Material Equations

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Newtons second law

- momentum balance

  $$\varrho\,\mathrm{D}_t\,v_k = \partial_i T_{ki} + f_k$$

- solid body, region $\mathcal{V}$
- velocity field spatially constant in $\mathcal{V}$
- $T_{ki} = 0$ at $\partial\mathcal{V}$
- integrate over $\mathcal{V}$

  $$M\,\mathrm{D}_t\;v_k = \int \mathrm{d}V\,f_k = F_k$$

- acceleration as felt by a co-moving observer

First law of TD for a fluid medium

- A slowly moving fluid is characterized by
  $$T_{ki} = -p\delta_{ki}$$
- internal energy balance
  $$\varrho\,\mathrm{D}_t\,u = -\partial_i J^{\mathrm{u}}_i - p\,\partial_i v_i$$
- no friction, no electric field, u and p spatially constant in small region $\mathcal{V}$
- divergence of velocity is
  $$\partial_i v_i = \varrho\,\mathrm{D}_t\,\varrho^-1$$
- Integration over volume of a constant mass
  $$\mathrm{D}_t\,U = -I^{\mathrm{u}} - p\;\mathrm{D}_t\,V$$
- or
  $$\mathrm{d}U = \mathrm{d}Q - p\,\mathrm{d}V$$
- $\mathrm{d}U$ is internal energy change, $\mathrm{d}Q = -\mathrm{d}t\,I^{\mathrm{u}}$ the inflow of heat, and $\mathrm{d}V$ the increase in volume of a constant mass

Liquids and gases

- a fluid medium, liquid or gas, cannot support reversible shear stresses
- recall that

  $$\mathrm{d}F_k = -T_{ki}\,\mathrm{d}A_i$$

  is the force on a surface element $\mathrm{d}A_i$
- $T'_{ik} = 0$ for $i \neq k$
- therefore

  $$T'_{ik} = -p\delta_{ik}$$
- $p = p(t, \boldsymbol{x})$ is the pressure field

Model: water

- in good approximation, water is incompressible
- as mentioned before

  $$0 \approx \varrho \, \mathrm{D}_t \, \varrho^{-1} = \partial_i v_i = 0$$

- in good approximation, friction is proportional to the velocity gradient
- Newtonian fluid

  $$T''_{ki} = 2\eta \, G_{ki} = \eta \, \{\partial_k v_i + \partial_i v_k\}$$

- Navier-Stokes equation

  $$\varrho \partial_t v_k + \varrho \partial_i v_k v_i = -\partial_k p + \eta \Delta v_k + f_k$$

- nonlinear term $\partial_i v_k v_i$ makes Navier-Stokes equation complicated

Reynold's number

- external forces are usually irrelevant in hydrodynamics
- select a suitable reference length ℓ_* and a reference velocity v_*
- then $v = \hat{v}\, v_*$ etc., where $\hat{v}$ is dimensionless
- dimensionless Navier-Stokes equation is
  $$\hat{\partial}_t \hat{v}_k + \mathtt{Re}\, \hat{\partial}_i \hat{v}_k \hat{v}_i = -\hat{\partial}_k \hat{p} + \hat{\Delta} \hat{v}_k$$
- dimensionless Reynold's number
  $$\mathtt{Re} = \frac{\varrho\, \ell_*\, v_*}{\eta}$$
- solutions can be scaled, i.e. model ships, model rivers, model water turbines etc.

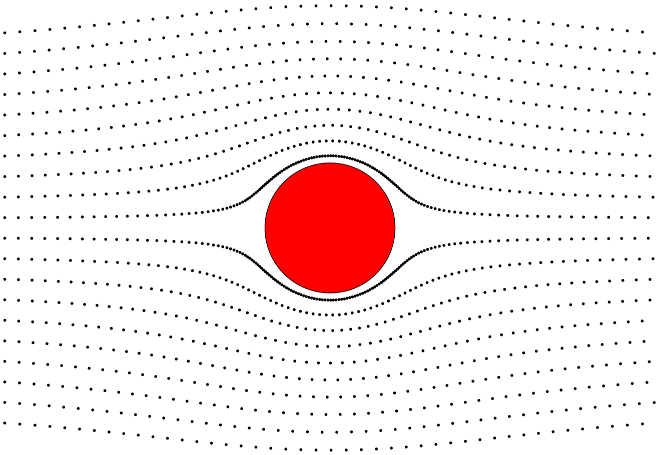
Stokes's law

- Re $\lessapprox 1$: creeping flow; viscosity dominates
- Re $\lessapprox 2000$: laminar, or sheet-wise flow
- Re $\gtrapprox 2000$: turbulence
- creeping stationary flow around a sphere
- solve

  $$\Delta v_k = \partial_k p \;\text{ and }\; \partial_i v_i = 0$$

- where $\boldsymbol{v}(\boldsymbol{x}) = (0, 0, v_\infty)$ for $|\boldsymbol{x}| \to \infty$
- and $\boldsymbol{v}(\boldsymbol{x}) = 0$ for $|\boldsymbol{x}| = R$
- stream function method
- force F on sphere is along 3-direction

  $$F = 6\pi\eta R v_\infty$$



Creeping flow around a sphere. The force on it grows *linearly* with radius R.

Ideal gas

- for sufficiently low pressure, all gases behave alike
- for N particles in a volume V at temperature T

$$p = \frac{N \mathsf{k}_\mathsf{B} T}{V}$$

- universal gas constant $R = N_\mathrm{A} \mathsf{k}_\mathsf{B}$
- molar mass $M = N_\mathrm{A} m$
- relation between pressure, temperature and mass density

$$p = \frac{\varrho}{M} R T$$

- diatomic ideal gas, adiabatic process

$$\frac{p_1}{p_2} = \left\{ \frac{T_1}{T_2} \right\}^{2/7}$$

- example: convection labile atmosphere

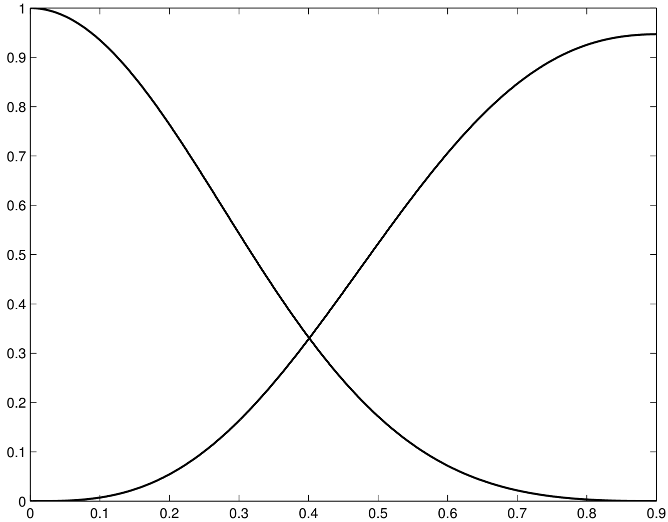
Normal, white dwarf, neutron stars

- normal stars (like the sun) produce energy
- $\pi(U)$ describes 4 H $\rightarrow$ He + 2 e$^-$ + 2 ν nuclear reactions
- momentum and internal energy balance equations
- radiation pressure $p \propto T^4$ dominates in reaction core
- ideal gas law outside
- white dwarf matter is a plasma of electrons and carbon/oxygen nuclei
- for $T = 0$ degeneracy pressure

$$p = a \frac{\hbar^2}{m_\mathrm{e}} \left\{ \frac{\varrho}{2m_\mathrm{p}} \right\}^{5/3}$$

- neutron star is a gas/liquid/solid of neutrons
- for $T = 0$

$$p = a \frac{\hbar^2}{m_\mathrm{p}} \left\{ \frac{\varrho}{m_\mathrm{p}} \right\}^{5/3}$$



Pressure p (decreasing) and mass M (increasing) of a white dwarf vs. distance r from the center in natural units. $r = 1$ corresponds to 6500 km, $M = 1$ to 0.85 sun masses.

Strain tensor

- consider neighboring material points at $\boldsymbol{x}$ and $\boldsymbol{x}+\mathrm{d}\boldsymbol{x}$
- if medium is deformed, they are at $\boldsymbol{x}+\boldsymbol{u}(\boldsymbol{x})$
- and $\boldsymbol{x}+\mathrm{d}\boldsymbol{x}+\boldsymbol{u}(\boldsymbol{x}+\mathrm{d}\boldsymbol{x})$
- displacement field $u_i = u_i(t,\boldsymbol{x})$
- by deformation, $\mathrm{d}x_i$ becomes
  $\mathrm{d}\bar{x}_i = (\delta_{ij} + \partial_j u_i)\mathrm{d}x_j$
- distance changes according to
  $\mathrm{d}\bar{s}^2 = \mathrm{d}s^2 + 2S_{jk}\mathrm{d}x_j\mathrm{d}x_k$
- where
  $2S_{jk} = \partial_j u_k + \partial_k u_j + (\partial_j u_i)(\partial_k u_i)$
- last term is quadratic in displacement gradient and may be neglected
- distance changes described by strain tensor
  $$\mathrm{d}\bar{s} - \mathrm{d}s = S_{jk}\mathrm{d}x_j\mathrm{d}x_k \quad \text{with} \quad S_{jk} = \frac{\partial_j u_k + \partial_k u_j}{2}$$

Hooke's law

- no strain - no stress
- little strain - little stress
- Hooke's law

  $T'_{ij} = \Lambda_{ijkl} S_{kl}$
- up to 21 independent elasticity constants
- 3 for cubic crystals, 2 for isotropic media
- Hooke's law for an isotropic elastic medium

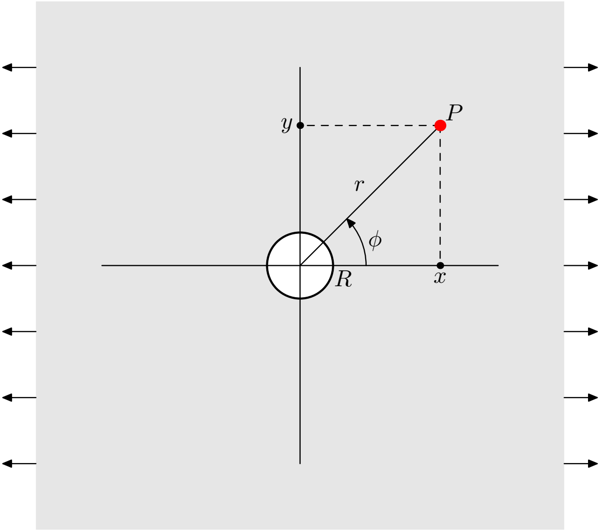
  $$T'_{ij} = \frac{E}{1+\nu} \left\{ S_{ij} + \frac{\nu}{1-2\nu} \delta_{ij} S_{kk} \right\}$$
- E is elasticity, or Young's module (dimension of a pressure)
- ν is Poissons's number, varies between 0 and $1/2$

Some examples

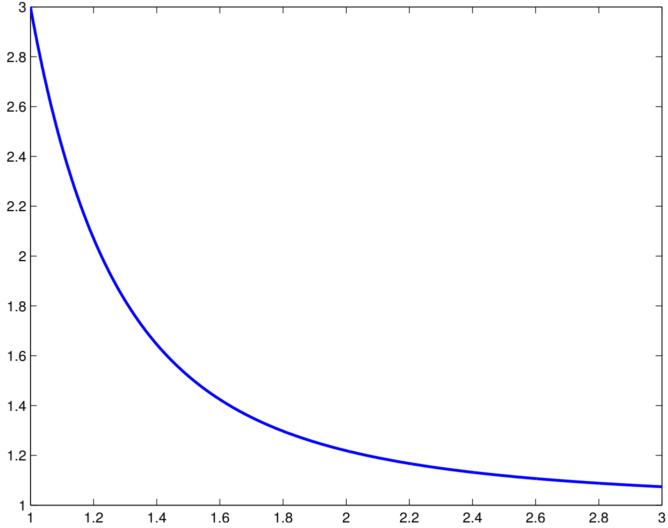
- in most cases, investigate structural stability
- $\varrho\,\mathrm{D}_t\,v_k$ vanishes, $T_{ki} = T'_{ki}$
- to be solved $u \to S \to T$ and

  $\partial_i T_{ki} + f_k = 0$
- houses, bridges, tools, cars, ship, etc.
- material imperfections, such as stress enhancement
- but also elastic waves

  $\varrho \ddot{u}_k = \partial_i T_{ki}$
- transversal and longitudinal waves (TA and LA), different sound velocities
- surface acoustic waves (SAW)
- seismology



A thin plate with a circular hole. Uniform stress at infinity.



Stress increase versus distance from hole in units of its radius. At the hole, the stress is enhanced by a factor 3.

Dielectric permittivity

- relation between light field and displacement of matter
  $\tilde{D}_i(\omega) = \epsilon(\omega)_{ij}\tilde{E}_j(\omega)$
- ϵ_{ij} is hermitian and symmetric (with $\mathcal{B}_k \to -\mathcal{B}_k$)
- isotropic and birefringent:
  $\epsilon_{ij} = \epsilon^{0,0}_{ij}$
- Pockels effect:
  $+\epsilon^{1,0}_{ijk}\mathcal{E}_k$
- Faraday effect:
  $+\epsilon^{0,1}_{ijk}\mathcal{B}_k$
- Kerr effect:
  $+\epsilon^{2,0}_{ijkl}\mathcal{E}_k\mathcal{E}_l$
- and so forth

More on optics

- Maxwell's equations play role of balance equations
- must be augmented by material equations
- behavior of light at interfaces, lenses, dielectric waveguides etc. are typical problems of continuum optics
- also metamaterials and photonic crystals
- calculation of permittivities, absorption etc. within the framework of quantum statistical theory
- linear response theory
- lasers, quantum dots etc. belong to the field of quantum optics proper

Ohms law and Hall effect

- for a static or quasi-static electric field
  $J^{\mathrm{e}}_i = \sigma_{ij}\mathcal{E}_j$
- huge range of applicability
- valid also if driving force is a gradient of the electron chemical potential
- electro-chemical potential
  $$\psi = \phi^{\mathrm{e}} - \frac{\mu^*}{e}$$
- μ^* is chemical potential of mobile electrons in a conducting material
- generalized Ohm's law
  $J^{\mathrm{e}}_i = -\sigma_{ij}\partial_j\psi$
- electro-chemistry: batteries, fuel cells, photo-voltaic modules
- conduction in an external magnetic field: Hall effect
  $E_z = R_{\mathrm{H}}\, J^{\mathrm{e}}_x\, \mathcal{B}_y$

Brownian Motion

- Brownian particle large enough to be seen in a microscope
- small enough to be kicked visibly by surrounding liquid
- random force F

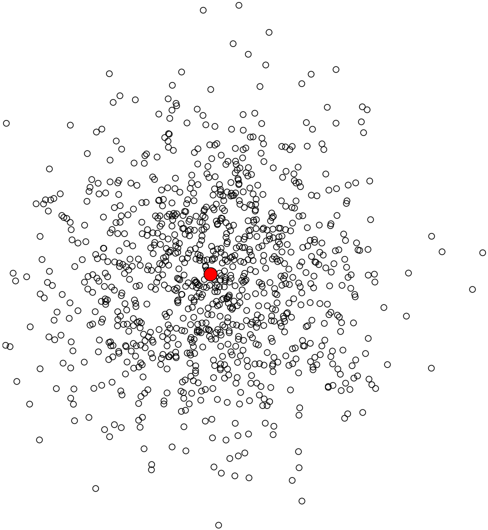
  $m(\dot{v} + \Gamma v) = F$
- instant time correlation

  $\langle F(t+\tau)F(t)\rangle = K_F(\tau) = K\delta(\tau)$
- energy per degree of freedom

  $\frac{m}{2}\langle v^2\rangle = \frac{1}{2}\mathsf{k_B}T$
- results in

  $< x(t)^2 >= \frac{2\mathsf{k_B}T}{\Gamma}\,t$
- diffusion is mass-wise Brownian motion

Random walk of a Brownian particle



Many Brownian particles have started at the same location and traveled the same time.

Diffusion

- one species of particles diffuses; density n, diffusion current $\boldsymbol{J}$
- particles diffuse because chemical potential μ has a gradient
  $$\boldsymbol{J} = -\frac{\Lambda}{T}\,\boldsymbol{\nabla}\mu$$
- $\Lambda > 0$ by second main law of TD
- T assumed constant, and
  $$\frac{\partial\mu(T,n)}{\partial n} > 0$$
- therefore
  $$\boldsymbol{J} = -D\,\boldsymbol{\nabla}n$$
- comparison with Brownian motion
  $$D = \frac{\mathsf{k_B}T}{6\pi\eta R}$$
  where R is (effective) radius of diffusing particle, η viscosity of liquid

Heat conduction

- heat conduction is phonon diffusion !
- see contribution to volumetric entropy production rate

$$\pi(S) = \dots + J_i^{\mathrm{u}}\, \partial_i \, \frac{1}{T} + \dots$$

- Fourier's law

$$\boldsymbol{J}^{\mathrm{u}} = -\lambda \, \boldsymbol{\nabla} \, T$$

- second main law ✔
- if specific internal energy u depends on location via T only

$$\varrho \, \mathrm{D}_t \, u = \varrho \frac{\partial u}{\partial T} \, \mathrm{D}_t \, T = \varrho c \, \mathrm{D}_t \, T$$

- c is specific heat. In a resting medium

$$\dot{T} = \frac{1}{\varrho c} \boldsymbol{\nabla} \lambda \boldsymbol{\nabla} T \approx \kappa \Delta T$$

- ϱ, c and λ usually depend on T only
- heat equation $\dot{T} = \kappa \Delta T$ may contain a heat production term (friction, radio-activity)

Gray-Scott model - Reactions

- two species of particles U and V with densities $u = u(x, y)$ and $v = v(x, y)$
- U is the substrate
- auto-catalytic reaction U + 2V $\rightarrow$ 3V
- law of mass action
- production of U particles
  $\pi^{\mathrm{u}} = -Ruv^2 + F(\bar{u} - u)$
- production of V particles
  $\pi^{\mathrm{v}} = +Ruv^2 - (F + K)v$
- outside concentration of U particles is maintained at $\bar{u}$, inflow proportional to concentration difference
- outgoing V particles are removed, i.e. $\bar{v} = 0$

Gray-Scott model - Diffusion

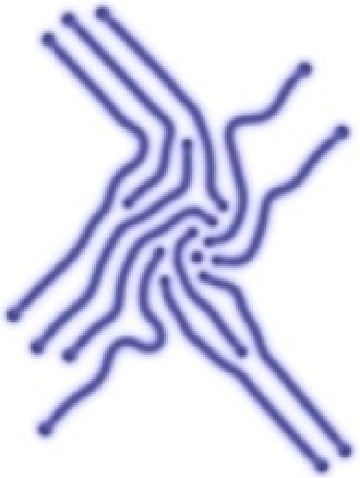
- U and V particles also diffuse
- diffusion equation for U

  $\dot{u} = D_{\mathrm{u}} \Delta u + \pi^{\mathrm{u}}$
- diffusion equation for V

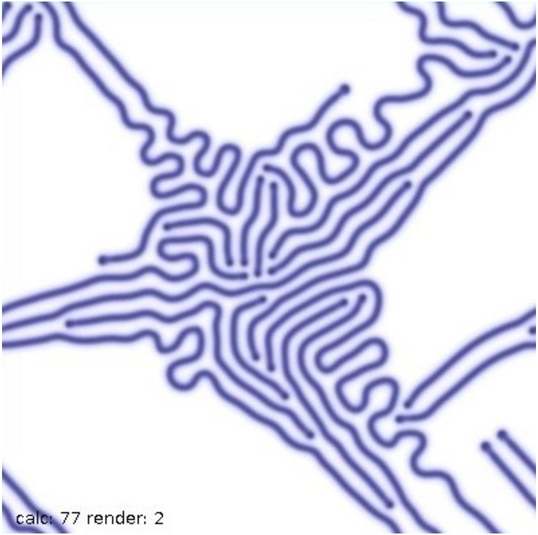
  $\dot{v} = D_{\mathrm{v}} \Delta v + \pi^{\mathrm{v}}$
- by choosing an appropriate reference length and time, the system can be rewritten such that only dimensionless quantities show up
- U equation

  $\dot{u} = \Delta u - uv^2 + f(1-u)$
- V equation

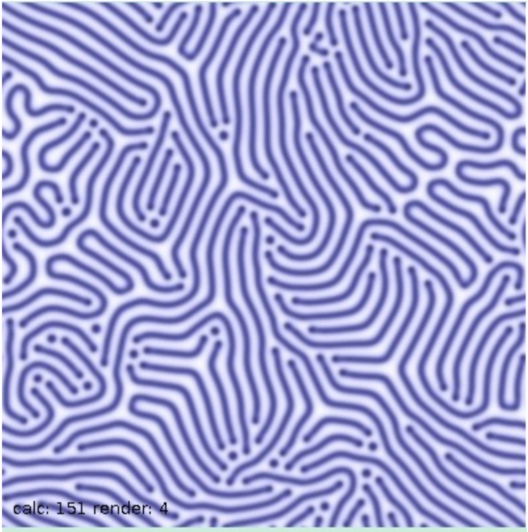
  $\dot{v} = \frac{1}{\sigma} + uv^2 - (f+k)v$
- σ is ratio of diffusion constants, f describes inflow of U, $(f+k)$ outflow of V



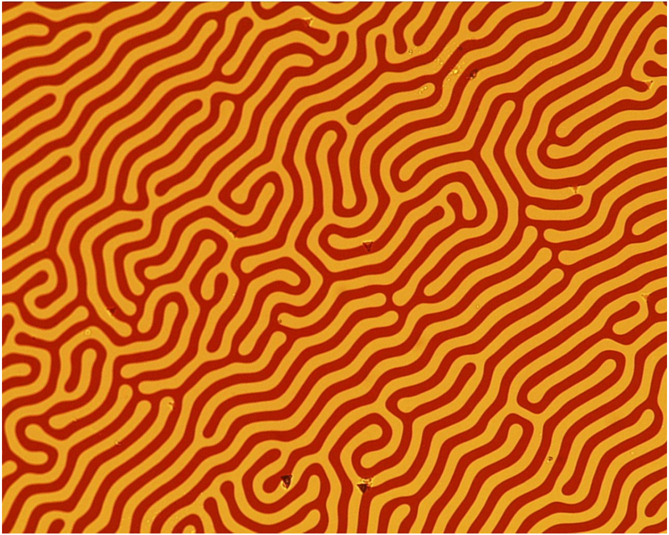
Concentration of V particles. $\sigma = 2$, $f = 0.050$ and $k = 0.065$. Early stage. Periodic boundary conditions. Random initial particle disbribution.



Intermediate stage. Note the effect of periodic boundary conditions.



Final and stationary stage.



Magnetic domains in a YIG film. What is the relation with the Gray-Scott model?