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

Paul Bartholomew
Sylvain Laizet

- Introduction
  - Motivation
  - The Low Mach Number (LMN) approximation
- `QuasIncompact3D`: the implementation of LMN in `Incompact3D`
  - Algorithm to solve LMN
  - Treatment of pressure equation
- Testcases
  - Scaling on `ARCHER` and `MARCONI`
  - 2D mixing layer
  - 2D non-Boussinesq lock-exchange
- Conclusion

Introduction

What problem are we trying to solve?

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

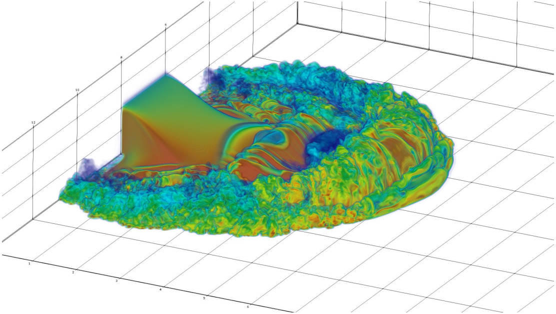


Figure: Gravity-driven flow simulated by `Incompact3D`[1]

[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.*

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

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

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

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

$$\begin{aligned}
p^{(0)} &= \rho^{(0)} T^{(0)} \\
\frac{\partial \rho^{(0)}}{\partial t} + \boldsymbol{\nabla} \cdot \rho^{(0)} \boldsymbol{u}^{(0)} &= 0 \\
\boldsymbol{0} &= \boldsymbol{\nabla} p^{(0)} \\
\rho^{(0)} \frac{\partial T^{(0)}}{\partial t} + \rho^{(0)} \boldsymbol{u}^{(0)} \cdot \boldsymbol{\nabla} T^{(0)} &= \frac{\boldsymbol{\nabla} \cdot k \boldsymbol{\nabla} T^{(0)}}{RePrT^{(0)}} + \frac{dp^{(0)}}{dt} \\
\frac{\partial \rho^{(0)} \boldsymbol{u}^{(0)}}{\partial t} + \boldsymbol{\nabla} \cdot \rho^{(0)} \boldsymbol{u}^{(0)} \boldsymbol{u}^{(0)} &= -\boldsymbol{\nabla} p^{(1)} + \frac{\boldsymbol{\nabla} \cdot \boldsymbol{\tau}^{(0)}}{Re}
\end{aligned}$$

- Combining continuity and temperature equations yields velocity divergence constraint

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

- Boundary condition follows

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

- Open domains

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

Numerical Method

Overview

- Advance density in time[2]

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

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

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

- Integrate momentum via fractional step method[3]

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

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

[2] Alternative algorithm updates temperature

[3] Chorin (1997)

- Like incompressible approach, take divergence of momentum directly

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

+ Constant coefficient Poisson equation: direct solution possible

− Need an approximation for $\boldsymbol{\nabla}\cdot(\rho\boldsymbol{u})^{k+1}$

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

- Alternatively, $\boldsymbol{\nabla} \cdot \boldsymbol{u}^{k+1}$ is available as a constraint[4]

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

- Cannot solve directly using spectral solver
- Iterative solver

$$\nabla^2 \widetilde{p^{(1)}}^{\nu+1} = \nabla^2 \widetilde{p^{(1)}}^{\nu} + \widetilde{\rho} \left[\frac{1}{\Delta t} \left(\boldsymbol{\nabla} \cdot \boldsymbol{u}^{\star} - \boldsymbol{\nabla} \cdot \boldsymbol{u}^{k+1} \right) - \boldsymbol{\nabla} \cdot \frac{1}{\rho} \boldsymbol{\nabla} \widetilde{p^{(1)}}^{\nu} \right]$$

$$\left|\left| \Delta \widetilde{p^{(1)}} \right|\right| \leq \mathtt{tol}$$

[4] *c.f.* incompressible flow: $\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$

Numerical Method

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

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

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

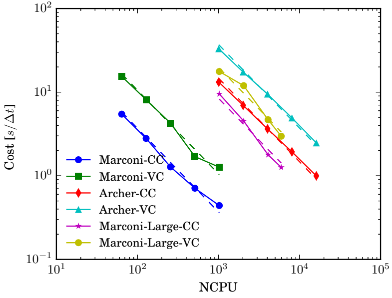
\+ Harmonic average is proportional to local minimum - promoting stability

- **Constant coefficient**
  - \+ Direct solver → fast solution
  - − Extrapolation is potential source of error
  - − Does not recover $\nabla \cdot \boldsymbol{u}^{k+1} = 0$ in inviscid case[5]
- **Variable coefficient**
  - \+ Obeys $\nabla \cdot \boldsymbol{u}^{k+1}$ constraint
  - − Iteration is potentially very expensive!

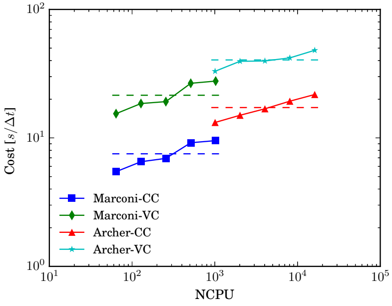
[5] Nicoud (2000)

Testcases

Scalability tests



(a) Strong scaling



(b) Weak scaling

Figure: Strong and weak scaling of QuasIncompact3D, performed on `ARCHER` and `MARCONI` with periodic BCs

- Hyperbolic tangent velocity profile

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

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

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

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

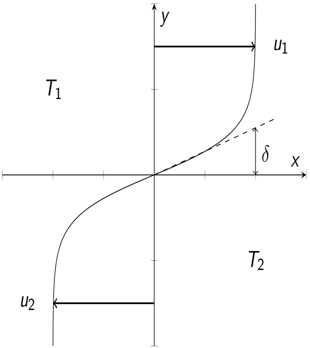


Figure: Diagram of non-isothermal mixing layer

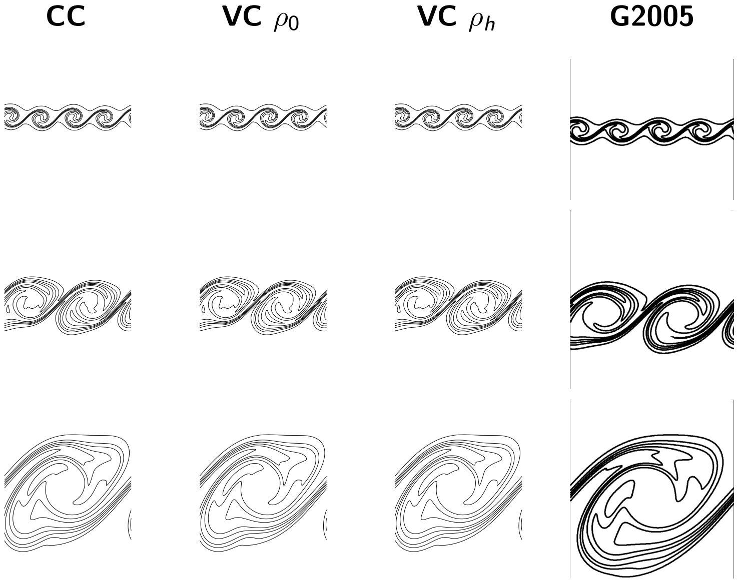
Testcases

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

CC	VC ρ_0	VC ρ_h	G2005

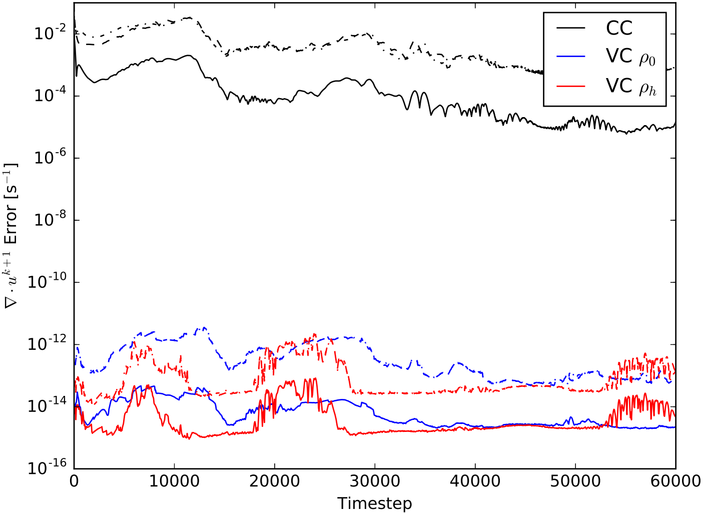
Testcases

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



Testcases

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



Testcases

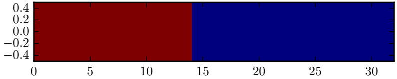
2D Non-Isothermal Mixing Layer - Results (Performance Comparison)

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)

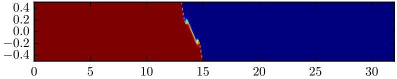
Testcases

2D Non-Boussinesq Lock-Exchange Problem[6]

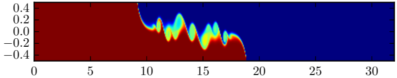
- Two fluids of different densities $\rho_2 > \rho_1$ horizontally separated in a vertical gravity field
- $\nu_1 = \nu_2 \Rightarrow$ test of variable viscosity implementation
- Results to be validated against data of Birman *et al.* (2005)



(a) $t = 0$



(b) $t = 2$



(c) $t = 10$

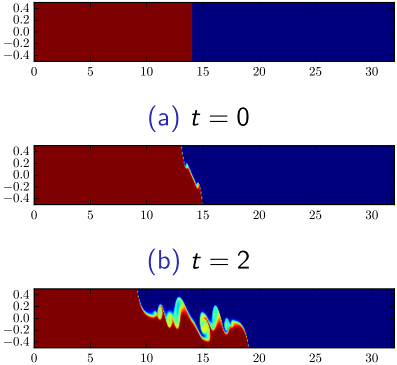
Figure: Lock-exchange $\dfrac{\rho_2}{\rho_1} = 0.998$

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

Testcases

2D Non-Boussinesq Lock-Exchange Problem[7]

- 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) $t = 10$

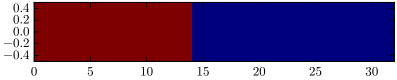
Figure: Lock-exchange $\dfrac{\rho_2}{\rho_1} = 0.92$

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

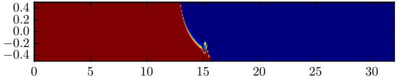
Testcases

2D Non-Boussinesq Lock-Exchange Problem[8]

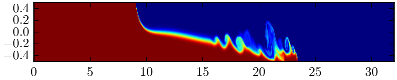
- Two fluids of different densities $\rho_2 > \rho_1$ horizontally separated in a vertical gravity field
- $\nu_1 = \nu_2 \Rightarrow$ test of variable viscosity implementation
- Results to be validated against data of Birman *et al.* (2005)



(a) $t = 0$



(b) $t = 2$



(c) $t = 10$

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

[8]Anecdotally, 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!