PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF in Olin 103

Notes on Lecture 39

Continuing review

1. Mathematical methods
2. Classical mechanics concepts

35	Fri, 11/17/2023	Chap. 11	Heat conduction	#28
36	Mon, 11/20/2023	Chap. 12	Viscous effects in hydrodynamics	
	Wed, 11/22/2023	Thanksgiving		
	Fri, 11/24/2023	Thanksgiving		
	Mon, 11/27/2023		Presentations I	
	Wed, 11/29/2023		Presentations 2	
	Fri, 12/01/2023		Presentations 3	
37	Mon, 12/04/2023	Chap. 12	Viscous effects in hydrodynamics	
38	Wed, 12/06/2023		Review	
39	Fri, 12/08/2023		Review	

Please fill out the course evaluation form for PHY 711 at the end of today's class

Final exam during finals week

Exam will be available at end of class today

Due < Monday 12/18/2023 at 11 AM

Brief comment on numerical methods --

Consider a continuous function $x(t)$

A Taylor expansion in the neighborhood of t :

$$x(t+h) = x(t) + h\frac{dx(t)}{dt} + \frac{1}{2}h^2\frac{d^2x(t)}{dt^2} + \frac{1}{3!}h^3\frac{d^3x(t)}{dt^3} + \ldots\ldots$$

Let $x_n \equiv nh$

$$x_{n+1} = x_n + hv_n + \frac{1}{2}h^2 a_n + \ldots\ldots$$

Here it is assumed that h is small and $h^3 << h^2$

Example differential equation (one dimension);

$$\frac{d^2x}{dt^2} = f(t) \qquad \text{Let} \quad t = nh \qquad (n = 1, 2, 3 \ldots)$$

$$x_n \equiv x(nh); \qquad f_n \equiv f(nh)$$

Euler's method:

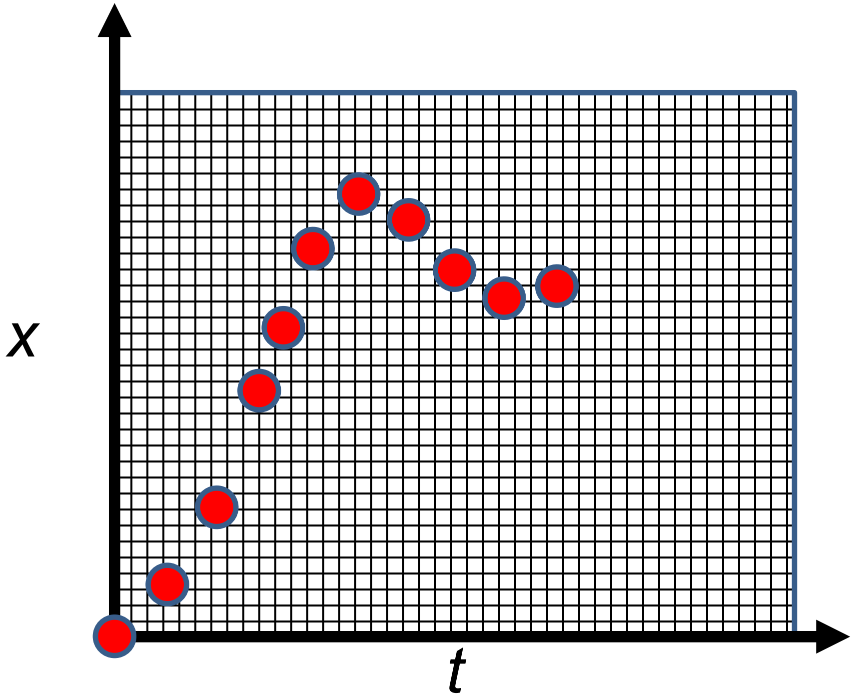
$$x_{n+1} = x_n + hv_n + \frac{1}{2}h^2 f_n$$

$$v_{n+1} = v_n + hf_n$$

Velocity Verlet algorithm:

$$x_{n+1} = x_n + hv_n + \frac{1}{2}h^2 f_n$$

$$v_{n+1} = v_n + \frac{1}{2}h\left(f_n + f_{n+1}\right)$$



Note that it is possible to check the magnitude of the terms that you are neglecting and estimate the error. Also, one needs to be careful of device-dependent restrictions. In general, it is useful to use scaled coordinates.

$$\text{For example,} \quad 1+1\times10^{-15} = 1.000000000000001$$
$$= 1.0 \text{ for most devices.}$$

When you perform numerical work, you need to take care about your algorithms both in terms of software and hardware.

Notions of phase space and Liouville's Theorem (1838)

The density of representative points in phase space corresponding to the motion of a system of particles remains constant during the motion.

Denote the density of particles in phase space: $D = D\left(\{q_\sigma(t)\},\{p_\sigma(t)\},t\right)$

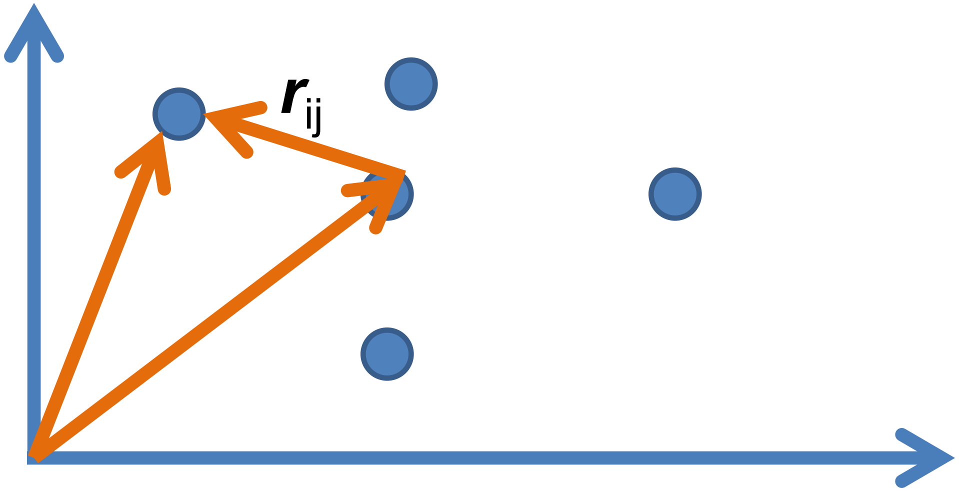
$$\frac{dD}{dt} = \sum_\sigma \left(\frac{\partial D}{\partial q_\sigma}\dot{q}_\sigma + \frac{\partial D}{\partial p_\sigma}\dot{p}_\sigma \right) + \frac{\partial D}{\partial t}$$

According to Liouville's theorem: $\dfrac{dD}{dt} = 0$

$$\frac{dD}{dt} = 0$$

Importance of Liouville's theorem to statistical mechanical analysis:

In statistical mechanics, we need to evaluate the probability of various configurations of particles. The fact that the density of particles in phase space is constant in time, implies that each point in phase space is equally probable and that the time average of the evolution of a system can be determined by an average of the system over phase space volume. Computationally this can be approximated using molecular dynamics or sampling methods.



$$L = L(\{\mathbf{r}_i(t)\},\{\dot{\mathbf{r}}_i(t)\}) = \sum_i \tfrac{1}{2} m_i |\dot{\mathbf{r}}_i|^2 - \sum_{i<j} u(|\mathbf{r}_i - \mathbf{r}_j|)$$

More generally $U(\{r_j\})$

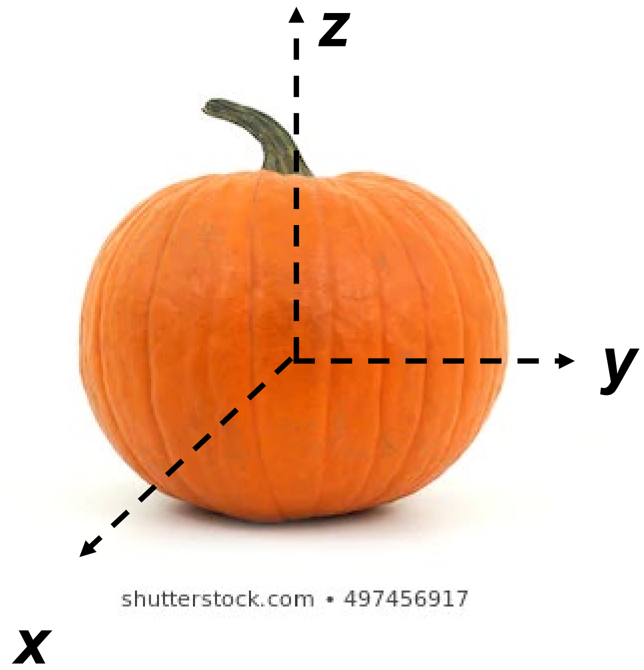
➔From this Lagrangian, can find the 3N coupled 2nd order differential equations of motion and/or find the corresponding Hamiltonian, representing the system at constant energy, volume, and particle number N (N,V,E ensemble).

Rigid body motion

Moment of inertia tensor :

$$\overleftrightarrow{\mathbf{I}} \equiv \sum_p m_p \left(\mathbf{1} r_p^2 - \mathbf{r}_p \mathbf{r}_p \right) \qquad \text{(dyad notation)}$$

In a reference frame attached to the object, there are 3 moments of inertia and 3 distinct principal axes



Representation of rotational kinetic energy:

$$T(\alpha, \beta, \gamma, \dot{\alpha}, \dot{\beta}, \dot{\gamma}) = \frac{1}{2} I_1 \tilde{\omega}_1^2 + \frac{1}{2} I_2 \tilde{\omega}_2^2 + \frac{1}{2} I_3 \tilde{\omega}_3^2$$

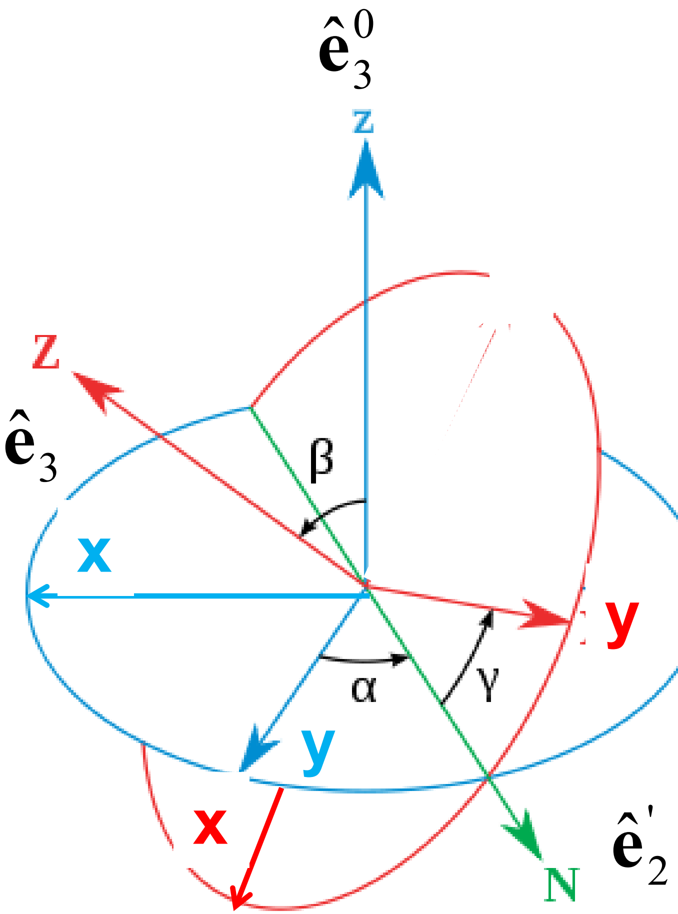
$$= \frac{1}{2} I_1 \left[\dot{\alpha} (-\sin\beta \cos\gamma) + \dot{\beta} \sin\gamma \right]^2$$

$$+ \frac{1}{2} I_2 \left[\dot{\alpha} (\sin\beta \sin\gamma) + \dot{\beta} \cos\gamma \right]^2$$

$$+ \frac{1}{2} I_3 \left[\dot{\alpha} \cos\beta + \dot{\gamma} \right]^2$$

Euler's transformation between body fixed and inertial reference frames

$$\tilde{\boldsymbol{\omega}} = \dot{\alpha}\,\hat{\mathbf{e}}_3^0 + \dot{\beta}\,\hat{\mathbf{e}}_2^{'} + \dot{\gamma}\,\hat{\mathbf{e}}_3$$

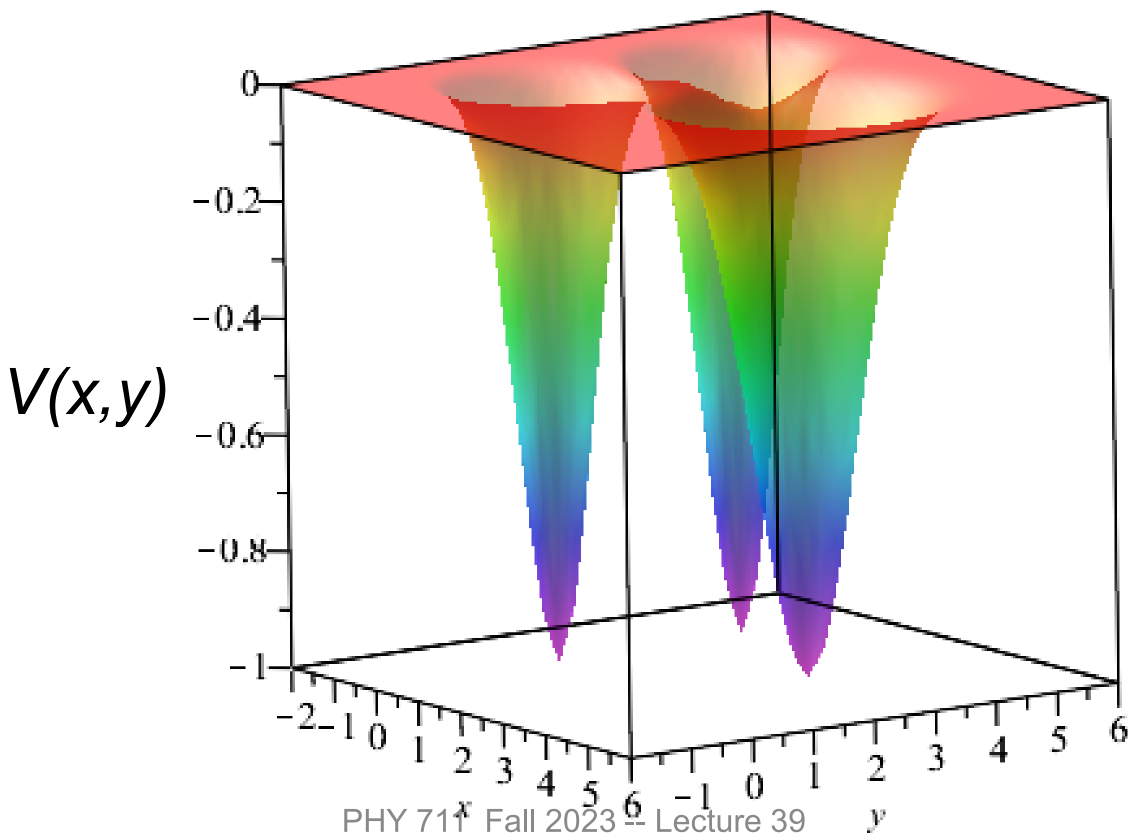


$$\begin{aligned}\tilde{\boldsymbol{\omega}} &= \left[\dot{\alpha}\left(-\sin\beta\cos\gamma\right) + \dot{\beta}\sin\gamma\right]\hat{\mathbf{e}}_1 \\ &+ \left[\dot{\alpha}\left(\sin\beta\sin\gamma\right) + \dot{\beta}\cos\gamma\right]\hat{\mathbf{e}}_2 \\ &+ \left[\dot{\alpha}\cos\beta + \dot{\gamma}\right]\hat{\mathbf{e}}_3\end{aligned}$$

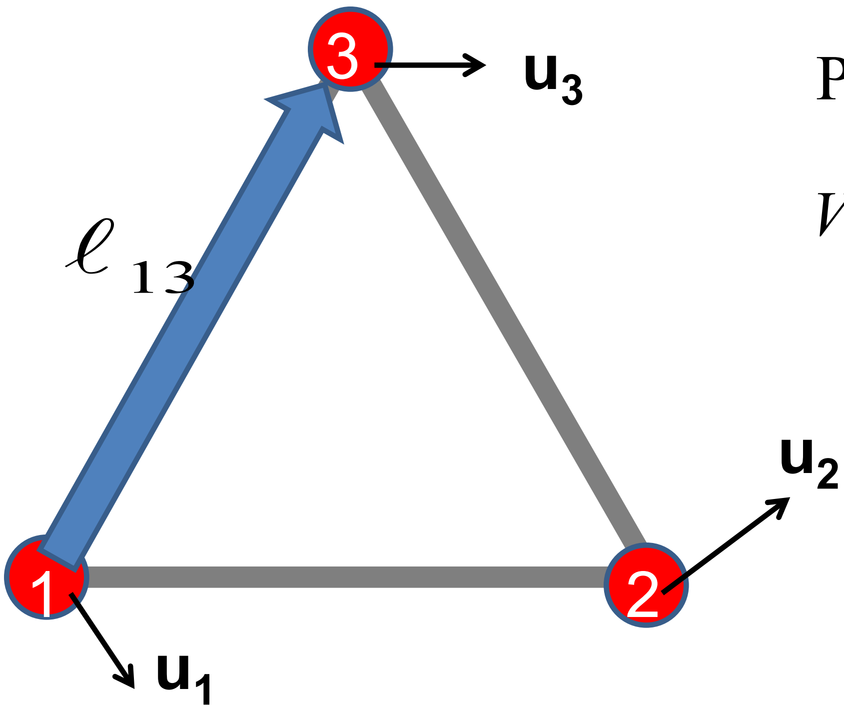
Normal modes of vibration -- potential in 2 and more dimensions

$$V(x,y) \approx V(x_{eq}, y_{eq}) + \tfrac{1}{2}(x - x_{eq})^2 \left.\frac{\partial^2 V}{\partial x^2}\right|_{x_{eq}, y_{eq}}$$

$$+ \tfrac{1}{2}(y - y_{eq})^2 \left.\frac{\partial^2 V}{\partial y^2}\right|_{x_{eq}, y_{eq}} + (x - x_{eq})(y - y_{eq}) \left.\frac{\partial^2 V}{\partial x \partial y}\right|_{x_{eq}, y_{eq}}$$



Example – normal modes of a system with the symmetry of an equilateral triangle -- continued



$$\boldsymbol{\ell}_{13} = |\boldsymbol{\ell}_{13}| \left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}} \right)$$

Potential contribution for spring 13:

$$V_{13} = \frac{1}{2}k\left(|\boldsymbol{\ell}_{13} + \mathbf{u}_3 - \mathbf{u}_1| - |\boldsymbol{\ell}_{13}|\right)^2$$

$$\approx \frac{1}{2}k\left(\frac{\boldsymbol{\ell}_{13} \cdot (\mathbf{u}_3 - \mathbf{u}_1)}{|\boldsymbol{\ell}_{13}|} \right)^2$$

$$\approx \frac{1}{2}k\left(\frac{1}{2}(u_{x3} - u_{x1}) + \frac{\sqrt{3}}{2}(u_{y3} - u_{y1}) \right)^2$$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

Potential contributions: $V = V_{12} + V_{13} + V_{23}$

$$\approx \frac{1}{2}k\left(\frac{\ell_{12}\cdot(\mathbf{u}_2-\mathbf{u}_1)}{|\ell_{12}|}\right)^2 + \frac{1}{2}k\left(\frac{\ell_{13}\cdot(\mathbf{u}_3-\mathbf{u}_1)}{|\ell_{13}|}\right)^2$$

$$+\frac{1}{2}k\left(\frac{\ell_{23}\cdot(\mathbf{u}_3-\mathbf{u}_2)}{|\ell_{23}|}\right)^2$$

$$\approx \frac{1}{2}k\left(u_{x2}-u_{x1}\right)^2$$

$$+\frac{1}{2}k\left(\frac{1}{2}(u_{x3}-u_{x1})+\frac{\sqrt{3}}{2}(u_{y3}-u_{y1})\right)^2$$

$$+\frac{1}{2}k\left(\frac{1}{2}(u_{x2}-u_{x3})-\frac{\sqrt{3}}{2}(u_{y2}-u_{y3})\right)^2$$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

$$\frac{k}{m}\begin{bmatrix} \frac{5}{4} & -1 & -\frac{1}{4} & \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} \\ -1 & \frac{5}{4} & -\frac{1}{4} & 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 \\ \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} & \frac{3}{4} & 0 & -\frac{3}{4} \\ 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 & \frac{3}{4} & -\frac{3}{4} \\ -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 & -\frac{3}{4} & -\frac{3}{4} & \frac{3}{2} \end{bmatrix}\begin{bmatrix} u_{x1} \\ u_{x2} \\ u_{x3} \\ u_{y1} \\ u_{y2} \\ u_{y3} \end{bmatrix} = \omega^2 \begin{bmatrix} u_{x1} \\ u_{x2} \\ u_{x3} \\ u_{y1} \\ u_{y2} \\ u_{y3} \end{bmatrix}$$

Discrete particle interactions → continuous media → The wave equation

Initial value solutions $\mu(x,t)$ to the wave equation; attributed to D'Alembert:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \qquad \text{where } \mu(x,0) = \varphi(x) \text{ and } \frac{\partial \mu}{\partial t}(x,0) = \psi(x)$$

$$\Rightarrow \mu(x,t) = \frac{1}{2}\Big(\varphi(x-ct) + \varphi(x+ct)\Big) + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(x')dx'$$

Mechanical motion of fluids

Newton's equations for fluids

Use Euler formulation; following "particles" of fluid

$$\text{Variables:} \quad \text{Density} \quad \rho(x,y,z,t)$$

$$\text{Pressure} \quad p(x,y,z,t)$$

$$\text{Velocity} \quad \mathbf{v}(x,y,z,t)$$

Navier-Stokes equation

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = \mathbf{f} - \frac{1}{\rho}\nabla p + \frac{\eta}{\rho}\nabla^2\mathbf{v} + \frac{1}{\rho}\left(\zeta + \frac{1}{3}\eta\right)\nabla(\nabla\cdot\mathbf{v})$$

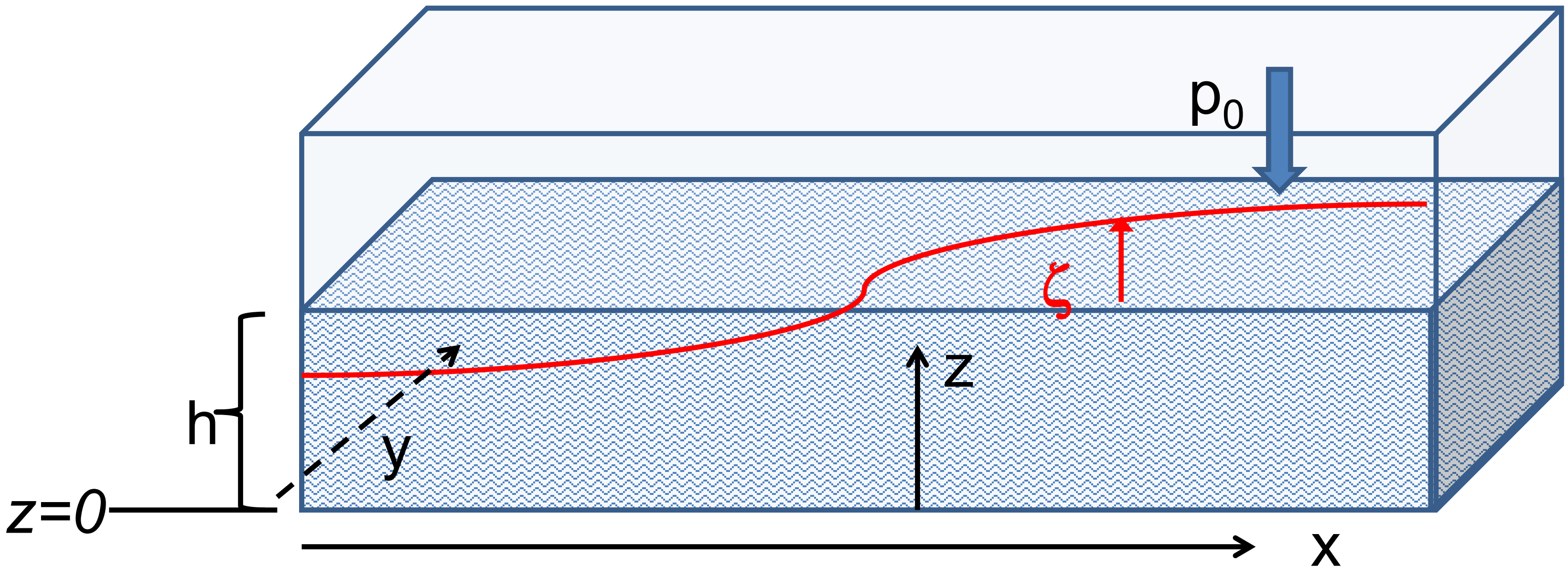
Continuity condition

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0$$

Viscosity contributions

Fluid mechanics of incompressible fluid plus surface

Non-linear effects in surface waves:



Dominant non-linear effects $\Rightarrow$ soliton solutions

$$\zeta(x,t) = \eta_0 \operatorname{sech}^2\left(\sqrt{\frac{3\eta_0}{h}}\frac{x-ct}{2h}\right) \qquad \eta_0 = \text{constant}$$

$$\text{where } c = \sqrt{\frac{gh}{1-\eta_0/h}} \approx \sqrt{gh}\left(1+\frac{\eta_0}{2h}\right)$$

Defining equations for $\Phi(x,z,t)$ and $\zeta(x,t)$

where $0 \leq z \leq h + \zeta(x,t)$

Continuity equation:

$$\nabla \cdot \mathbf{v} = 0 \quad \Rightarrow \quad \frac{\partial^2 \Phi(x,z,t)}{\partial x^2} + \frac{\partial^2 \Phi(x,z,t)}{\partial z^2} = 0$$

Bernoulli equation (assuming irrotational flow) and gravitation potential energy

$$-\frac{\partial \Phi(x,z,t)}{\partial t} + \frac{1}{2}\left[\underbrace{\left(\frac{\partial \Phi(x,z,t)}{\partial x} \right)^2}_{v_x^2} + \underbrace{\left(\frac{\partial \Phi(x,z,t)}{\partial z} \right)^2}_{v_z^2} \right] + g(z-h) = 0.$$

Boundary conditions on functions –

Zero velocity at bottom of tank:

$$\frac{\partial \Phi(x,0,t)}{\partial z} = 0.$$

Consistent vertical velocity at water surface

$$v_z(x,z,t)\Big|_{z=h+\zeta} = \frac{d\zeta}{dt} = \mathbf{v}\cdot\nabla\zeta + \frac{\partial \zeta}{\partial t}$$

$$= v_x \frac{\partial \zeta}{\partial x} + \frac{\partial \zeta}{\partial t}$$

$$\Rightarrow -\frac{\partial \Phi(x,z,t)}{\partial z} + \frac{\partial \Phi(x,z,t)}{\partial x}\frac{\partial \zeta(x,t)}{\partial x} - \frac{\partial \zeta(x,t)}{\partial t}\Bigg|_{z=h+\zeta} = 0$$

Bernoulli equation evaluated at surface:

$$-\frac{\partial\Phi(x,z,t)}{\partial t}+\frac{1}{2}\left[\left(\frac{\partial\Phi(x,z,t)}{\partial x}\right)^2+\left(\frac{\partial\Phi(x,z,t)}{\partial z}\right)^2\right]\Bigg|_{z=h+\zeta}+g\zeta(x,t)=0.$$

Consistency of surface velocity

$$-\frac{\partial\Phi(x,z,t)}{\partial z}+\frac{\partial\Phi(x,z,t)}{\partial x}\frac{\partial\zeta(x,t)}{\partial x}-\frac{\partial\zeta(x,t)}{\partial t}\Bigg|_{z=h+\zeta}=0$$

Analysis follows a number of steps based on a knowledge of the velocity potential at *z=0* and discarding small and high order non-linearities.

Coupled equations: $$-\frac{\partial \phi}{\partial t}+\frac{h^2}{2}\frac{\partial^3 \phi}{\partial t \partial x^2}+\frac{1}{2}\left(\frac{\partial \phi}{\partial x}\right)^2+g\zeta=0.$$

$$\frac{\partial}{\partial x}\left((h+\zeta(x,t))\frac{\partial \phi}{\partial x}\right)-\frac{h^3}{3!}\frac{\partial^4 \phi}{\partial x^4}-\frac{\partial \zeta}{\partial t}=0.$$

Traveling wave solutions with new notation:

$u \equiv x-ct \qquad \phi(x,t) \equiv \chi(u) \qquad$ and $\quad \zeta(x,t) \equiv \eta(u)$

Note that the wave “speed” c will be consistently determined

$$c\frac{d\chi(u)}{du}-\frac{ch^2}{2}\frac{d^3\chi(u)}{du^3}+\frac{1}{2}\left(\frac{d\chi(u)}{du}\right)^2+g\eta(u)=0.$$

$$\frac{d}{du}\left((h+\eta(u))\frac{d\chi(u)}{du}\right)-\frac{h^3}{6}\frac{d^4\chi(u)}{du^4}+c\frac{d\eta(u)}{du}=0.$$

Integrating and re-arranging coupled equations

$$c\frac{d\chi(u)}{du}-\frac{ch^2}{2}\frac{d^3\chi(u)}{du^3}+\frac{1}{2}\left(\frac{d\chi(u)}{du}\right)^2+g\eta(u)=0.$$

$$\chi'=-\frac{g}{c}\eta+\frac{h^2}{2}\chi'''-\frac{1}{2c}(\chi')^2\approx-\frac{g}{c}\eta-\frac{h^2 g}{2c}\eta''-\frac{g^2}{2c^3}\eta^2$$

$$\frac{d}{du}\left((h+\eta(u))\frac{d\chi(u)}{du}\right)-\frac{h^3}{6}\frac{d^4\chi(u)}{du^4}+c\frac{d\eta(u)}{du}=0.$$

$$\Rightarrow(h+\eta)\frac{d\chi(u)}{du}-\frac{h^3}{6}\frac{d^3\chi(u)}{du^3}+c\eta(u)=0$$

Now we can express $\frac{d\chi(u)}{du}=\chi'$ in terms of η:

$$\chi'\approx-\frac{g}{c}\eta-\frac{h^2 g}{2c}\eta''-\frac{g^2}{2c^3}\eta^2$$

Solution of the famous Korteweg-de Vries equation

Modified surface amplitude equation in terms of η

$$\Rightarrow \left(1-\frac{hg}{c^2}\right)\eta(u)-\frac{h^2}{3}\eta''(u)-\frac{3}{2h}\left[\eta(u)\right]^2=0.$$

Soliton solution

$$\zeta(x,t)=\eta(x-ct)=\eta_0 \ \mathrm{sech}^2\left(\sqrt{\frac{3\eta_0}{h}}\,\frac{x-ct}{2h}\right)$$

$$c=\sqrt{\frac{gh}{1-\eta_0/h}}\approx\sqrt{gh}\left(1+\frac{\eta_0}{2h}\right) \quad \text{where } \eta_0 \text{ is a constant}$$