PHY 711 Classical Mechanics and Mathematical Methods
11-11:50 AM MWF Olin 102

Plan for Lecture 38

General review

- Classical mechanics – traditional topics
- Classical mechanics – related topics
- Mathematical methods
- Course assessment

23	Wed, 10/26/2016	Chap. 9	Introduction to hydrodynamics		
24	Fri, 10/28/2016	Chap. 9	Introduction to hydrodynamics	#18	10/31/2016
25	Mon, 10/31/2016	Chap. 9	Sound waves	#19	11/02/2016
26	Wed, 11/02/2016	Chap. 9	Sound waves	#20	11/04/2016
27	Fri, 11/04/2016	Chap. 9	Non-linear sound	#21	11/07/2016
28	Mon, 11/07/2016	Chap. 10	Surface waves in fluids		
29	Wed, 11/09/2016	Chap. 10	Surface waves in fluids	#22	11/11/2016
30	Fri, 11/11/2016	Chap. 11	Heat conductivity	#23	11/14/2016
31	Mon, 11/14/2016	Chap. 12	Viscous fluids	#24	11/16/2016
32	Wed, 11/16/2016	Chap. 12	Viscous fluids	#25	11/18/2016
33	Fri, 11/18/2016	Chap. 12	Viscous fluids	#26	11/21/2016
34	Mon, 11/21/2016	Chap. 13	Elastic continua	Prepare presentations	
	Wed, 11/23/2016		Thanksgiving Holiday -- no class		
	Fri, 11/25/2016		Thanksgiving Holiday -- no class		
35	Mon, 11/28/2016	Chap. 13	Elastic continua	Prepare presentations	
36	Wed, 11/30/2016		Math methods	Prepare presentations	
37	Fri, 12/02/2016		Math methods	Prepare presentations	
38	Mon, 12/05/2016		Review	Prepare presentations	
	Wed, 12/07/2016		Presentations I		
	Fri, 12/09/2016		Presentations II		

PHY 711 Presentation Schedule -- Fall 2016

Please enter your name and title next to your prefered time --

Wednesday, Dec. 7, 2016

	Presenter name	Title of presentation
11:00-11:25 AM	Hamna Haneef	Unravelling a classical mechanics brain twister
11:25-11:50 AM	Matt Roveto	Numerical Solutions to the Classical Three Body Problem

Friday, Dec. 9, 2016

	Presenter name	Title of presentation
11:00-11:25 AM	Colin Tyznik	Normal Modes of Perovskite crystal

Review of course topics

- Classical mechanics – traditional topics
  - Particle scattering; scattering cross section
  - Inertial and accelerated reference frames
  - Calculus of variations
  - Lagrangian and Hamiltonian formalisms
  - Small oscillations near equilibrium
  - Rigid body rotations
- Classical mechanics – additional topics
  - Mechanics of continuous media
  - Mechanics of fluids; bulk and surface motions
  - Heat conduction
  - Elastic continua
- Mathematical methods

Scattering theory:

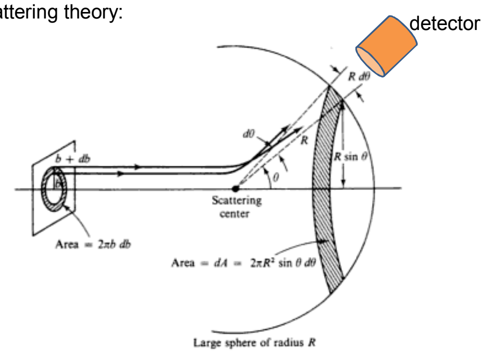
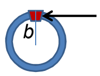


Figure 5.5 The scattering problem and relation of cross section to impact parameter.

Differential cross section

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{Number of detected particles at } \theta \text{ per target particle}}{\text{Number of incident particles per unit area}}$$

$$= \text{Area of incident beam that is scattered into detector at angle } \theta$$



$d\varphi b db$

If we can assume that the process is isotropic in ϕ, results depend on b and θ:

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{d\varphi\, b\, db}{d\varphi \sin\theta\, d\theta} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

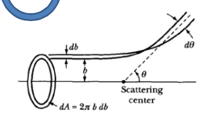


Figure from Marion & Thorton, Classical Dynamics

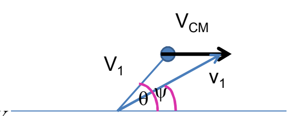
In general, scattering is most easily analyzed in the center of mass frame -- relationship between center of mass and laboratory frames of reference:

lab CM

$$\mathbf{v}_1 = \mathbf{V}_1 + \mathbf{V}_{CM}$$

$$v_1 \sin\psi = V_1 \sin\theta$$

$$v_1 \cos\psi = V_1 \cos\theta + V_{CM}$$



$$\tan\psi = \frac{\sin\theta}{\cos\theta + V_{CM}/V_1} = \frac{\sin\theta}{\cos\theta + m_1/m_2} \quad \text{for elastic case}$$

$$\text{Also:} \quad \cos\psi = \frac{\cos\theta + m_1/m_2}{\sqrt{1 + 2m_1/m_2 \cos\theta + (m_1/m_2)^2}}$$

Differential cross sections in different reference frames

$$\left(\frac{d\sigma_{LAB}(\psi)}{d\Omega_{LAB}}\right) = \left(\frac{d\sigma_{CM}(\theta)}{d\Omega_{CM}}\right)\frac{d\Omega_{CM}}{d\Omega_{LAB}}$$

$$\frac{d\Omega_{CM}}{d\Omega_{LAB}} = \left|\frac{\sin\theta}{\sin\psi}\frac{d\theta}{d\psi}\right| = \left|\frac{d\cos\theta}{d\cos\psi}\right|$$

Using:

$$\cos\psi = \frac{\cos\theta + m_1/m_2}{\sqrt{1 + 2(m_1/m_2)\cos\theta + (m_1/m_2)^2}}$$

$$\left|\frac{d\cos\psi}{d\cos\theta}\right| = \frac{(m_1/m_2)\cos\theta + 1}{\left(1 + 2(m_1/m_2)\cos\theta + (m_1/m_2)^2\right)^{3/2}}$$

Differential cross sections in different reference frames –

$$\left(\frac{d\sigma_{LAB}(\psi)}{d\Omega_{LAB}}\right) = \left(\frac{d\sigma_{CM}(\theta)}{d\Omega_{CM}}\right)\left|\frac{d\cos\theta}{d\cos\psi}\right|$$

$$\left(\frac{d\sigma_{LAB}(\psi)}{d\Omega_{LAB}}\right) = \left(\frac{d\sigma_{CM}(\theta)}{d\Omega_{CM}}\right)\frac{\left(1+2m_1/m_2\cos\theta+(m_1/m_2)^2\right)^{3/2}}{(m_1/m_2)\cos\theta+1}$$

$$\text{where :}\quad \tan\psi = \frac{\sin\theta}{\cos\theta + m_1/m_2}$$

$$\left(\frac{d\sigma_{CM}}{d\Omega_{CM}}\right) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

Scattering angle equation in CM frame for interaction potential $V(r)$:

$$\theta = -\pi + 2b\int_0^{1/r_{\min}} du\left(\frac{1}{\sqrt{1-b^2u^2-\frac{V(1/u)}{E}}}\right)$$

where:

$$1-\frac{b^2}{r_{\min}^2}-\frac{V(r_{\min})}{E}=0$$

Rutherford scattering example: $\frac{V(r)}{E}\equiv\frac{\kappa}{r}$

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{\kappa^2}{16}\frac{1}{\sin^4(\theta/2)}$$

Physics of rotating coordinate system

Consider a vector $\mathbf{V}$ in a frame rotating with angular velocity $\boldsymbol{\omega}$:

$$\left(\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\frac{d\mathbf{V}}{dt}\right)_{body} + \sum_{i=1}^{3} V_i\frac{d\hat{e}_i}{dt}$$

$$\left(\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\frac{d\mathbf{V}}{dt}\right)_{body} + \boldsymbol{\omega}\times\mathbf{V}$$

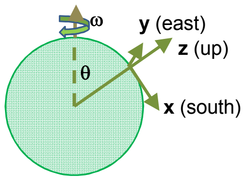
Effects on acceleration (rotation only):

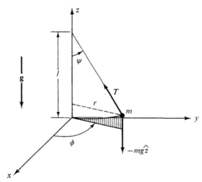
$$\left(\frac{d}{dt}\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\left(\frac{d}{dt}\right)_{body} + \boldsymbol{\omega}\times\right)\left\{\left(\frac{d\mathbf{V}}{dt}\right)_{body} + \boldsymbol{\omega}\times\mathbf{V}\right\}$$

$$\left(\frac{d^2\mathbf{V}}{dt^2}\right)_{inertial} = \left(\frac{d^2\mathbf{V}}{dt^2}\right)_{body} + 2\boldsymbol{\omega}\times\left(\frac{d\mathbf{V}}{dt}\right)_{body} + \frac{d\boldsymbol{\omega}}{dt}\times\mathbf{V} + \boldsymbol{\omega}\times\boldsymbol{\omega}\times\mathbf{V}$$

Equation of motion on Earth's surface

$$m\left(\frac{d^2\mathbf{r}}{dt^2}\right)_{earth} = -\frac{GM_e m}{r^2}\hat{\mathbf{r}} + \mathbf{F}' - 2m\boldsymbol{\omega}\times\left(\frac{d\mathbf{r}}{dt}\right)_{earth} - m\frac{d\boldsymbol{\omega}}{dt}\times\mathbf{r} - m\boldsymbol{\omega}\times\boldsymbol{\omega}\times\mathbf{r}$$





$$\boldsymbol{\omega} \approx -\omega\sin\theta\hat{\mathbf{x}} + \omega\cos\theta\hat{\mathbf{z}}$$

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Calculus of variation example for a pure integral functions

Find the function $y(x)$ which extremizes $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$

where $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) \equiv \int_{x_i}^{x_f} f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) dx.$

Necessary condition : $\delta L = 0$

At any x, let $y(x) \rightarrow y(x) + \delta y(x)$

$$\frac{dy(x)}{dx} \rightarrow \frac{dy(x)}{dx} + \delta\frac{dy(x)}{dx}$$

$$\Rightarrow \left(\frac{\partial f}{\partial y}\right)_{x,\frac{dy}{dx}} - \frac{d}{dx}\left[\left(\frac{\partial f}{\partial(dy/dx)}\right)_{x,y}\right] = 0 \quad \text{for all } x_i \le x \le x_f$$

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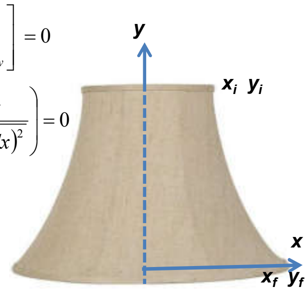
Example : Lamp shade shape *y(x)*

$$A = 2\pi\int_{x_i}^{x_f} x\sqrt{1+\left(\frac{dy}{dx}\right)^2}\,dx \quad \Rightarrow f\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right) = x\sqrt{1+\left(\frac{dy}{dx}\right)^2}$$

$$\left(\frac{\partial f}{\partial y}\right)_{x,\frac{dy}{dx}} - \frac{d}{dx}\left[\left(\frac{\partial f}{\partial(dy/dx)}\right)_{x,y}\right] = 0$$

$$\Rightarrow -\frac{d}{dx}\left(\frac{x\,dy/dx}{\sqrt{1+(dy/dx)^2}}\right) = 0$$



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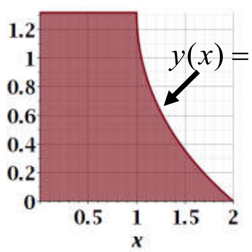
$$-\frac{d}{dx}\left(\frac{x\,dy/dx}{\sqrt{1+(dy/dx)^2}}\right)=0$$

$$\frac{x\,dy/dx}{\sqrt{1+(dy/dx)^2}}=K_1$$

$$\frac{dy}{dx}=-\frac{1}{\sqrt{\left(\frac{x}{K_1}\right)^2-1}}$$

$$\Rightarrow y(x)=K_2-K_1\ln\left(\frac{x}{K_1}+\sqrt{\frac{x^2}{K_1^2}-1}\right)$$



$$y(x)=\ln\left(\frac{2+\sqrt{3}}{x+\sqrt{x^2-1}}\right)$$

Application of calculus of variation to Lagrangian mechanics:

Now consider the Lagrangian defined to be:

$$L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)\equiv T-U$$

Kinetic energy (T); Potential energy (U)

Hamilton's principle states:

$$S\equiv\int_{t_i}^{t_f}L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)dt \quad \text{is minimized for physical } y(t):$$

Lagrange's equations of motion:

$$\left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma}-\frac{\partial L}{\partial q_\sigma}\right)=0 \quad \text{for} \quad L=L\left(\{q_\sigma\},\{\dot{q}_\sigma\},t\right)\equiv T-U$$

Extension of results in presence of electromagnetic field (using cartesian coordinates)

where $\mathbf{E}(\mathbf{r},t) = -\nabla\Phi(\mathbf{r},t) - \frac{1}{c}\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}$ $\quad \mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$

$$L = L(x,y,z,\dot{x},\dot{y},\dot{z},t) \equiv T - U$$

$$T = \tfrac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right) \qquad U = U_0(\mathbf{r},t) + q\Phi(\mathbf{r},t) - \frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)$$

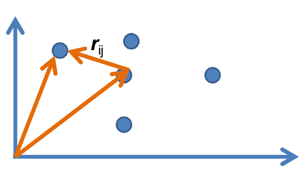
$$L = \tfrac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right) - U_0(\mathbf{r},t) - q\Phi(\mathbf{r},t) + \frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)$$

Recipe for constructing the Hamiltonian and analyzing the equations of motion

1. Construct Lagrangian function : $L = L(\{q_\sigma(t)\},\{\dot{q}_\sigma(t)\},t)$
2. Compute generalized momenta : $p_\sigma \equiv \dfrac{\partial L}{\partial \dot{q}_\sigma}$
3. Construct Hamiltonian expression : $H = \sum_\sigma \dot{q}_\sigma p_\sigma - L$
4. Form Hamiltonian function : $H = H(\{q_\sigma(t)\},\{p_\sigma(t)\},t)$
5. Analyze canonical equations of motion :

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \qquad \frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$

Use of Lagrangian/Hamiltonian formalism for molecular dynamics



Pairwise interaction between particles

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

➔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).

H. C. Andersen's effective Lagrangian for constant pressure simulations

$$L\left(\{\boldsymbol{\rho}_i(t)\},\{\dot{\boldsymbol{\rho}}_i(t)\},Q,\dot{Q}\right)=Q^{2/3}\sum_i \tfrac{1}{2}m_i\left|\dot{\boldsymbol{\rho}}_i\right|^2-\sum_{i<j}u\left(Q^{1/3}\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|\right)+\tfrac{1}{2}M\dot{Q}^2-\alpha Q$$

$$H\left(\{\boldsymbol{\rho}_i(t)\},\{\boldsymbol{\pi}_i(t)\},Q,\Pi\right)=\sum_i \frac{\left|\boldsymbol{\pi}_i\right|^2}{2m_iQ^{2/3}}+\sum_{i<j}u\left(Q^{1/3}\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|\right)+\frac{\Pi^2}{2M}+\alpha Q$$

Equations of motion in "original" coordinates:

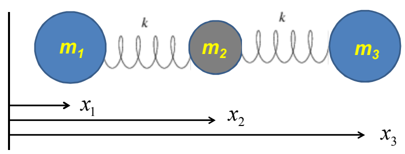
$$\frac{d\mathbf{r}_i}{dt}=\frac{\mathbf{p}_i}{m_i}+\frac{1}{3}\mathbf{r}_i\frac{d\ln V}{dt}$$

$$\frac{d\mathbf{p}_i}{dt}=-\sum_{j<i}\frac{\mathbf{r}_i-\mathbf{r}_j}{\left|\mathbf{r}_i-\mathbf{r}_j\right|}u'\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)-\frac{1}{3}\mathbf{p}_i\frac{d\ln V}{dt}$$

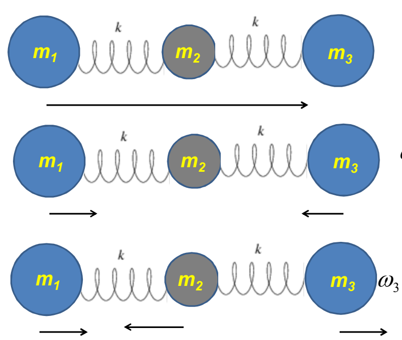
$$M\frac{d^2V}{dt^2}=-\alpha+\frac{1}{V}\left(\frac{2}{3}\sum_i\frac{\mathbf{p}_i\cdot\mathbf{p}_i}{m_i}-\frac{1}{3}\sum_{j<i}\left|\mathbf{r}_i-\mathbf{r}_j\right|u'\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)\right)$$

Normal modes of vibration about equilibrium:

Example – linear molecule



$$L=\frac{1}{2}m_1\dot{x}_1^2+\frac{1}{2}m_2\dot{x}_2^2+\frac{1}{2}m_3\dot{x}_3^2$$
$$-\frac{1}{2}k\left(x_2-x_1-\ell_{12}\right)^2-\frac{1}{2}k\left(x_3-x_2-\ell_{23}\right)^2$$

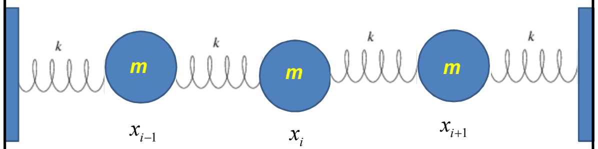


$$\omega_1=0$$

$$\omega_2=\sqrt{\frac{k}{m_O}}$$

$$\omega_3=\sqrt{\frac{k}{m_O}+\frac{2k}{m_C}}$$

Consider an extended system of masses and springs:



Note: each mass coordinate is measured relative to its equilibrium position x_i^0

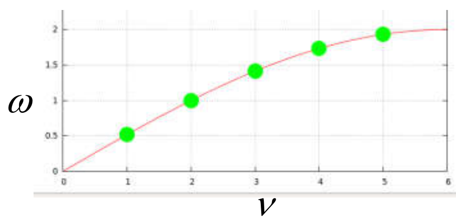
$$L = T - V = \frac{1}{2} m \sum_{i=1}^{N} \dot{x}_i^2 - \frac{1}{2} k \sum_{i=0}^{N} \left(x_{i+1} - x_i\right)^2$$

Note: In fact, we have N masses; x_0 and x_{N+1} will be treated using boundary conditions.

Summary of results:

$$\Rightarrow \omega_\nu^2 = \frac{4k}{m} \sin^2\left(\frac{\nu\pi}{2(N+1)}\right) \qquad x_n = \Re\left(2iA \sin\left(\frac{\nu\pi n}{N+1}\right)\right)$$

$$\nu = 0,1,...N \qquad n = 1,2,.....N$$



Extension of ideas --

3-dimensional periodic lattices

Example – face-centered-cubic unit cell (Al or Ni)

Diagram of atom positions

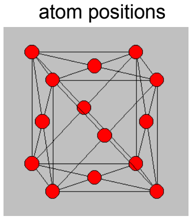
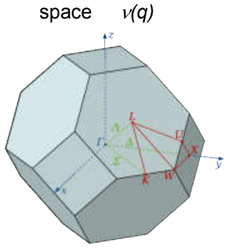


Diagram of q-space $\nu(q)$



From: PRB **59** 3395 (1999); Mishin et. al. $\nu(q)$

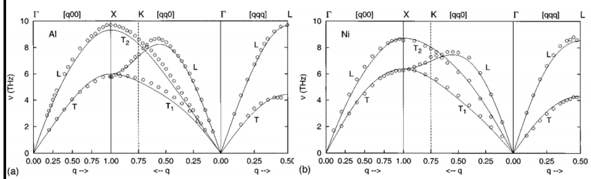
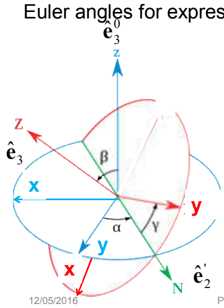


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point X were included in the fitting database with low weight.

Rigid body rotation -- Moment of inertia tensor :

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

Euler angles for expressing rigid body rotation:



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

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

Rotational kinetic energy for "symmetric" top:

If $I_1 = I_2$:

$$T(\alpha,\beta,\gamma,\dot{\alpha},\dot{\beta},\dot{\gamma}) = \frac{1}{2} I_1 \left(\dot{\alpha}^2 \sin^2\beta + \dot{\beta}^2\right) + \frac{1}{2} I_3 \left[\dot{\alpha}\cos\beta + \dot{\gamma}\right]^2$$

Equations of motion for continuous media

Variables:

ρ density (mass/volume)

p pressure (force/area)

$\mathbf{f}$ force density (force/density)

$\mathbf{v}$ velocity

$\mathbf{r}$ (x_1, x_2, x_3) position

i^{th} component of momentum form of Newton-Euler equation:

$$\frac{\partial(\rho v_i)}{\partial t} + \sum_{i=1}^{3} \frac{\partial T_{ij}}{\partial x_j} = \rho f_i \quad \text{where } T_{ij} \text{ denotes stress tensor}$$

Continuity equation

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

Stress tensor for fluids

Total stress tensor: $T_{kl} = T_{kl}^{\text{ideal}} + T_{kl}^{\text{viscous}}$

$$T_{kl}^{\text{ideal}} = \rho v_k v_l + p\delta_{kl}$$

$$T_{kl}^{\text{viscous}} = -\eta\left(\frac{\partial v_k}{\partial x_l} + \frac{\partial v_l}{\partial x_k} - \frac{2}{3}\delta_{kl}(\nabla \cdot \mathbf{v})\right) - \zeta\delta_{kl}(\nabla \cdot \mathbf{v})$$

Navier-Stokes equation for fluid motion

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

Stress tensor for elastic media (Hooke's law in terms of displacement **u**; linear terms only)

Hooke's law: $T_{kl} = -K\delta_{kl}(\nabla \cdot \mathbf{u}) - 2\mu\left(\frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) - \frac{1}{3}\delta_{kl}(\nabla \cdot \mathbf{u})\right)$

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mu \nabla^2 \mathbf{u} + \left(K + \frac{1}{3}\mu\right)\nabla(\nabla \cdot \mathbf{u}) + \rho \mathbf{f}$$