Lect1: Fluid dynamics

October 8, 2007

Plan of the lecture

- Reactive flow fluid dynamics - equations
- Sound waves and shocks
- Flames and detonations
- Deflagration-to-detonation transition (DDT)
- Instabilities
- Turbulence
- An example

FLUID CHARACTERISTICS

ρ	-	mass density	(g/cm^3)
U_i	-	velocity, $i = 1, 2, 3$	(cm/s)
T	-	temperature	(K)
P	-	pressure	(ergs/cm^3)
E_{int}	-	internal energy density	(ergs/cm^3)
E	-	energy density ($= E_{int} + \frac{\rho U^2}{2}$)	(ergs/cm^3)
c_p	-	specific heat	(ergs/g/K)
ν,ζ	-	kinematic viscosity (shear and bulk)	(cm^2/s)
κ	-	heat diffusivity	(cm^2/s)
C_s	-	mass diffusivity (of chemical species)	(cm^2/s)
X_s	-	"chemical" variables (e.g., mass fractions)	
R_s	-	net reaction rates ($= \frac{dX_s}{dt}$)	(s^{-1})

Equation of state (EoS):

$$P(\rho, T, X_s), \quad E_{int}(\rho, T, X_s). \tag{1}$$

Sound speed, specific heat:

$$a_s = \left(\frac{\partial P}{\partial \rho}\right)_{S,X_s}, \quad c_V = \left(\frac{\partial E_{int}/\rho}{\partial T})\right)_{\rho,X_s}, \dots \tag{2}$$

Diffusion coefficients:

$$\nu(\rho, T, X_s), \quad \kappa(\rho, T, X_s), \quad C_i(\rho, T, X_s). \tag{3}$$

Reaction rates:

$$R_s(\rho, T, X_s). \tag{4}$$

EQUATIONS

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho U_k)}{\partial x_k} = 0, \tag{5}$$

Conservation of momentum:

$$\underbrace{\frac{\partial \rho U_i}{\partial t} + \frac{\partial}{\partial x_k}(\rho U_k U_i)}_{\text{Inertia}} = \underbrace{-\frac{\partial P}{\partial x_k}}_{\text{Pressure}} \underbrace{+ \rho g_i}_{\text{Gravity}} \underbrace{- \frac{\partial \Sigma_{ik}}{\partial x_k}}_{\text{Viscosity}}, \tag{6}$$

where

$$\Sigma_{ij} = \rho\nu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial U_k}{\partial x_k} \right) + \rho\zeta\delta_{ij}\frac{\partial U_k}{\partial x_k} \quad - \quad \text{viscous stress.} \tag{7}$$

Conservation of energy:

$$\frac{\partial E}{\partial t} + \frac{\partial(EU_k)}{\partial x_k} = \underbrace{-\frac{\partial(PU_k)}{\partial x_k}}_{\text{Pressure}} + \underbrace{\rho g_k U_k}_{\text{Gravity}} + \underbrace{\frac{\partial \Sigma_{ik} U_i}{\partial x_k}}_{\text{Viscosity}} + \underbrace{\frac{\partial}{\partial x_k}\left(\rho c_p \kappa \frac{\partial T}{\partial x_k}\right)}_{\text{Heat conduction}} \tag{8}$$

Reactions:

$$\frac{\partial \rho X_s}{\partial t} + \frac{\partial \rho X_s U_k}{\partial x_k} = \underbrace{\rho R_s(\rho, T, \vec{X})}_{\text{Reactions}} + \underbrace{\frac{\partial}{\partial x_k}\left(\rho C_s \frac{\partial X_s}{\partial x_k}\right)}_{\text{Mass diffusion}} \tag{9}$$

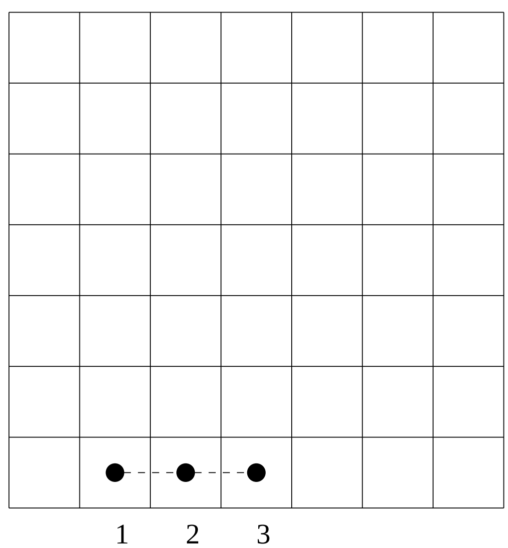
Gravity:

$$g_i(\vec{x}) = -G \int \rho' \frac{(\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^3}\, d^3x' \tag{10}$$

NUMERICAL SIMULATIONS OF FLUID MOTIONS

1. Computational mesh: Space is divided into computational cells. At each time t every cell is characterized by values of $\rho(t)$, $T(t)$, $P(t)$, etc. Number of cells, N may be very large, e.g., $N \sim 10^9 - 10^{10}$. Typical number of cells in each direction is then $\sim N^{1/3}$.

2. Discretization: Equations of hydrodynamics are converted into a large system of algebraic equations (finite-difference, finite-volume, finite-element equations) for variables at time t (which are known) and variables at time $t + \Delta t$ (which are unknowns); Δt is a time-step.



$$(dU/dt)_2 = U_3 - U_1$$

3. Numerical integration: algebraic equations are solved on a computer to find values of variables at $t + dt$. The procedure is repeated many times, say, $n \sim 10^4 - 10^5$ times.

SOUND WAVE

Consider a uniform base state of a fluid: $U = 0$, $\rho = const$, $P = const$, $X_s = const$. No reactions, gravity, viscosity, heat and mass transport.

Sound wave is a small adiabatic perturbation of a uniform state. Wave equation follows from (6) and (5):

$$\frac{\partial^2 h}{\partial t^2} + a_s^2 \frac{\partial^2 h}{\partial {x_i}^2} = 0, \quad \text{where } h = U_i, \delta\rho, \delta P \tag{11}$$

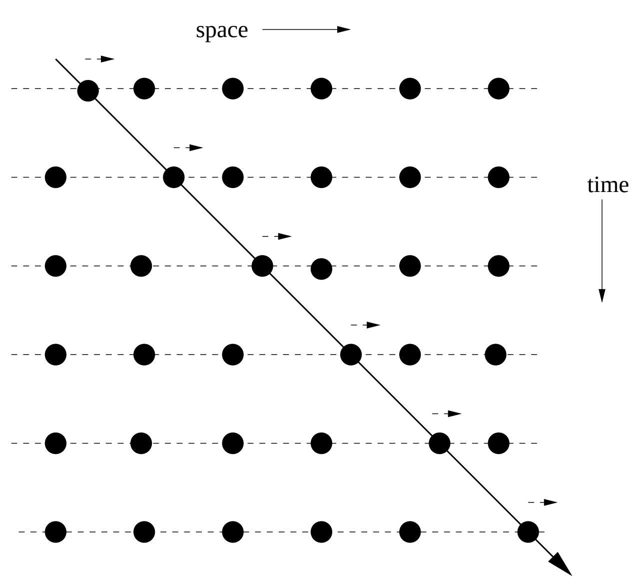
Planar sound wave is a one-dimensional solution of (11),

$$U = f(x \pm a_s t), \quad \delta\rho = \rho U / a_s, \quad \delta P = \rho a_s U. \tag{12}$$

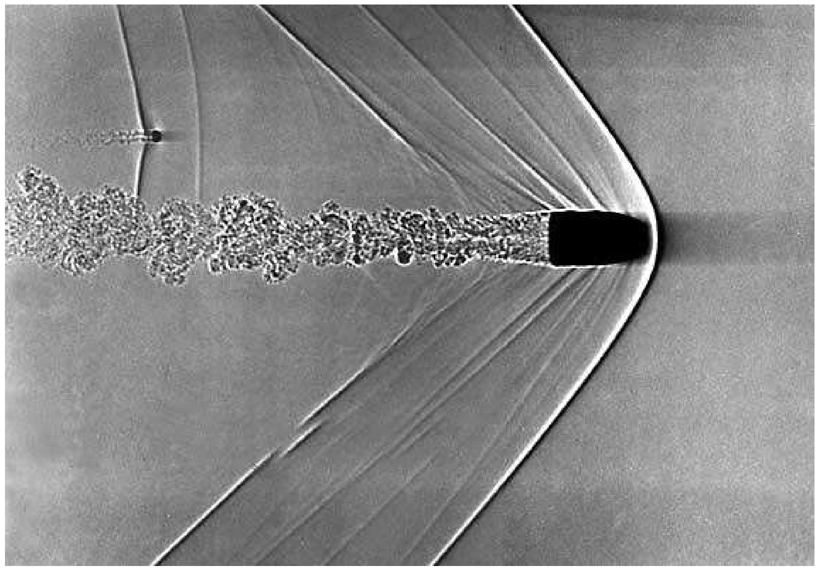
Monochromatic planar wave is

$$U = sin(x \pm a_s t). \tag{13}$$

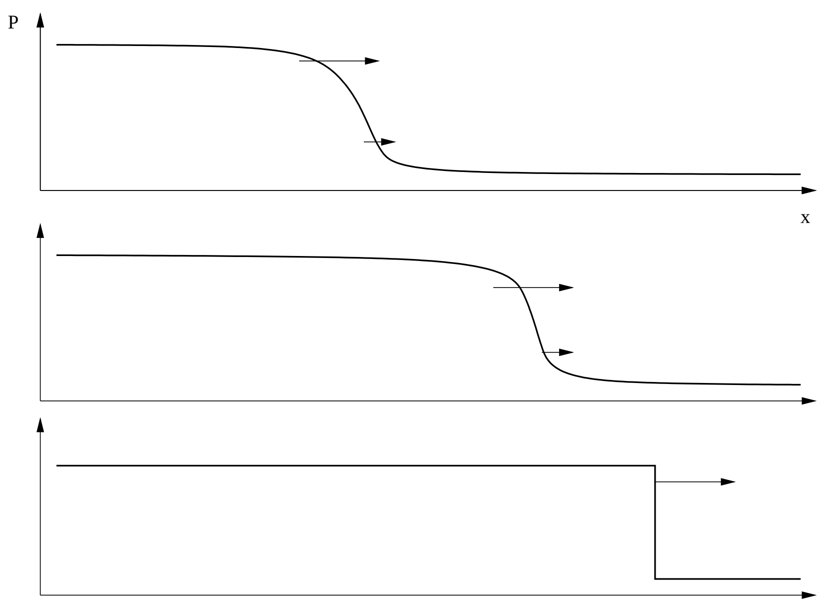
Sound is propagated by collisions of particles:



SHOCK WAVE



Sound speed increases with density. As a result, a large amplitude sound wave may turn into a shock.



Shock wave also propagates due to collisions of particles, but its speed D is greater than the sound speed, $D > a_s$.

FLAME

Premixed Flame - fuel and oxidant are mixed before flame is ignited (e.g., ethylene + air).

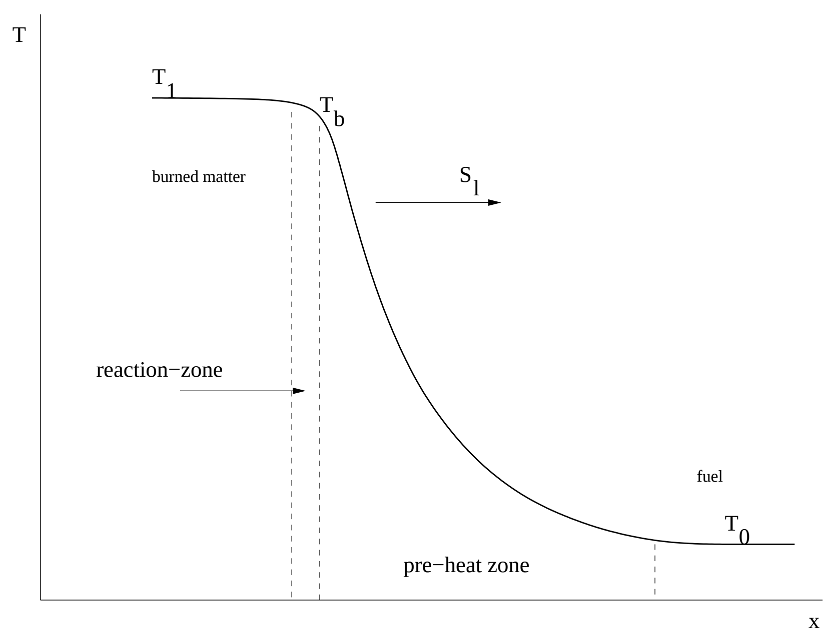
Flame in a supernova is similar to a terrestrial premixed flame: leading reaction is ${}^{12}C + {}^{12}C$, matter is ready to burn.

Reaction rate increases with T exponentially: $R \sim e^{-Q/T}$ or $R \sim e^{-Q/T^{1/3}}$.

Flame $=$ wide pre-heat zone $+$ very thin reaction zone. In pre-heat zone fuel is heated from $T_0 << T_1$. Reaction occurs at $T_b \simeq T_1$, where T_1 - temperature in burned matter.

Flame speed $S_l \simeq (\kappa/\tau)$, where τ is a reaction time-scale at T_b.

In terrestrial flames diffusion of species is important as well. In SNIa flame it is not.



DETONATION

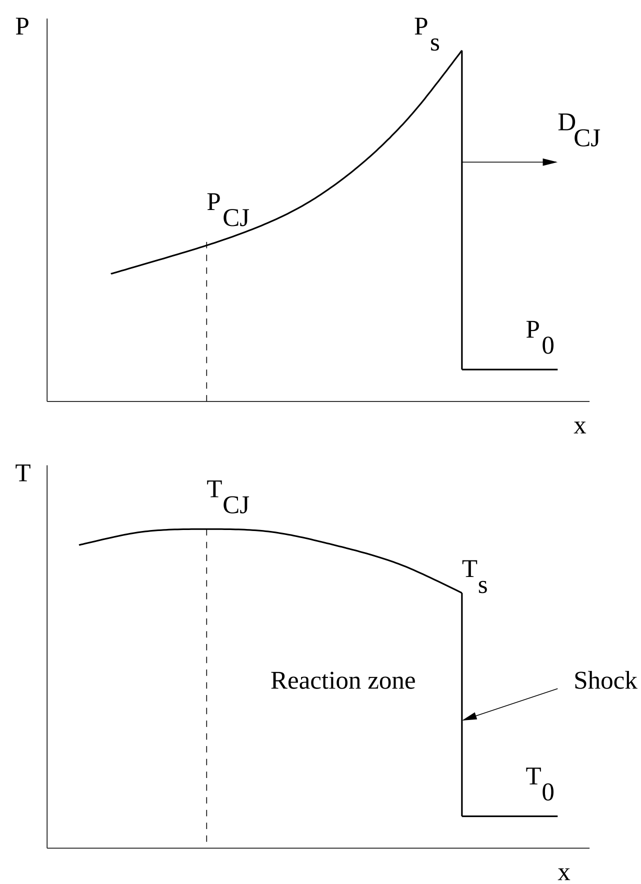
In a detonation wave matter is shocked to a high temperature $T_s > T_0$.

Burning starts immediately behind the shock. Matter expands while it burns, P and ρ decrease, T increases.

Chapman-Jouguet detonation: Burning terminates and $U - D_{CJ} = a_s$ (matter outflows with the sound speed) simultaneously at the CJ point.

Detonation speed is $D_{CJ} \simeq q^{1/2}$ where q is the energy released in by reactions behind the shock (ergs/g).

Detonation does not need heat or species diffusion to propagate. Speed of detonation $D_{CJ} > a_s >> S_l$.



KELVIN-HELMHOLTZ INSTABILITY

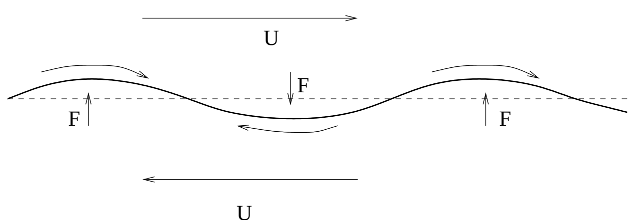
Two fluids move with relative velocity U with respect to each other.

Centrifugal force appears when interface between fluids is perturbed (bended). The force acts to increase the aplitude of perturbations.

Growth rate ω (sec^{-1} depends on velocity U and wavelength of perturbation λ:

$$\omega \sim \frac{U}{\lambda}\frac{\sqrt{\rho_1\rho_2}}{\rho_1+\rho_2}. \tag{14}$$

Instability occurs regardless of whether densities of the fluids are equal or not.



RAYLEIGH-TAYLOR INSTABILITY

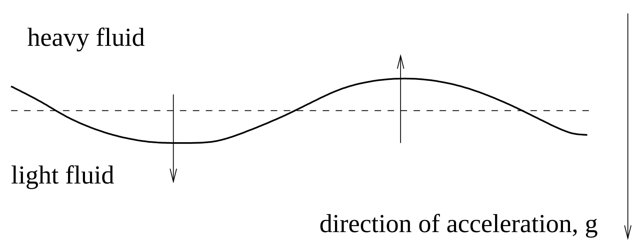
Heavy fluid (ρ_1) is on top of a light fluid ($\rho_2 < \rho_1$) subject to acceleration g.

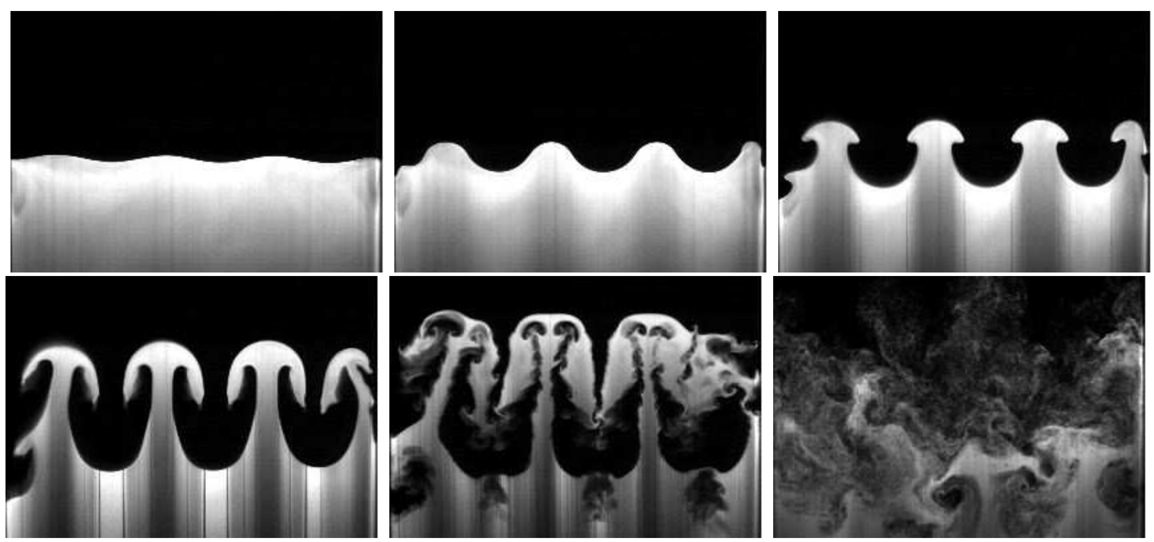
Boyancy forces light fluid to float and heavy fluid to sink.

Growth rate ω depends on g, λ and density contrast,

$$\omega \simeq \left(\frac{g}{\lambda}A\right)^{1/2}, \quad A = \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2} \tag{15}$$

Acceleration may be caused by gravity or time-dependent fluid motions.





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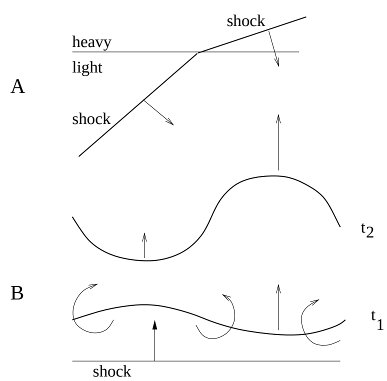
RICHTMYER-MESHKOV INSTABILITY

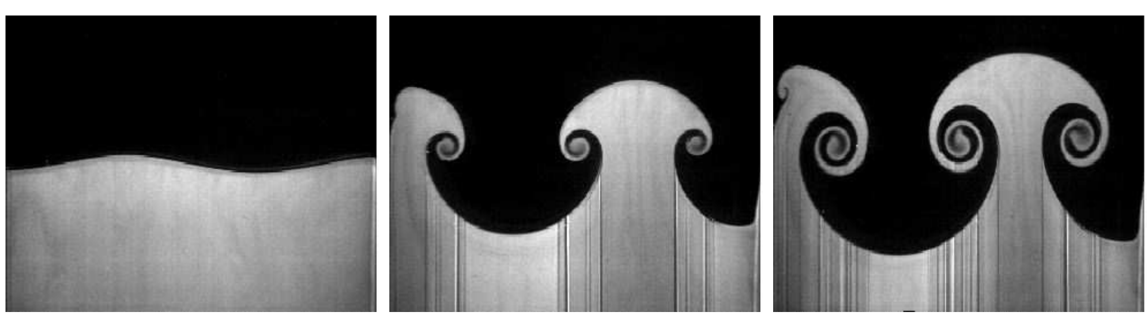
Distortion of a density discontinuity by an impulsive acceleration, e.g, by a shock passage.

A: An oblique shock changes its direction when it passes through an interface between two fluids with different sound speed a_s.

B: When a shock passes through a curved interface it generates vortical motions (t_1). Vortical motions distort the interface behind the shock ($t_2 > t_1$).

The rate of distortion depends on shock strength, sound speeds, and interface cuvature.





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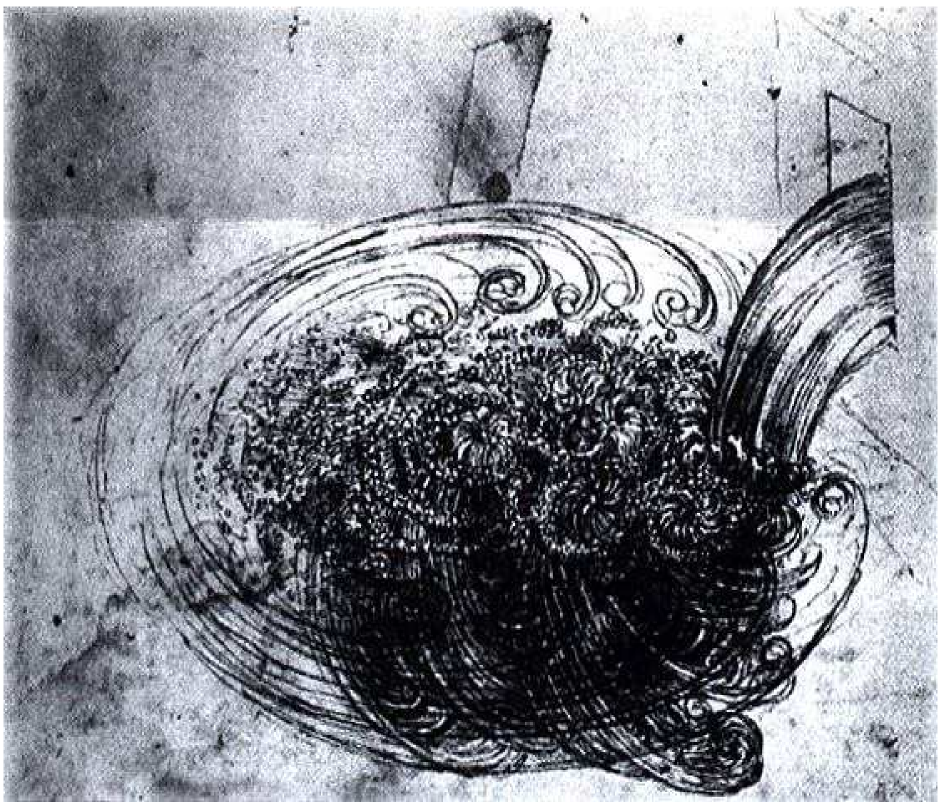
TURBULENCE

da Vinci: "... the water has eddying motions, one part of which is due to the principal current, the other to the random and reverse motion."



Reynolds Number: relative importance of inertia and viscosity in (6) can be characterized by

$$Re = \frac{LU}{\nu}, \tag{16}$$

where L - system size, U - large scale velocity.

Flow usually becomes turbulent when $Re >> 1$.

Kolmogorov cascade: in turbulence, energy cascades from large-scale to small-scale eddies. In a steady-state turbulence,

$$U_\lambda \simeq U_L \left(\frac{\lambda}{L}\right)^{1/3}, \quad \lambda_K < \lambda < L,$$

U_λ - velocity of eddies of size λ;

$$\lambda_K = L\, Re^{-3/4} \tag{17}$$

is a viscous micro-scale (a scale at which local Reinolds number $\lambda U_\lambda/\nu \sim 1$).

Examples:

System	L, cm	U, cm/s	ν, cm^2/s	λ_K, cm	Re	N	Gbytes
cup of coffee	10	10	0.01	10^{-2}	10^4	10^9	100
star	10^{10}	10^5	0.1	10^{-2}	10^{16}	10^{24}	10^{20}
SNIa	10^8	10^8	0.1	10^{-5}	10^{17}	10^{25}	10^{21}

Implications to first-principles numerical modeling: number of grid points required to model a turbulent system is $N > (L/\lambda_K)^3 \sim Re^{9/4}$. This number could be extremely large.

System	Grid points	Required memory (Gb)
cup of coffee	10^9	100
star	10^{24}	10^{20}
supernova	10^{25}	10^{21}

At present we can model a cup of coffee :-).

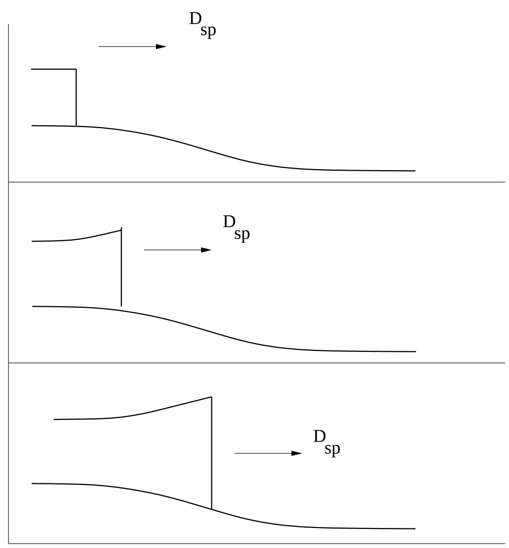
DEFLAGRATION-TO-DETONATION TRANSITION

Spontaneous wave of burning: burning can propagate with *any* speed as a result of non-uniform initial condtions (Zeldovich). Spontaneous burning has been experimentally observed.

Suppose $T = T(x)$. Reaction rate R and reaction timescale $\tau = R^{-1}$ depend on T. Therefore reaction may spread spontaneously with a speed

$$D_{sp} \simeq \left(\frac{\partial \tau(T(x))}{\partial x} \right)^{-1} . \tag{18}$$

For certain $T(x)$ spontaneous burning will spread supersonically, $S_{sp} \simeq a_s$, and then transition to a detonation.



Given initial $T(x)$ it is very easy to calculate spontaneous wave and transition to a detonation.

It is very difficult to predict what the exact initial conditions, $T(x)$, should be. For two reasons: (a) it involves instabilities and turbulence, (b) we usually do not know initial initial conditions :-).