Things that can wrong in computational astrophysics

Simulations are *approximations* to reality! It is the mark of a good computational astrophysicist to recognise the limitations of numerical solutions instead of identifying artificial results with “nature”. Simulations can produce spurious results for many reasons:

- Insufficient resolution/low-order convergence (many of the other problems are also resolution problems in disguise, but can't be fixed because the required resolution is not affordable)
- Different fluid regimes require different numerical methods
- The hydro solver may be prone to purely numerical instabilities
- Problems with boundary conditions
- The grid geometry spoils the results
- Instabilities due to the coupling of hydrodynamic fluid flow and combustion/radiative transfer
- Bugs

Numerical Diffusivity and Viscosity

- The most obvious approximation is the use of discrete grid, which introduces a discretisaion error.
- Our investigation of the modified equation earlier on is an a important step.
- For some simple first-order advection methods, we showed that the modified equation is essentially characterised by the appearance of a numerical diffusion term.
- For non-linear Riemann solvers and higher-order reconstruction methods, this is no longer a straightforward procedure, but one can use heuristic strategies to analyse these methods as well.

A Concrete Example – Neutron Star Cooling

- Consider a young proto-neutron star left behind by a supernova explosions. It will emit $\sim 10^{53}\,\mathrm{erg}$ by neutrinos within the first $\tau_\mathrm{cool} \sim 5\,\mathrm{s}$.
- What numerical scheme do we need to simulate this initial "Kelvin-Helmholtz" cooling phase and the neutrino signal from it?
- If we user a first-order scheme with the Rusanov or HLLE flux, than the numerical diffusivity is: $D_\mathrm{num} \sim \Delta r\, c_s$ and the corresponding diffusion time-scale is

$$\tau_\mathrm{num} \sim \frac{R^2}{D} = \frac{R^2}{\Delta r\, c_s} = N_r \tau_\mathrm{sound}.$$

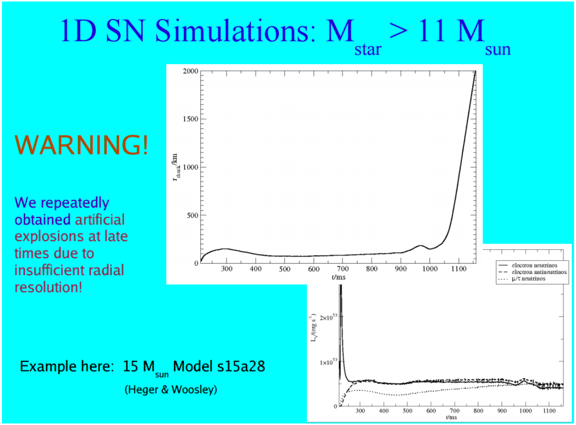
- So unless $N_r \tau_\mathrm{sound} \gg \tau_\mathrm{cool}$, numerical diffusion will compete with physical diffusion, and the neutron star will cool too fast in the simulation.
- With $c_s \approx c/\sqrt{3}$ and $R = 15\,\mathrm{km}$, the sound crossing time becomes $\approx 0.9 \times 10^{-4}\,\mathrm{s}$.
- So we would need $N_r \gg 60,000$ radial zones to model with with HLLE and first-order reconstruction.
- Most likely, we need at least ten times more zones to be on the safe side and get anywhere close to convergence.

Numerical Diffusivity for Higher-Order Methods

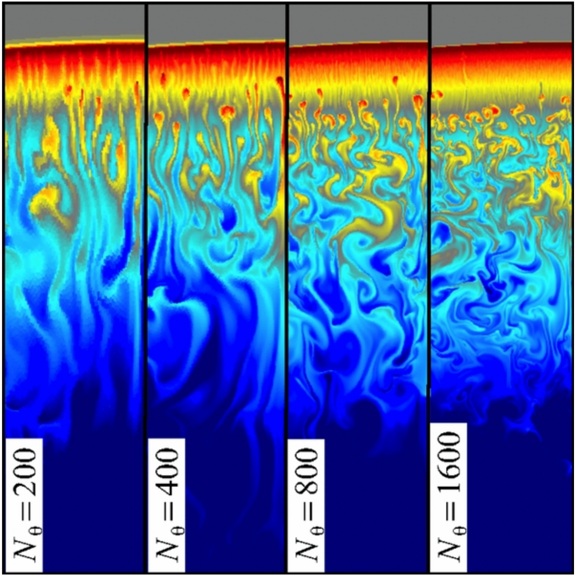
- For a second-order method, the diffusion will be *of the same order* on the grid-scale!
- The reason for this is that for the reconstruction reverts back to first order for the smallest possible mode, which is an odd-even mode with $\lambda_{\mathrm{grid}} = 2\Delta r$.
- Because of higher-order reconstruction, the effective diffusivity is no longer given by a linear diffusion term in the modified equation, but we can still characterise it by a *scale-dependent* numerical diffusivity.
- If the order of convergence is n, we can assume that the error and the numerical diffusivity on a larger scale λ will scale as $D \sim D_{\mathrm{grid}}(2\Delta r/\lambda)^{n-1}$.
- For a second-order method, the numerical diffusion time-scale for the entire neutron star then becomes

$$\tau_{\mathrm{num}} \sim \frac{R^2}{(\Delta r\, c_s)(2\Delta r/R)} = \frac{N_r^2}{2}\tau_{\mathrm{sound}}$$

- Hence $N_r \gg 333$ and if we calculate with a sufficient safety margin, this implies that at least several thousand zones would be needed to avoid spurious numerical diffusion.



Insufficient resolution is usually a "benign" problem, because it is one of the first things people think about. But sometimes reminders are helpful. . .



Duffell & MacFadyen 2013, ApJ 775,87

Viscosity and Turbulence

- Importance of advective vs. viscous terms in Navier-Stokes equations characterised by *Reynolds number* $\mathrm{Re} = vL/\nu$, where L is the typical length scale and ν is the kinematic viscosity.
- For typical astrophysical explosions, Re is large. For thermonuclear explosions of white dwarfs: $\mathrm{Re} \sim 10^{14}$.
- Flow at such high Reynolds numbers is turbulent (except under very rare circumstances), and is characterised by a cascade of eddies, whose typical velocities scale with $v \propto l^{1/3}$ (l: eddy size).
- Can this be simulated?

- The numerical kinematic viscosity is the numerical diffusivity (dimensions L^2/T) in the momentum equation.
- Thus, for HLLE/Rusanov, we have $\nu_{\mathrm{num}} \sim \Delta l \, c_s$ for small velocities on the grid scale.
- For Riemann solvers that resolve the contact discontinuity, the effective kinematic viscosity is $\nu_{\mathrm{num}} \sim \Delta l \, v$ on the grid scale.

The numerical Reynolds number that can be reached for a certain resolution ($N = L/\Delta l$: number of zones in one direction) is therefore

$$\mathrm{Re} \sim \frac{vL}{c_s \Delta l} \approx \mathrm{Ma}\, N$$

for HLLE/Rusanov-type solvers, and

$$\mathrm{Re} \sim \frac{vL}{v_{\mathrm{grid}} \Delta l} = \left(\frac{L}{\Delta l}\right)^{4/3} = N^{4/3}$$

for solvers like HLLC, Marquina, Roe, or the exact Riemann solver.

Numerical Reynolds Number

This implies:

- The maximum numerical Reynolds number that can be reached nowadays with ~ 2048 per direction is of the order of 2×10^4.
- Thus, we can barely enter the regime of fully developed turbulence.
- Astrophysical Reynolds numbers are far out of reach.
- If the turbulent region occupies only part of the numerical domain, the Reynolds number is much smaller.
- Riemann solvers that don't resolve all the waves in the Riemann fan are much less suited for capturing turbulent flow, especially at low Mach numbers!

Why simulations still work for many purposes

- For sufficiently high Reynolds number, the turbulent structures become self-similar over a wide range of scales ("turbulent cascade").
- Thus flows with different Reynolds numbers will look similar.
- For many purposes it doesn't matter for the overall solution at which scales dissipation occurs.
- As long as the numerical dissipation mimics the effect of turbulent dissipation, the results remain trustworthy.
- This is known as the ILES (**I**mplicit **L**arge **E**ddy **S**imulations) approach.
- But: For magnetohydrodynamic turbulence or systems with extreme ratios of the heat conductivity, kinematic viscosity, and the diffusivity for different fluid components (e.g nuclear species), this assumption may be break down.
- Even for "normal" subsonic turbulence, unexpected phenomena can still happen at $\mathrm{Re} \sim 10^5$, such as the "drag crisis" (the effect that makes dimpled golf balls fly faster than smooth ones).

Extreme Flow Regimes – Low Mach Number

- At low Mach number, time-explicit finite-volume schemes introduce artificial sound wave activity.
- This smears out and distorts features in low Mach number flow.
- This is shown on the right using the Gresho vortex as an example.
- In the vortex, the pressure gradient and the centrifugal force balance exactly, and it should be perfectly stationary.
- Specialised numerical methods are needed in this regime.

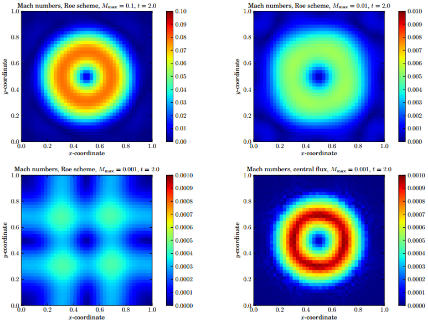


Figure 4.2: Mach number distributions at the end of the simulation time

Fabian Miczek, PhD thesis

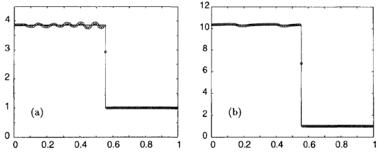


Fig. 7.2. Oscillations generated in a slowly-moving shock. The shock was initially at $x = 0.5$ and has moved to $x = 0.555$ at time $t = 0.5$. **(a)** Density **(b)** Pressure

Leveque, in *Computational Methods for Astrophysical Fluid Flow*

Ringing behind a slowly moving shock

Solution: Play with your reconstruction method...

Numerical Instabilities of Shocks

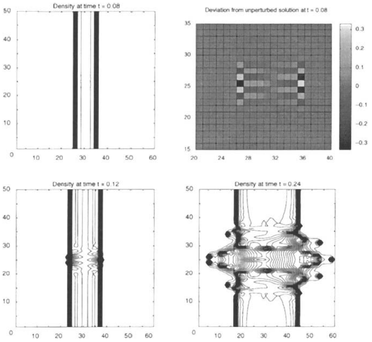


Fig. 7.3. Colliding winds give rise to two outgoing shock waves. An initial density perturbation of magnitude 10^{-6} grows due to numerical instability

Leveque, in *Computational Methods for Astrophysical Fluid Flow*

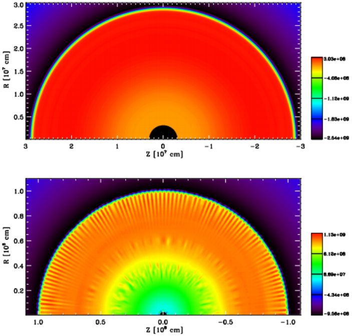
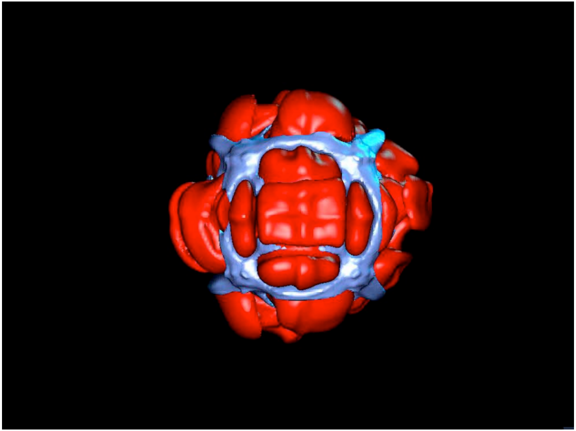


Figure 3.23: Odd-even decoupling in the test calculation (see text). Note that while (R, Z) coordinates of the cylindrical grid which was used for plotting are indicated in the Figure, the calculations have been performed in spherical coordinates. From top to bottom: a) Radial velocity (in cm/s) of the unperturbed model, at $t = 30$ ms. b) Radial velocity at $t = 108$ ms, after seed perturbations have been added to the model shown in a).

K. Kifonidis, PhD thesis

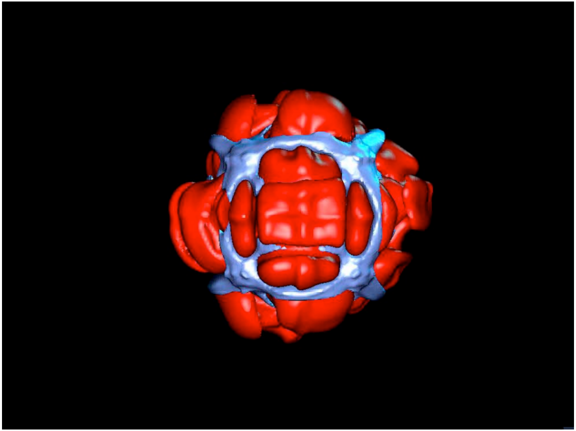
The exact Riemann solver and the Roe solver are prone odd-even decoupling behind grid-aligned shocks and to the carbuncle phenomenon (protrusion of shocks where they are locally aligned with the grid). This gets worse at high resolution.
Solution: Switch to a more dissipative solver near strong shocks.

The Effect of the Grid Geometry



Burrows, Emerging Themes in the Theory of CC SNe Explosions, KITP Conference 2009

The Effect of the Grid Geometry



Burrows, Emerging Themes in the Theory of CC SNe Explosions, KITP Conference 2009

The grid geometry often dictates in which direction instabilities grow fastest. This happens for Cartesian coordinates (strong $m = 4$ modes) and spherical polar coordinate (singular at the axis) alike. Sometimes it matters, sometimes it doesn't.

Sonic Points

- The exact Riemann solver has a mild instability at sonic points ($v = \pm c_s$), where it can give expansion shocks (though not as bad as the Roe solver).
- This can happen, e.g., in the transonic neutrino-driven wind from a young neutron star.
- **Solution:** Switch to a more dissipative solver if this occurs.

Nuclear Burning

- Nuclear burning rates often have an extremely steep temperature dependence
- Sometimes the burning time-scale is so short that cells burn instantly once they exceed a certain ignition temperature
- Under these circumstances, numerical diffusion can determine the propagation of burning fronts
- Suspicion is in order if a burning front always propagates by one grid cell per time-step
- **Solution:** Switch off burning in shocks, use special front-tracking methods.

Bugs

Scientists can be very creative at coming up with new bugs, but some are particularly popular:

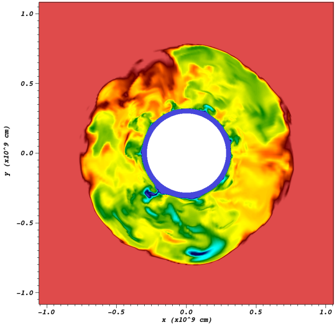
- Index errors (debuggers sometimes help)
- Sign errors
- Wrong brackets
- Unit conversion errors
- Typos involving the * and ** operators (multiplication and exponentiation) in Fortran
- Search-and-replace errors

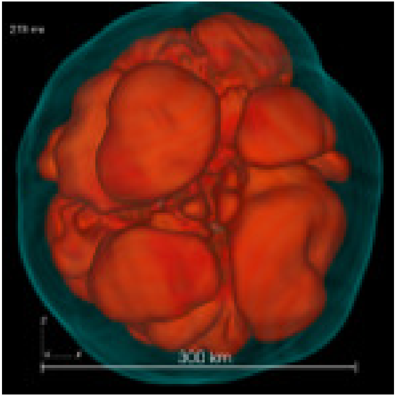
Failsafe Strategies

- Analyse simulation results early while the simulation is running.
- "Conservative" coding – don't rewrite your code more often than necessary once it works.
- Understand the physics behind the problem and use analytic results and rule-of-thumb estimates to check your simulation.
- Run test cases with known solutions.
- Run your code in 1D before you run it in 2D, and in 2D before you run in it in 3D (if you can).
- Know the strengths and weakness of your numerical method. There is often a fix available for some of its shortcomings already.
- Consult with colleagues.
- Don't be intimated: Not all bugs and numerical artefacts are lethal!

Beyond shock tubes: Multi-dimensional problems from real life

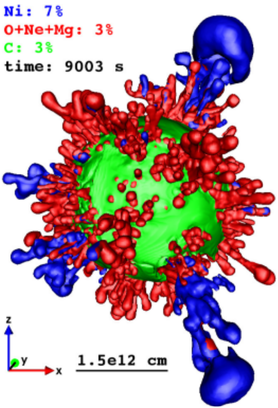
Buoycancy-Driven Instabilities – Convection

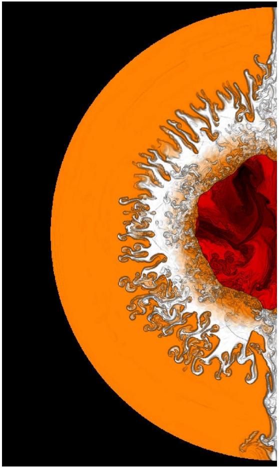




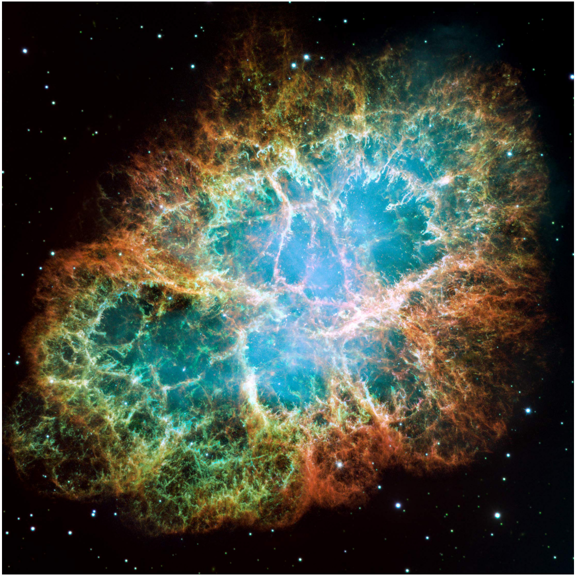
Rayleigh-Taylor Instability

Mixing in supernova envelopes:





Rayleigh-Taylor Instability

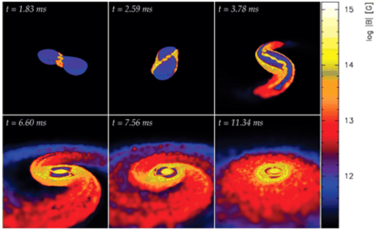


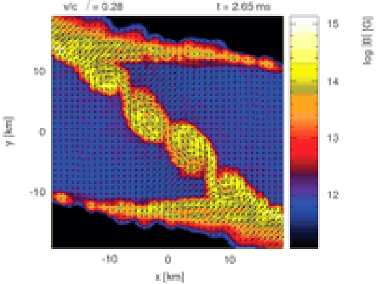
Crab Nebula

Shear-Driven Instabilities - Kelvin-Helmholtz Instability

Kelvin-Helmholtz instability between different atmospheric layers.

This is what we REALLY want to simulate! Where do these instabilities come from?





KH instability in neutron star mergers.

If we have $\rho = \mathrm{const.}$, then the continuity equation and the momentum equation simplify to:

$$\begin{aligned} \nabla \cdot \mathbf{v} &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} + \frac{\nabla P}{\rho} &= \mathbf{g} \end{aligned}$$

Obviously, the continuity equation is no longer a time-evolution equation. Instead it is now a *constraint equation* that states that the velocity vector field is *divergence-free*. Because of this constraint, we can also get rid of the energy equation. If the velocity field is to remain divergence-free, then we must have $\partial(\nabla \cdot \mathbf{v})/\partial t = 0$ and hence:

$$\begin{aligned} \nabla \cdot [(\mathbf{v} \cdot \nabla)\mathbf{v}] + \frac{\Delta P}{\rho} &= \nabla \cdot \mathbf{g} \\ \Delta P &= \rho \nabla \cdot \mathbf{g} - \rho \nabla \cdot [(\mathbf{v} \cdot \nabla)\mathbf{v}] \end{aligned}$$

Thus, we get an elliptic (Poisson-like) equation for the pressure, i.e. the gravitational acceleration and the velocity field at a given time completely determine the pressure (together with the boundary conditions). Since the pressure is determined by an elliptic equation and the density is constant, this also implies that we the internal energy density is determined everywhere. Only the momentum equation remains as an evolution equation.

The fact that the pressure is determined by an elliptic equation means that some signal velocities are infinite in the incompressible approximation. The pressure adjusts instantaneously to perturbations elsewhere in the fluid. A more rigorous analysis shows that the incompressible case corresponds to the limit of vanishing Mach number $|v| \ll c_s$ or $c_s \to \infty$, i.e. it is the sound waves that propagate at an infinite speed.

In practice, the assumption of incompressible flow is adequate up to $\mathrm{Ma} \approx 0.3$ in many terrestrial applications. In stratified media (where ρ varies strongly, but the flow is still subsonic), one can make similar approximations in this flow regime (anelastic approximation, Boussinesq approximation).

Let us linearise the incompressible Euler equations around the background state. For the background state, we have $\mathbf{v}_{1,2} = (\pm u, 0, 0)$ and $\partial P_{1,2}/\partial z = -\rho_{1,2} g$. Let the velocity perturbation be $\delta \mathbf{v} = (\delta u, 0, \delta w)$ and let δP be the pressure perturbation. Then we have

$$
\begin{aligned}
\frac{\partial u}{\partial t} + u \frac{\partial \delta u}{\partial x} + \frac{1}{\rho} \frac{\partial \delta P}{\partial x} &= 0 \\
\frac{\partial w}{\partial t} + u \frac{\partial \delta w}{\partial x} + \frac{1}{\rho} \frac{\partial \delta P}{\partial z} &= 0
\end{aligned}
$$

for the two fluids above and below the interface. In addition,

$$
\frac{\partial \delta u}{\partial x} + \frac{\partial \delta w}{\partial z} = 0
$$

must hold.

Let us use the ansatz

$$\delta u = Ae^{\omega t + ikx + \lambda z}, \quad \delta w = Be^{\omega t + ikx + \lambda z}, \quad \delta P = Ce^{\omega t + ikx + \lambda z}$$

where A, B, C, and D are complex. This ansatz using oscillating/evanescent wave can be applied because the equations are translationally invariant *within* either region. Similarly, for the displacement ζ of the fluid interface, we use:

$$\zeta = De^{\omega t + ikx}.$$

The solenoidal constraint $\partial \delta u / \partial x + \partial \delta w / \partial x = 0$ leads to:

$$\begin{aligned} ikA + \lambda B &= 0 \\ \lambda &= -\frac{ikA}{B} \end{aligned}$$

Moreover, the condition $\nabla \cdot (\partial \delta \mathbf{v}/\partial t) = 0$ leads to:

$$\begin{aligned} u(-k^2 A + ik\lambda B) + \frac{1}{\rho}(\lambda^2 - k^2) C &= 0 \\ u(-k^2 A + k^2 A) - \frac{1}{\rho}\left(\frac{k^2 A^2}{B^2} + k^2\right) C &= 0 \\ \left(\frac{k^2 A^2}{B^2} + k^2\right) C &= 0 \end{aligned}$$

We therefore must have $B^2 = -A^2$, or $B = \pm iA$, which then implies

$$\lambda = \begin{cases} k, & B = -iA, \quad \text{region 1} \\ -k, & B = iA, \quad \text{region 2} \end{cases}$$

for positive wave vectors k. For negative k, we must choose $\lambda = -k$ in region 1 and $\lambda = k$ in region 2, so that the perturbtions asymptote to zero far away from the discontinuity.

Again restricting ourselves to positive k, we therefore have

$$
\begin{aligned}
\omega B_1 + ikuB_1 + k\frac{C_1}{\rho_1} &= 0, \\
\omega B_2 - ikuB_2 - k\frac{C_2}{\rho_2} &= 0,
\end{aligned}
$$

in region 1 and region 2 from the momentum equation for δw. The equation for δu does not add any new condition. Two more equations are needed to obtain a dispersion relation $\omega(k)$.

Linear Stability Analysis – Jump Conditions

The interface between the two fluids is a contact discontinuity, so we must have

$$P_1(x,\delta z,t) = P_2(x,\delta z,t), \quad w_1(x,\delta z,t) = w_2(x,\delta z,t). \tag{1}$$

First we impose continuity of the pressure. Bearing in mind that we can neglect second order terms like $\delta z\, \partial \delta P/\partial z$, this implies

$$\zeta \frac{\partial P_1}{\partial z} + \delta P_1(x,0,t) = \zeta \frac{\partial P_2}{\partial z} + \delta P_2(x,0,t).$$

Then we replace $\partial P/\partial z$ using $\partial P/\partial z = -\rho g$ for the unperturbed system, and substitute our ansatz for δP:

$$\begin{aligned}
-\rho_1 g \zeta + C_1 e^{\omega t + ikx} &= -\rho_2 g \zeta + C_2 e^{\omega t + ikx}, \\
-\rho_1 g D e^{\omega t + ikx} + C_1 e^{\omega t + ikx} &= -\rho_2 g D e^{\omega t + ikx} + C_2 e^{\omega t + ikx}, \\
C_1 - C_2 &= D(\rho_1 - \rho_2) g
\end{aligned}$$

In the *comoving* frame on each side, time derivative of ζ is just given by δw,

$$\left(\frac{\mathrm{d}\zeta}{\mathrm{d}t}\right)_{1,2} = \frac{\partial\zeta}{\partial t} \pm u\frac{\partial\zeta}{\partial x} = \delta w_{1,2}.$$

If ζ is to be continuous across the jump, we must have

$$\left(\frac{\partial\zeta}{\partial t}\right)_1 = \left(\frac{\partial\zeta}{\partial t}\right)_2,$$

which implies

$$\begin{aligned}
\frac{\partial\zeta}{\partial t} + u\frac{\partial\zeta}{\partial x} &= \delta w_1 \\
\frac{\partial\zeta}{\partial t} - u\frac{\partial\zeta}{\partial x} &= \delta w_2 \\
D(\omega + iku) &= B_1 \\
D(\omega - iku) &= B_2
\end{aligned}$$

Combining $D(\omega \pm iku) = B_{1,2}$ and $C_1 - C_2 = D(\rho_1 - \rho_2)g$, and $B_{1,2}(\omega \pm iku) \pm kC_{1,2}/\rho_{1,2} = 0$ yields:

$$
\begin{aligned}
D(\omega \pm iku)^2 \pm \frac{kC_{1,2}}{\rho_{1,2}} &= 0 \\
C_1 &= -\frac{\rho_1}{k} D(\omega + iku)^2 \\
C_2 &= \frac{\rho_2}{k} D(\omega + iku)^2
\end{aligned}
$$

$$
-\frac{\rho_1}{k} D(\omega + iku)^2 - \frac{\rho_2}{k} D(\omega - iku)^2 = D(\rho_1 - \rho_2)g
$$

$$
-(\rho_1 + \rho_2)\omega^2 + 2iku(\rho_2 - \rho_1)\omega + \left[(\rho_1 + \rho_2)k^2u^2 + (\rho_2 - \rho_1)gk\right] = 0
$$

The dispersion relation can be further simplified using the Atwood number $At = (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$:

$$
\omega^2 - 2iku\,\mathrm{At}\,\omega - \left[k^2u^2 + \mathrm{At}\,gk\right] = 0
$$

The general case with non-zero At and u will be left as a homework problem.
Let us first consider what happens for $\rho_1 = \rho_2$ $(\mathrm{At} = 0)$:

$$\omega^2 - k^2 u^2 = 0$$

We thus have one unstable (exponentially growing) mode with $\omega = ku$ and a stable mode with $\omega = -ku$.
This is the Kelvin-Helmholtz instability. It occurs for all wave numbers, and grows fastest for small wavelengths (high wave numbers).

For $u = 0$, we have

$$\omega^2 - \mathrm{At}\, gk = 0$$

For $\mathrm{At} > 0$ ($\rho_2 > \rho_1$), we get an unstable mode with $\omega = \sqrt{\mathrm{At}\ gk}$. This is the Rayleigh-Taylor instability. For $\rho_2 < \rho_1$, i.e. for light fluid on top of heavy fluid, both modes are purely oscillatory.

General case

- One can show than in the general case of non-zero u and At a fluid interface is unstable only if

$$u^2 > -\frac{\mathrm{At}}{1-\mathrm{At}^2} g k^{-1}.$$

- This means that a fluid interface can always be driven to the unstable regime by increasing u.
- For positive Atwood number, all wavelengths are unstable. For negative Atwood number, buoyancy has a stabilizing effect, and only short wavelengths with $k > |\mathrm{At}|/(1-\mathrm{At}^2) g/u^2$ are unstable.