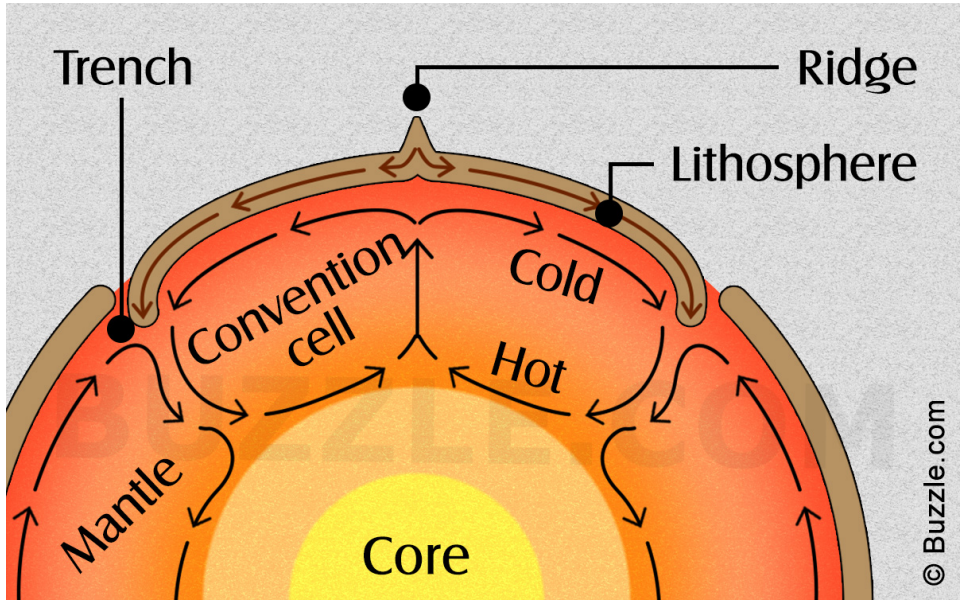


Applying class concepts to describe convection cells

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Applied Math 205
Harvard University

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Outline for solving problems numerically:

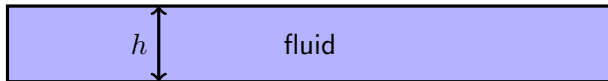
1. What are the equations?
2. What are the units?
3. Which parts of the equations are important?
4. What does a simplified model suggest the answer should be? **This is critical!**
5. What is the specific discretized equation to be solved?
6. What method is appropriate given the problem parameters?

What are the equations?

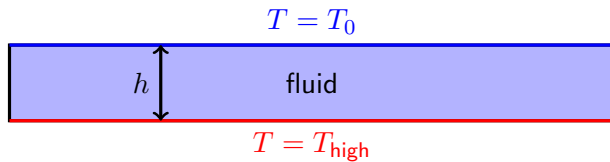


fluid

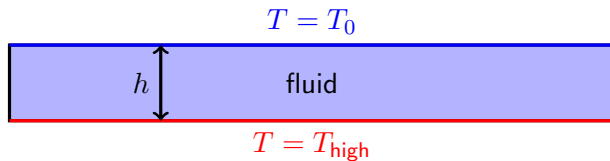
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What's evolving?

► density: $\rho = \rho_0 [1 - \alpha(T - T_0)]$

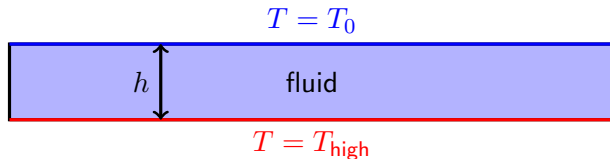
parameters:

- coeff. of thermal expansion α

variables:

- density ρ
► temperature T

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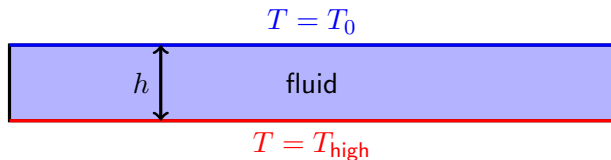
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► density: $\rho = \rho_0 [1 - \alpha(T - T_0)]$

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$$\rho_0 \frac{D\mathbf{u}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{u} - \rho g \hat{\mathbf{z}},$$

► temperature:

$$\frac{DT}{Dt} = \kappa \nabla^2 T + \left(\frac{\mu}{\rho_0 c} \right) \nabla \mathbf{u} : \nabla \mathbf{u},$$

parameters:

- coeff. of thermal expansion α
- gravitation g
- viscosity μ
- therm. diffusivity K
- spec. heat capacity c

variables:

- density ρ
- temperature T
- velocity \mathbf{u}
- pressure p

What are the units?

- ▶ The bits storing values in our simulations have no concept of units
- ▶ Square plot of land, width 10 ft, height 5 m. Plug 5 and 10 into calculation for area 50. Is this wrong?
- ▶ No! Our chosen **computational units** are
 - ▶ width: feet
 - ▶ height: meters
 - ▶ area: foot-meters The result makes perfect sense in this context!
- ▶ It is **vital** to know what your computational units are. A few common approaches:
 1. use physical units. Most of us do this without thinking about it, e.g.

$$[\text{force}] = \text{N} = \frac{\text{kg m}}{\text{s}^2}, \quad [\text{time}] = \text{s}, \quad [\text{length}] = \text{m}.$$

2. non-dimensionalize and use problem-relevant scalings. **Why do this?**

What are the units? (scalings for temperature equations)

- ▶ From the density equation $\rho = \rho_0 [1 - \alpha (T - T_0)]$, it's clear $T - T_0$ is the “real” temperature variable [note $d(T - T_0) = dT$ so derivatives are unchanged.]

$$\text{Scale: } \Delta T = T_{\text{high}} - T_0, \quad \text{Dim'less temp: } \boxed{\theta = \frac{T - T_0}{\Delta T}}.$$

- ▶ We can use the height h as a length scale.
- ▶ Introduce a velocity scale U , so $\boxed{\mathbf{v} = U \mathbf{u}}$. Time scale: $\tau = h/U$ and $\boxed{t = \tau s}$,

$$\underbrace{\left(\frac{U \Delta T}{h}\right)}_{\text{const.}} \underbrace{\frac{D\theta}{Ds}}_{\text{vars.}} = \underbrace{\left(\frac{\kappa \Delta T}{h^2}\right)}_{\text{c}} \underbrace{\nabla^2 \theta}_{\text{v}} + \underbrace{\left(\frac{\mu U^2}{\rho_0 c h^2}\right)}_{\text{c}} \underbrace{\nabla \mathbf{v} : \nabla \mathbf{v}}_{\text{v}}.$$

- ▶ Letting $U = \kappa/h$:

$$\frac{D\theta}{Ds} = \nabla^2 \theta + \left[\frac{\mu(\kappa/h^2)}{\rho_0 c \Delta T} \right] \nabla \mathbf{v} : \nabla \mathbf{v}$$

Which parts of the equations are important?

- ▶ We have a non-dimensional parameter M , with

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- ▶ What does M represent? Let's look at units more.

$$[\mu] = \frac{\text{energy}}{\text{volume} \times \text{time}}, \quad [\kappa] = \frac{\text{length}^2}{\text{time}}, \quad [\rho_0 c] = \frac{\text{energy}}{\text{volume} \times \text{temperature}}.$$

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$$[M] = \left[\frac{\mu(\kappa/h^2)}{\rho_0 c \Delta T} \right] = \frac{\text{viscous energy density}}{\text{thermal energy density}} = \text{dim'less.}$$

In water? Substituting in material constants: $M = 10^{-4} \left(\frac{\mu \text{m}^2 \text{ } ^\circ\text{C}}{h^2 \Delta T} \right).$

Given temp. difference of one degree, would need **fluid thickness of 10 nm!**

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- ▶ We have a non-dimensional parameter M , with

$$\frac{D\theta}{Ds} = \nabla^2\theta + M\nabla\mathbf{v} : \nabla\mathbf{v}, \quad \boxed{M \ll 1 \implies \frac{D\theta}{Ds} = \nabla^2\theta.}$$

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What are the units? (Reprise I)

Scalings (computational units):

$$[\text{velocity}] = U = \frac{\kappa}{h}, \quad [\text{length}] = h,$$

$$[\text{density}] = \rho_0, \quad [\text{temperature}] = \Delta T, \quad [\text{time}] = \tau = h^2/\kappa.$$

Dimensionless variables:

$$\mathbf{u} = U\hat{\mathbf{u}}, \quad \rho = \hat{\rho}\rho_0, \quad T = T_0 + \Delta\theta, \quad t = \tau\hat{t}.$$

Equations:

$$\hat{\rho} = 1 - \alpha\Delta T\theta, \quad \frac{D\theta}{D\hat{t}} = \nabla^2\theta,$$

Our choice of scaling has greatly simplified these two! What about velocity?

What are the units? (Reprise II)

The cost of choosing scalings that simplify the temperature equation is that we have non-trivial terms in the velocity equation! Letting $\nu = \mu/\rho_0$ and doing some algebra,

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_0}\nabla p + \nu\nabla^2\mathbf{u} - \frac{\rho}{\rho_0}g\hat{\mathbf{z}},$$

Some simplifying: let $\tilde{p} = \hat{p} + (gh^2/\nu\kappa)(z/h)$,

Prandtl number and Rayleigh number:

$$\frac{\kappa}{\nu} = \frac{1}{\text{Pr}} = \frac{\text{thermal diffusion}}{\text{momentum diffusion}}, \quad \frac{\alpha\Delta Tgh^3}{\nu\kappa} = \text{Ra} = \frac{\text{convection}}{\text{conduction}}$$

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What are the equations? (Reprise)

Eliminating ρ , we have three equations for three variables, and two parameters Pr and Ra :

$$\frac{D\theta}{Dt} = \nabla^2 \theta, \quad \frac{1}{Pr} \frac{D\mathbf{u}}{Dt} = -\nabla \tilde{p} + \nabla^2 \mathbf{u} + Ra \theta \hat{\mathbf{z}}, \quad \nabla \cdot \mathbf{u} = 0.$$

Some static part of the pressure must be dedicated to balancing the thermal gradient. Let $\mathbf{u} = \mathbf{0}$ and look for static solutions $\partial_t = 0$. The solutions are given by \tilde{P} and Θ , with $\Theta = 1 - z$ and

$$\nabla \tilde{P} = Ra \theta \hat{\mathbf{z}} \implies \tilde{P} = Ra z \left(1 - \frac{z}{2}\right).$$

Now we can look for perturbations from this solution, $\tilde{p} = \tilde{P} + \delta p$, $\theta = \Theta + \delta\theta$, $\mathbf{u} = \delta\mathbf{u}$:

$$\frac{1}{Pr} \frac{\partial \delta\mathbf{u}}{\partial t} = -\nabla \delta p + \nabla^2 \delta\mathbf{u} + Ra \delta\theta \hat{\mathbf{z}}, \quad \frac{\partial \delta\theta}{\partial t} = \delta\mathbf{u} \cdot \hat{\mathbf{z}} + \nabla^2 \delta\theta.$$

Now we have two coupled linear equations. Let's combine to get one!

What are the equations? (Reprise II)

Assume $\delta\theta = \delta\theta(z)$. Apply $(\partial_z \nabla \cdot)$ to velocity equation:

$$\nabla^2 \partial_z \delta p = \text{Ra} \partial_z \delta\theta.$$

Apply $(\nabla^2 \hat{z} \cdot)$...

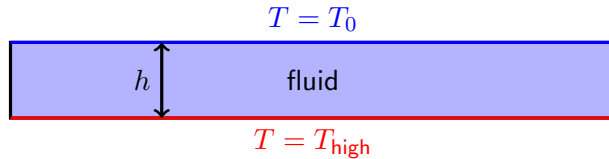
$$\nabla^2 \partial_z \delta p = \nabla^4 w + \text{Ra} \nabla^2 \delta\theta - \frac{1}{\text{Pr}} \nabla^2 \partial_t w,$$

and combine:

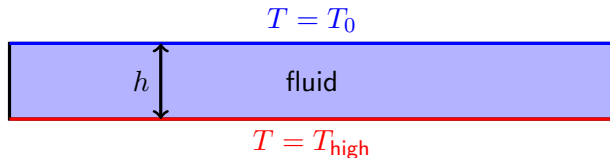
$$\nabla^2 \left(\frac{1}{\text{Pr}} \partial_t - \nabla^2 \right) w = \text{Ra} (\nabla^2 - \partial_z^2) \delta\theta, \quad \partial_t \delta\theta = w + \nabla^2 \delta\theta.$$

Vector + scalar equation \rightarrow two scalar equations! Almost there...

What are the boundary conditions?

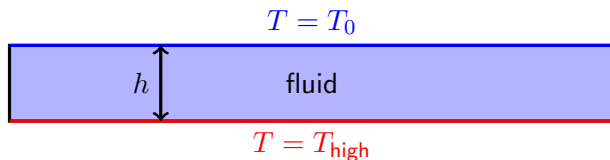


What are the boundary conditions?



- $T = T_0$ at top, $T = T_{\text{high}}$ at bottom $\implies \theta = 0$ at $z = 1$, $\theta = 1$ at $z = 0$,
 $\implies \boxed{\delta\theta = 0 \text{ at } z = 0, 1.}$

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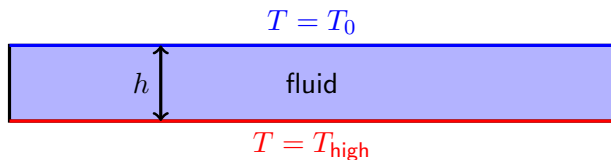
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- No divergence: $\nabla \cdot \mathbf{u} = 0$. Split into vertical and horizontal parts:

$$\mathbf{u} = w\hat{\mathbf{z}} + \mathbf{u}_h \implies \nabla \cdot \mathbf{u} = \partial_z w + \nabla_h \cdot \mathbf{u}_h.$$

No-slip condition (no tangential velocity) at top or bottom:

$$\implies \boxed{\partial_z w = 0 \text{ at } z = 0, 1.}$$

What are the equations? (Finale)

Now, if we're just interested in the spacing between convection cells, we can omit time derivatives:

$$-\nabla^4 w = \text{Ra} (\nabla^2 - \partial_z^2) \delta\theta, \quad \boxed{0 = w + \nabla^2 \delta\theta.}$$

We've got everything down to one equation!

$$\nabla^6 \delta\theta = \text{Ra} (\nabla^2 - \partial_z^2) \delta\theta.$$

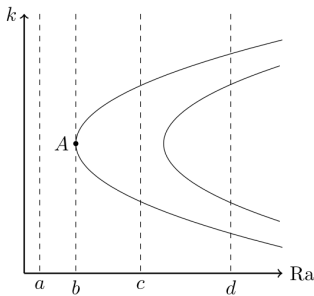
Linear stability analysis: let $\delta\theta = f(z) \exp(i\mathbf{k} \cdot \mathbf{x}_h)$. (What does this mean?)

$$\boxed{\frac{-1}{k^2} \left(\frac{d}{dz^2} - k^2 \right)^3 f = \text{Ra} f, \quad f = 0, \quad f'' = k^2 f, \quad f''' = k^2 f' \text{ on } z = 0, 1.}$$

Why is this sufficient for what we want to know? What is \mathbf{k} ? What is Ra?

This is an eigenvalue problem.

There won't be an f satisfying our equation for any combination of k and Ra : the solutions lie on different contours representing different modes of instability:



The lowest value of Ra allowing for convection is at point A : finding that point will tell us the critical value of Ra at which convection cells will form.

What is the specific discretized equation to be solved?

Let $D_k = -k^{-2} (d_z^2 - k^2)$. Then

$$D_k f = \text{Ra } f$$

looks a lot like a matrix equation. What are ways that we could solve this?

- ▶ analytics / algebra
- ▶ shooting method
- ▶ represent D_k as a matrix and find the eigenvalues (“chalkboard”)

Group project problem:

In quantum mechanics, the steady wavefunction $\psi = \psi(\mathbf{x}, t)$ for a particle of mass m is described by the Schrödinger equation,

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right] \psi(\mathbf{x}) = E\psi(\mathbf{x}),$$

where $V(\mathbf{x})$ is the potential energy around the particle, \hbar is the reduced Planck constant, and E is the particle's energy. In general, solutions only exist for certain values of the energy (it is quantized.) The form of the wavefunction and corresponding energy level represents an eigenvector/-value pair of the operator on the LHS.

Consider a 1D potential $V(x)$ which is infinite outside of the range $x \in [-L/2, L/2]$. Within the range, $V = 0$ for $|x| > w/2$ and otherwise $V = V_0$. Formulate the steady Schrödinger equation in dimensionless variables. What are the dimensionless parameters?

Let $w = L/3$. Choose three values for (the dimensionless analogue to) V_0 . Report the first four energy levels and plot the probability ($p = \psi\psi^*$) distribution of the particle for each mode.