(0)} T^{(0)}$$

$$\frac{\partial \rho^{(0)}}{\partial t} + \nabla \cdot \rho^{(0)} \mathbf{u}^{(0)} = 0$$

$$\mathbf{0} = \nabla p^{(0)}$$

$$\rho^{(0)} \frac{\partial T^{(0)}}{\partial t} + \rho^{(0)} \mathbf{u}^{(0)} \cdot \nabla T^{(0)} = \frac{\nabla \cdot k \nabla T^{(0)}}{Re Pr T^{(0)}} + \frac{dp^{(0)}}{dt}$$

$$\frac{\partial \rho^{(0)} \mathbf{u}^{(0)}}{\partial t} + \nabla \cdot \rho^{(0)} \mathbf{u}^{(0)} \mathbf{u}^{(0)} = -\nabla p^{(1)} + \frac{\nabla \cdot \boldsymbol{\tau}^{(0)}}{Re}$$

Introduction

The Low Mach Number Approximation (cont.)

- Combining continuity and temperature equations yields velocity divergence constraint

$$\nabla \cdot \mathbf{u} = \frac{1}{p^{(0)}} \left(\frac{\nabla \cdot k \nabla T}{RePr} - \frac{dp^{(0)}}{dt} \right)$$

- Boundary condition follows

$$\int_{\partial\Omega} \mathbf{u} \cdot \hat{\mathbf{n}} dS = \frac{1}{p^{(0)}} \left(\frac{1}{RePr} \int_{\partial\Omega} k \nabla T \cdot \hat{\mathbf{n}} dS - \frac{dp^{(0)}}{dt} V_{\Omega} \right)$$

- Open domains

$$\frac{dp^{(0)}}{dt} = 0 \Rightarrow p^{(0)} = p_a$$

- Advance density in time²

$$\rho^{k+1} = \rho^k + \Delta t \nabla \cdot (\rho \mathbf{u})^k$$

- Update temperature via EOS and compute $\nabla \cdot \mathbf{u}^{k+1}$

$$T^{k+1} = \frac{p^{(0)}}{\rho^{k+1}} \Rightarrow \nabla \cdot \mathbf{u}^{k+1} = \frac{\nabla \cdot k \nabla T^{k+1}}{p^{(0)} RePr}$$

- Integrate momentum via fractional step method³

$$(\rho \mathbf{u})^* = (\rho \mathbf{u})^k - \Delta t \left(\nabla \cdot (\rho \mathbf{u} \mathbf{u})^k - \frac{\nabla \cdot \boldsymbol{\tau}^k}{Re} \right)$$

$$(\rho \mathbf{u})^{k+1} = (\rho \mathbf{u})^* - \Delta t \nabla \widetilde{p^{(1)}}^{k+1} \Rightarrow \mathbf{u}^{k+1} = \frac{(\rho \mathbf{u})^{k+1}}{\rho^{k+1}}$$

²Alternative algorithm updates temperature

³Chorin (1997)

Numerical Method

The Poisson Equation - Constant Coefficient

- Like incompressible approach, take divergence of momentum directly

$$\nabla^2 \widetilde{p^{(1)}}^{k+1} = \frac{1}{\Delta t} \left(\nabla \cdot (\rho \mathbf{u})^* - \nabla \cdot (\rho \mathbf{u})^{k+1} \right)$$

- + Constant coefficient Poisson equation: direct solvers available
- Need an approximation for $\nabla \cdot (\rho \mathbf{u})^{k+1}$

$$\nabla \cdot (\rho \mathbf{u})^{k+1} = - \left. \frac{\partial \rho}{\partial t} \right|^{k+1} \approx - \frac{\rho^{k+1} - \rho^k}{\Delta t} + \mathcal{O}(\Delta t)$$

Numerical Method

The Poisson Equation - Variable Coefficient

- Alternatively, $\nabla \cdot \mathbf{u}^{k+1}$ is available as a constraint⁴

$$\Rightarrow \nabla \cdot \frac{1}{\rho} \nabla \widetilde{p^{(1)}}^{k+1} = \frac{1}{\Delta t} \left(\nabla \cdot \mathbf{u}^* - \nabla \cdot \mathbf{u}^{k+1} \right)$$

- Cannot solve directly using spectral solver
- Iterative solver

$$\begin{aligned} \nabla^2 \widetilde{p^{(1)}}^{\nu+1} &= \nabla^2 \widetilde{p^{(1)}}^{\nu} + \tilde{\rho} \left[\frac{1}{\Delta t} \left(\nabla \cdot \mathbf{u}^* - \nabla \cdot \mathbf{u}^{k+1} \right) - \nabla \cdot \frac{1}{\rho} \nabla \widetilde{p^{(1)}}^{\nu} \right] \\ \left\| \Delta \widetilde{p^{(1)}} \right\| &\leq \text{tol} \end{aligned}$$

⁴c.f. incompressible flow: $\nabla \cdot \mathbf{u} = 0$

Numerical Method

The Poisson Equation - Discussion

- **Constant coefficient**

- + Direct solver \rightarrow fast solution
- Extrapolation is potential source of error
- Does not recover $\nabla \cdot \mathbf{u}^{k+1} = 0$ in inviscid case⁵

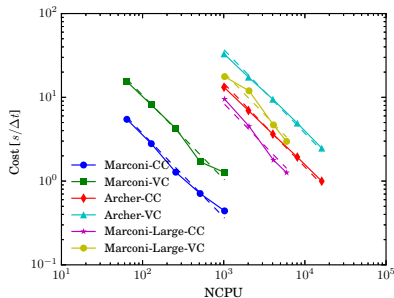
- **Variable coefficient**

- + Obeys $\nabla \cdot \mathbf{u}^{k+1}$ constraint
- Iteration is potentially very expensive!

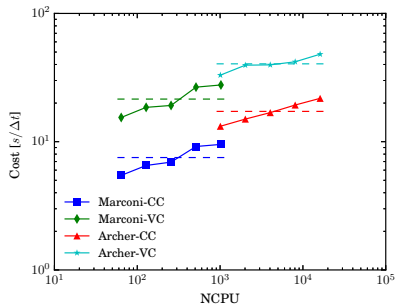
⁵Nicoud (2000)

Results

Scalability tests



(a) Strong scaling



(b) Weak scaling

Figure: Strong and weak scaling of QuasiIncompact3D, performed on ARCHER and MARCONI with periodic BCs

Results

2D Non-Isothermal Mixing Layer - Initial & Boundary Conditions

- Hyperbolic tangent velocity profile

$$u(y) = \frac{u_1 + u_2}{2} + \frac{u_1 - u_2}{2} \tanh\left(\frac{2y}{\delta}\right)$$

$$u_c = \frac{u_1 \sqrt{T_2} + u_2 \sqrt{T_1}}{\sqrt{T_1} + \sqrt{T_2}} = 0$$

$$\frac{T_2}{T_1} = \frac{1}{2}, \quad \frac{dp^{(0)}}{dt} = 0$$

- Initial perturbation applied to velocity field to promote transition
- Periodic in x no-slip on y

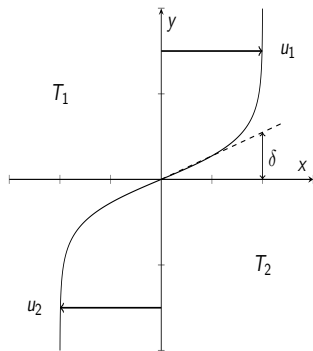


Figure: Diagram of non-isothermal mixing layer

Results

2D Non-Isothermal Mixing Layer - Results (Vorticity)

CC



VC ρ_0



VC ρ_h



G2005



Results

2D Non-Isothermal Mixing Layer - Results (Density)

CC



VC ρ_0



VC ρ_h

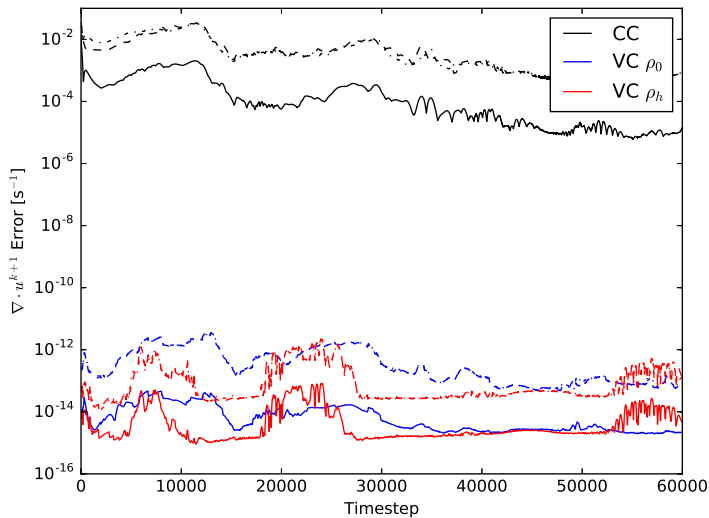


G2005



Results

2D Non-Isothermal Mixing Layer - Results (Error in $\nabla \cdot \mathbf{u}^{k+1}$)



Results

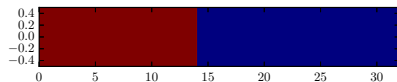
2D Non-Isothermal Mixing Layer - Results (Performance Comparison)

| Poisson Eq. | CPU / Δt [s] |
|-------------|---------------------------|
| CC | 4.48×10^{-2} |
| VC ρ_0 | 6.16×10^{-1} |
| VC ρ_h | 3.53×10^{-1} |
| | Cost (normalised) |
| CC | 1 |
| VC ρ_0 | 13.75 |
| VC ρ_h | 7.88 |
| | Time (its) in Poisson [%] |
| CC | 23.4 (1) |
| VC ρ_0 | 94.2 (34.1) |
| VC ρ_h | 89.9 (18.8) |

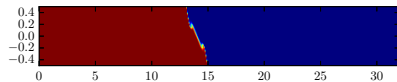
Results

2D Non-Boussinesq Lock-Exchange Problem⁶

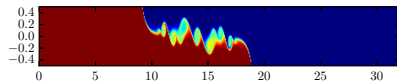
- Two fluids of different densities $\rho_2 > \rho_1$ horizontally separated in a vertical gravity field
- $\nu_1 = \nu_2 \Rightarrow$ test of variable viscosity implementation
- Results to be validated against data of Birman *et al.* (2005)



(a) $t = 0$



(b) $t = 2$



(c) $t = 10$

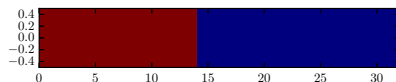
Figure: Lock-exchange $\frac{\rho_2}{\rho_1} = 0.998$

⁶Anecdotally, this case highlights the importance of the guess for $p^{\nu=0}$!

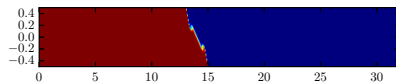
Results

2D Non-Boussinesq Lock-Exchange Problem⁷

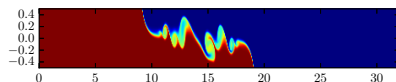
- Two fluids of different densities $\rho_2 > \rho_1$ horizontally separated in a vertical gravity field
- $\nu_1 = \nu_2 \Rightarrow$ test of variable viscosity implementation
- Results to be validated against data of Birman *et al.* (2005)



(a) $t = 0$



(b) $t = 2$



(c) $t = 10$

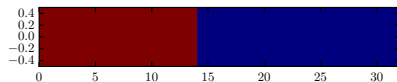
Figure: Lock-exchange $\frac{\rho_2}{\rho_1} = 0.92$

⁷Anecdotally, this case highlights the importance of the guess for $p^{\nu=0}$!

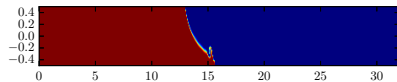
Results

2D Non-Boussinesq Lock-Exchange Problem⁸

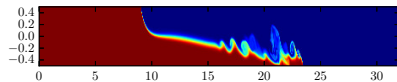
- Two fluids of different densities $\rho_2 > \rho_1$ horizontally separated in a vertical gravity field
- $\nu_1 = \nu_2 \Rightarrow$ test of variable viscosity implementation
- Results to be validated against data of Birman *et al.* (2005)



(a) $t = 0$



(b) $t = 2$



(c) $t = 10$

Figure: Lock-exchange $\frac{\rho_2}{\rho_1} = 0.2$

⁸Anecdotally, this case highlights the importance of the guess for $p^{\nu=0}$!

Conclusion and Future Work

- LMN implemented in Incompact3D
- Implemented constant and variable coefficient Poisson solvers
- Proposed new formulation for variable coefficient Poisson solver
- Complete simulation of buoyant, turbulent jets
- Complete validation of non-Boussinesq lock-exchange in 2D
- Investigate 3D non-Boussinesq lock-exchange problem

Thanks for listening!

Numerical Method

The Poisson Equation - Variable Coefficient, Choice of $\tilde{\rho}$

- Free choice of $\tilde{\rho}$
- Choice of $\tilde{\rho}$ will affect convergence
- Typical choices are an average or minimum value, $\tilde{\rho} = \rho_0$
 - Stems from '*brute force*' derivation of iteration equation
- Chain-rule suggests $\tilde{\rho}$ should vary in space

$$\begin{aligned}\nabla \cdot \frac{1}{\rho} \nabla \widetilde{p^{(1)}} &= \frac{1}{\rho} \nabla^2 \widetilde{p^{(1)}} + \nabla \frac{1}{\rho} \cdot \nabla \widetilde{p^{(1)}} \\ &= \frac{1}{\rho} \nabla^2 \widetilde{p^{(1)}} + \left(\nabla \cdot \frac{1}{\rho} \nabla \widetilde{p^{(1)}} - \frac{1}{\rho} \nabla^2 \widetilde{p^{(1)}} \right) \\ &\Rightarrow \tilde{\rho} = \left(\overline{1/\rho} \right)^{-1}\end{aligned}$$

- + Harmonic average is proportional to local minimum - promoting stability