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

Plan for Lecture 27:

Introduction to hydrodynamics

1. Motivation for topic
2. Newton's laws for fluids
3. Conservation relations

3	Mon, 9/03/2012	Chap. 1	Scattering theory continued	#3
4	Wed, 9/05/2012	Chap. 1 & 2	Scattering theory/Accelerated coordinate frame	#4
5	Fri, 9/07/2012	Chap. 2	Accelerated coordinate frame	#5
6	Mon, 9/10/2012	Chap. 3	Calculus of Variation	#6
7	Wed, 9/12/2012	Chap. 3	Calculus of Variation continued	
8	Fri, 9/14/2012	Chap. 3	Lagrangian	#7
9	Mon, 9/17/2012	Chap. 3 & 6	Lagrangian	#8
10	Wed, 9/19/2012	Chap. 3 & 6	Lagrangian	#9
11	Fri, 9/21/2012	Chap. 3 & 6	Lagrangian	#10
12	Mon, 9/24/2012	Chap. 3 & 6	Lagrangian and Hamiltonian	#11
13	Wed, 9/26/2012	Chap. 6	Lagrangian and Hamiltonian	#12
14	Fri, 9/28/2012	Chap. 6	Lagrangian and Hamiltonian	#13
15	Mon, 10/01/2012	Chap. 4	Small oscillations	#14
16	Wed, 10/03/2012	Chap. 4	Small oscillations	#15
17	Fri, 10/05/2012	Chap. 4	Small oscillations	
18	Mon, 10/08/2012	Chap. 7	Wave equation	Take Home Exam
19	Wed, 10/10/2012	Chap. 7	Wave equation	Take Home Exam
20	Fri, 10/12/2012	Chap. 7	Wave equation	Take Home Exam
21	Mon, 10/15/2012	Chap. 7	Wave equation	Exam due
22	Wed, 10/17/2012	Chap. 7, 5	Moment of inertia	
	Fri, 10/19/2012		Fall break	
23	Mon, 10/22/2012	Chap. 5	Rigid body rotation	#16
24	Wed, 10/24/2012	Chap. 5	Rigid body rotation	#17
25	Fri, 10/26/2012	Chap. 5	Rigid body rotation	#18
26	Mon, 10/29/2012	Chap. 8	Waves in elastic membranes	#19
27	Wed, 10/31/2012	Chap. 9	Introduction to hydrodynamics	

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WFU Joint Physics and Chemistry Colloquium

TITLE: Lithium ion batteries: From practice to theory

SPEAKER: Dr. Paul R. C. Kent,

Center for Nanophase Materials
Oak Ridge National Laboratories

TIME: Wednesday October 31, 2012 at 4 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge prior to the colloquium. All interested persons are cordially invited to attend.

ABSTRACT

Advances in rechargeable lithium ion batteries have led to their near ubiquitous use in mobile devices. However, significant improvements in energy density, power density, lifetime, and overall cost are desired for widespread use in new applications such as in the automotive industry. This will require the modification and adoption of new cathode, anode, and electrolyte materials, as well as insights into lifetime altering mechanisms such as solid-electrolyte interphase formation. In this talk I will provide a gentle introduction to the fundamental physical principles of these energy storage devices, outline the challenging scientific problems that remain, and describe how quantum mechanics based simulations will be able to address some of these problems. I will also describe some of the fundamental problems with current modeling approaches and recent attempts to improve simulation capability on supercomputers.

Motivation

1. Natural progression from strings, membranes, fluids; description of 1, 2, and 3 dimensional continua
2. Interesting and technologically important phenomena associated with fluids

Plan

1. Newton's laws for fluids
2. Continuity equation
3. Stress tensor
4. Energy relations
5. Bernoulli's theorem
6. Various examples
7. Sound waves

Newton's equations for fluids

Use Lagrange formulation; following "particles" of fluid

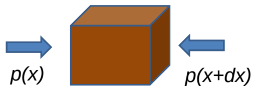
$$\text{Variables: Density } \rho(x,y,z,t)$$
$$\text{Pressure } p(x,y,z,t)$$
$$\text{Velocity } \mathbf{v}(x,y,z,t)$$

$$m\mathbf{a} = \mathbf{F}$$

$$m \rightarrow \rho dV$$

$$\mathbf{a} \rightarrow \frac{d\mathbf{v}}{dt}$$

$$\mathbf{F} \rightarrow \mathbf{F}_{applied} + \mathbf{F}_{pressure}$$



$$F_{pressure}\big|_x = \left(-p(x+dx,y,z)+p(x,y,z)\right)dydz$$
$$= \frac{\left(-p(x+dx,y,z)+p(x,y,z)\right)}{dx}dxdydz$$
$$= -\frac{\partial p}{\partial x}dV$$

Newton's equations for fluids -- continued

$$m\mathbf{a} = \mathbf{F}_{applied} + \mathbf{F}_{pressure}$$
$$\rho dV\frac{d\mathbf{v}}{dt} = \mathbf{f}_{applied}\,\rho dV - \nabla p dV$$
$$\rho\frac{d\mathbf{v}}{dt} = \rho\mathbf{f}_{applied} - \nabla p$$

Detailed analysis of acceleration term :

$$\mathbf{v} = \mathbf{v}(x,y,z,t)$$
$$\frac{d\mathbf{v}}{dt} = \frac{\partial\mathbf{v}}{\partial x}\frac{dx}{dt} + \frac{\partial\mathbf{v}}{\partial y}\frac{dy}{dt} + \frac{\partial\mathbf{v}}{\partial z}\frac{dz}{dt} + \frac{\partial\mathbf{v}}{\partial t}$$
$$\frac{d\mathbf{v}}{dt} = \frac{\partial\mathbf{v}}{\partial x}v_x + \frac{\partial\mathbf{v}}{\partial y}v_y + \frac{\partial\mathbf{v}}{\partial z}v_z + \frac{\partial\mathbf{v}}{\partial t}$$
$$\frac{d\mathbf{v}}{dt} = (\mathbf{v}\cdot\nabla)\mathbf{v} + \frac{\partial\mathbf{v}}{\partial t}$$

Note that :

$$\frac{\partial\mathbf{v}}{\partial x}v_x + \frac{\partial\mathbf{v}}{\partial y}v_y + \frac{\partial\mathbf{v}}{\partial z}v_z = \nabla\left(\frac{1}{2}\mathbf{v}\cdot\mathbf{v}\right) - \mathbf{v}\times(\nabla\times\mathbf{v})$$

Newton's equations for fluids -- continued

$$\rho\frac{d\mathbf{v}}{dt}=\rho\mathbf{f}_{applied}-\nabla p$$

$$\rho\left(\nabla\left(\frac{1}{2}\mathbf{v}\cdot\mathbf{v}\right)-\mathbf{v}\times(\nabla\times\mathbf{v})+\frac{\partial\mathbf{v}}{\partial t}\right)=\rho\mathbf{f}_{applied}-\nabla p$$

$$\frac{\partial\mathbf{v}}{\partial t}+\nabla\left(\tfrac{1}{2}v^2\right)-\mathbf{v}\times(\nabla\times\mathbf{v})=\mathbf{f}_{applied}-\frac{\nabla p}{\rho}$$

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Continuity equation:

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

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

Consider : $\frac{d\rho}{dt}=\frac{\partial\rho}{\partial t}+\nabla\rho\cdot\mathbf{v}$

$\Rightarrow \frac{d\rho}{dt}+\rho\nabla\cdot\mathbf{v}=0$ alternative form of continuity equation

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Solution of Euler's equation for fluids

$$\frac{\partial\mathbf{v}}{\partial t}+\nabla\left(\tfrac{1}{2}v^2\right)-\mathbf{v}\times(\nabla\times\mathbf{v})=\mathbf{f}_{applied}-\frac{\nabla p}{\rho}$$

Consider the following restrictions:

1. $(\nabla\times\mathbf{v})=0$ "irrotational flow"

   $\Rightarrow \mathbf{v}=-\nabla\Phi$

2. $\mathbf{f}_{applied}=-\nabla U$ conservative applied force

3. $\rho=$ (constant) incompressible fluid

$$\frac{\partial(-\nabla\Phi)}{\partial t}+\nabla\left(\tfrac{1}{2}v^2\right)=-\nabla U-\frac{\nabla p}{\rho}$$

$$\Rightarrow \nabla\left(\frac{p}{\rho}+U+\tfrac{1}{2}v^2-\frac{\partial\Phi}{\partial t}\right)=0$$

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Bernoulli's integral of Euler's equation

$$\nabla\left(\frac{p}{\rho}+U+\tfrac{1}{2}v^2-\frac{\partial\Phi}{\partial t}\right)=0$$

Integrating over space:

$$\frac{p}{\rho}+U+\tfrac{1}{2}v^2-\frac{\partial\Phi}{\partial t}=C(t)$$

where $\mathbf{v}=-\nabla\Phi(\mathbf{r},t)=-\nabla\big(\Phi(\mathbf{r},t)+C(t)\big)$

$$\Rightarrow \frac{p}{\rho}+U+\tfrac{1}{2}v^2-\frac{\partial\Phi}{\partial t}=0 \qquad \text{Bernoulli's theorem}$$

Examples of Bernoulli's theorem

$$\frac{p}{\rho}+U+\tfrac{1}{2}v^2-\frac{\partial\Phi}{\partial t}=0$$

Modified form; assuming $\frac{\partial\Phi}{\partial t}=0$

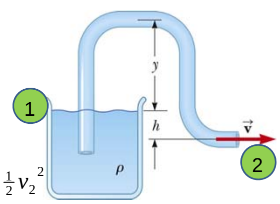
$$\frac{p}{\rho}+U+\tfrac{1}{2}v^2=\text{constant}$$

$p_1=p_2=p_{atm}$

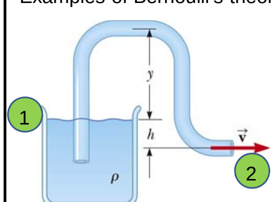
$U_1-U_2=gh$

$v_1\approx 0$

$$\frac{p_1}{\rho}+U_1+\tfrac{1}{2}{v_1}^2=\frac{p_2}{\rho}+U_2+\tfrac{1}{2}{v_2}^2$$



Examples of Bernoulli's theorem -- continued



$p_1=p_2=p_{atm}$

$U_1-U_2=gh$

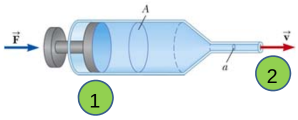
$v_1\approx 0$

$$\frac{p_1}{\rho}+U_1+\tfrac{1}{2}{v_1}^2=\frac{p_2}{\rho}+U_2+\tfrac{1}{2}{v_2}^2$$

$$v_2\approx\sqrt{2gh}$$

Examples of Bernoulli's theorem -- continued

$$\frac{p}{\rho}+U+\tfrac{1}{2}v^2=\text{constant}$$



$$p_1=\frac{F}{A}+p_{atm} \qquad p_2=p_{atm}$$

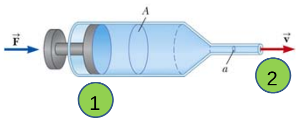
$$U_1=U_2$$

$$v_1A=v_2a \qquad \text{continuity equation}$$

$$\frac{p_1}{\rho}+U_1+\tfrac{1}{2}v_1{}^2=\frac{p_2}{\rho}+U_2+\tfrac{1}{2}v_2{}^2$$

Examples of Bernoulli's theorem -- continued

$$\frac{p}{\rho}+U+\tfrac{1}{2}v^2=\text{constant}$$



$$\frac{2F}{A}=v_2{}^2\left(1-\left(\frac{a}{A}\right)^2\right)$$

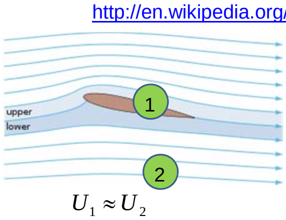
$$v_2=\sqrt{\frac{2F/A}{1-\left(\frac{a}{A}\right)^2}}$$

Examples of Bernoulli's theorem – continued

Approximate explanation of airplane lift

Cross section view of airplane wing

http://en.wikipedia.org/wiki/Lift_%28force%29



$$U_1\approx U_2$$

$$\frac{p_1}{\rho}+U_1+\tfrac{1}{2}v_1{}^2=\frac{p_2}{\rho}+U_2+\tfrac{1}{2}v_2{}^2$$

$$p_2-p_1=\tfrac{1}{2}\left(v_1{}^2-v_2{}^2\right)$$