Work all 5 problems.

1. Continuum mechanics.

(a) Give a clear and complete definition, in words and mathematically, or state the theorem or principle of each of the following terms related to the behavior of a continuous medium:

1. Motion.
2. Displacement.
3. Deformation gradient.
4. Right Cauchy-Green deformation tensor.
5. Green strain tensor.
6. Strain-displacement relations.
7. Linear momentum.

(b) The cube shown is subject to finite simple shear.

(1) Compute the deformation gradient $F$.
(2) Compute the deformation tensor $C$.
(3) Compute the principle directions of deformation for $\Delta = a$. 
2. **Transport.** Transport due to convection and diffusion arises in many application areas.

(a) Name 3 different transport applications where such models are appropriate.
(b) The "model" one-dimensional transport equation for scalar \( \varphi \) is

\[
\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} = k \frac{\partial^2 \varphi}{\partial x^2},
\]

where \( u \) and \( k \) are known positive constants.

(i) Identify the physical nature of the terms and variables in the equation.
(ii) Give initial and boundary conditions on a domain to complete a well posed mathematical model.
(iii) Also give an example of data where the problem is not well posed and explain why it is not.
(iv) What is the PDE type of the equation as stated?

(c) Introduce characteristic scales to construct a dimensionless form of the problem. Comment on how the choice of timescales influences the resulting dimensionless equation.
(d) What is the expected behavior of the mathematical model as \( u \) or \( k \) independently approach 0?
(e) For the steady-state problem with \( u \gg k \), explain qualitatively the idea of multiple scales and matched asymptotic expansions giving an illustrative example to support your reasoning. (Be brief.)

3. **Density calculation.** Consider a collection of particles in two dimensions, interacting through the potential

\[
E = \frac{1}{2} \sum_{i \neq j} \phi(r_{ij}),
\]

where

\[
\phi(r) = \phi_0 \exp(-r) \left( \frac{a}{r} - 1 \right),
\]

\( r_{ij} \) is the magnitude of the distance between particles \( i \) and \( j \) in two dimensions, and \( a \) is a constant. For \( a \) less than a critical value \( a_0 \), as the number \( N \) of particles becomes large, the energy of this collection of particles is unbounded below, and the particles collapse toward a state of infinite density. Find \( a_0 \). In performing calculations, assume that the particles can be replaced by a continuous distribution of particles of constant density, and neglect the fact that for any finite number of particles there must be a place where the density of particles falls to zero.
4. Boltzmann Transport. Consider the Boltzmann Transport Equation (BTE) for elastic collisions described by the equation

$$\partial_t f(t, x, v) - v \nabla_x f(t, x, v) = Q(f, f)(t, x, v), \quad (x, v) \in \mathbb{R}^3 \times \mathbb{R}^3, \quad t > 0,$$

where the collision operator $Q(f, f)$ satisfies the weak formulation

$$\int_{\mathbb{R}^n} Q(f, f) \phi(v) \, dv = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{S^{n-1}} f(v) f(v_*) [\phi(v') + \phi(v'_*) - \phi(v) - \phi(v_*)] |(v - v_*) \cdot \eta| \, d\eta \, dv_*, \, dv.$$

for any test function $\phi(v)$, for $v \in \mathbb{R}^3$, where the velocities $v, v_*, v', v'_*$ are related by the elastic collisional law

$$v' = v - ((v - v_*) \cdot \eta) \eta, \quad v'_* = v_* + ((v - v_*) \cdot \eta) \eta,$$

for a collision direction $\eta$.

(a) Since $\ln x$ is a monotone increasing function, show that

$$\int_{\mathbb{R}^n} Q(f, f) \ln f(v) \, dv \leq 0.$$

(b) If $f(v) = A \exp \left( \frac{|v - U|^2}{\beta} \right)$, show that

$$\int_{\mathbb{R}^n} Q(f, f) \ln f(v) \, dv = 0.$$

(c) Use the BTE equation in space-homogeneous regime ($x$-space independent case) and part (a) to show the $H$-theorem: The total entropy $H(t)$ satisfies

$$H(t) = \frac{d}{dt} \int_{\mathbb{R}^n} f \ln f \, dv \leq 0.$$

5. Homogenization. Use formal homogenization to find the limit function $u_0$ and the homogenized problem it satisfies for

$$-\nabla \cdot [a(x/\epsilon) \nabla u_\epsilon] + c(x/\epsilon) u_\epsilon = q(x) \quad \text{in} \ \Omega,$$

$$u_\epsilon = 0 \quad \text{on} \ \partial \Omega.$$

Assume that there exists a unique solution and that $a(x/\epsilon), c(x/\epsilon), \text{and } q(x/\epsilon)$ are smooth and periodic in $y = x/\epsilon$ on the unit cube.
Area C Qualifying Exam  
5 Problems

Problem 1:
The nodes of a simple contiguous cubic lattice are located at the positions \( \vec{x} = l(n_1, n_2, n_3) \), where \( l \) is the lattice spacing and \( n \)'s are integers. The nodes are connected by identical slender links, whose length is equal to \( l \), cross-sectional area is equal to \( A \), and electric conductivity is equal to \( k \). The boundary nodes of the lattice are subjected to the temperature \( T = \vec{g} \cdot \vec{x} \) where \( \vec{g} \) is a constant vector.

1. Determine the specific energy of the lattice defined as

\[
U = \frac{1}{2V} \int \kappa |\nabla u|^2 \, dV
\]

where \( V \) is the volume occupied by the lattice, including the vacuum, and \( V_L \) is the volume occupied by the links. Express your answer in terms of \( \vec{g} \), \( k \), \( l \), and \( A \).

2. For some applications, it is advantageous to replace the lattice with a hypothetical homogeneous material. How would you choose the conductivity of such a material.

Problem 2:
A Continuum Model of Viscous, Incompressible Flow

This problem has as its goal the development of a mathematical model of the flow of water through a long circular pipe of length \( L \) with an interior diameter of \( 2a \).

1. Kinematics. Define mathematically the velocity gradient tensor \( \mathbf{L} \) and its symmetric part \( \mathbf{D} \), the deformation rate tensor. Define all terms and notations used.


3. Momentum. State the local forms of the laws of balance of linear and angular momentum in terms of the Cauchy stress \( \mathbf{T} \), the density \( \rho \), and the body force \( \mathbf{f} \).

4. Conservation of Mass. Noting that \( (\det \mathbf{F})^* = (\det \mathbf{F}) \) \( \text{div} \, \mathbf{v} \), where \( \mathbf{F} \) is the deformation gradient, and that therefore \( \text{div} \, \mathbf{v} = 0 \) for flow without a volume change, show that the principle of conservation of mass implies that \( \rho = \text{constant} \) for incompressible fluid flow.
where $\mu$ is a constant, $D$ is the symmetric part of $L$, $p$ is the hydrostatic pressure, and $I$ is the identity tensor, derive the Navier Stokes equations in terms of $\rho$, the velocity $v$ and the pressure $p$ and the body force $f$ as a mathematical model of the flow.

6. **Boundary and Initial Conditions.** Comment briefly on possible boundary and initial conditions for the stated problem.

**Problem 3:**

a. You have joined General Motors in support of their mathematical modeling activities in the following application areas: (1). Engine design; (2) vehicle shape; (3) crashworthiness. **(5)**

Indicate the main steps you would use in constructing a mathematical model for one of these applications areas (your choice). **(5)**

List the main sources of error that might be associated with developing a mathematical model for an application of your choice. **(Note: Modeling error not numerical error).**

b. Certain experimental measurements are made for your problem application. Assume you have formulated a mathematical model that involves two parameters. State briefly what is meant in the experimental design context by: parameter optimization, and parameter sensitivity. **(8)**

If you compute the eigenvalues of the sensitivity matrix for this problem and find that one eigenvalue is zero, what does this imply about your choice of measurement in the associated experimental design problem?

c. What is meant by the term "multiscale" and how is this related to matched asymptotics in singular perturbation analysis. Give an example to illustrate your reasoning and show how the basic ideas of singular perturbation theory would be applied. **(9)**

Comment on the difference between an asymptotic approximation and approximation using a truncated converging series.
Problem 4:

Homogenization Problem.

In this exercise, you give a formal derivation of Darcy's Law from homogenization theory. Begin with an elementary representative cell $Y$, consisting of the solid part $Y_s$ and the fluid region $Y_f$. Let $\epsilon > 0$ and assume that the domain $\Omega$ is a union of translates of $\epsilon Y$, with fluid part $\Omega_f$ being the union of translates of $\epsilon Y_f$. The fluid obeys the Stokes equation

$$
\epsilon^2 \mu \Delta v^\epsilon = \nabla p^\epsilon \quad x \in \Omega_f,
$$

$$
\nabla \cdot v^\epsilon = 0 \quad x \in \Omega_f,
$$

$$
v^\epsilon = 0 \quad x \in \partial \Omega_f,
$$

where $\mu$ is the constant fluid viscosity. Formally expand both $p^\epsilon$ and $u^\epsilon$ and let $\epsilon \to 0$. You should obtain that the leading terms in the formal expansion, $u_0(x,y)$ and $p_0(x)$, satisfy a Darcy law

$$
\int_{Y_f} u_0(x,y) \, dy = -\frac{1}{\mu} K \nabla_x p_0(x),
$$

and also that $\nabla \cdot \int_{Y_f} u_0(x,y) \, dy = 0$. Show these facts, and also show how we can determine the permeability constant $K$.

Problem 5:

Schrödinger Problem.

Schrödinger's equation for a single particle in a one-dimensional potential $U(x)$ is an equation for a complex wave function $\psi$:

$$
\hbar \frac{\partial}{\partial t} \psi(x) = \left(-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + U(x)\right) \psi(x)
$$

(1)

1. Consider $\psi(x)$ where $x \in [0, L]$. There is a constraint on $\psi$ corresponding to the condition that there is one particle and it must be located somewhere. Write down this constraint mathematically.

2. When $U(x) = 0$, there is a collection of solutions of Schrödinger's equation that are periodic on the domain $x \in [0, L]$. Write down these solutions. Make sure that the constraint in the first part of the problem is obeyed, and that the function is periodic over the required domain.
Area C Exam Question

1. Develop a mathematical model of the flow of water through a rigid trough with a square cross section. This involves setting up a reference frame, writing down the appropriate balance laws, choosing constitutive equations, and proposing boundary and initial conditions.

(Define carefully and completely all terms.)

2. Next, suppose a stainless steel rod is welded to the bottom of the trough. Describe a mathematical model of the dynamic behavior of the rod assuming the flow surrounding it is known.
CAM AREA C PRELIMINARY EXAM:
HOMOGENIZATION PROBLEM

In this exercise, you give a formal derivation of Darcy's Law from homogenization theory. Begin with an elementary representative cell $Y$, consisting of the solid part $Y_s$ and the fluid region $Y_f$. Let $\varepsilon > 0$ and assume that the domain $\Omega$ is a union of translates of $\varepsilon Y$, with fluid part $\Omega_f$ being the union of translates of $\varepsilon Y_f$. The fluid obeys the Stokes equation

$$
\varepsilon^2 \mu \Delta v^\varepsilon = \nabla p^\varepsilon \quad x \in \Omega_f, \\
\nabla \cdot v^\varepsilon = 0 \quad x \in \Omega_f, \\
v^\varepsilon = 0 \quad x \in \partial \Omega_f,
$$

where $\mu$ is the constant fluid viscosity. Formally expand both $p^\varepsilon$ and $u^\varepsilon$ and let $\varepsilon \to 0$. You should obtain that the leading terms in the formal expansion, $u_0(x,y)$ and $p_0(x)$, satisfy a Darcy law

$$
\int_{Y_f} u_0(x,y) \, dy = -\frac{1}{\mu} K \nabla_x p_0(x),
$$

and also that $\nabla \cdot \int_{Y_f} u_0(x,y) \, dy = 0$. Show these facts, and also show how we can determine the permeability constant $K$. 
Problem 1

State or define the following:

a) The Cauchy Stress Principle
b) The Piola Transformation
c) The First Piola-Kirchhoff Stress Tensor
d) The Principle of Conservation of Energy
e) The Principle of Balance of Linear Momentum

The block of lime jello shown in (a) is a cube (square) in its reference configuration, and undergoes a motion that leads to the current configuration shown in (b) (in which the material lines originally parallel to the $X_2$-axis form quadratic curves, as shown)

a) Determine the motion $\varphi(X)$
b) Determine the right Cauchy-Green deformation tensor $C$
c) Determine the Green strain component $E_{22}$ at the point $(X_1, X_2) = (a,a)$. 
Problem 2

Density calculation Consider a collection of $N$ particles in two dimensions whose energy is

$$\mathcal{E} = \frac{1}{2} \sum_{i \neq j} \phi(r_{ij})$$

(1)

where

$$\phi(r) = \begin{cases} \phi_0 \exp(-r)\left(\frac{1}{r^4} - 5\right) & \text{if } r < 1.5 \\ 0 & \text{else,} \end{cases}$$

(2)

Suppose that these particles form a two-dimensional triangular lattice of lattice spacing $a$ and that $N$ is very large. Find

1. the value of $a$ that minimizes the system energy, and
2. compute the energy per particle $\mathcal{E}/N$. 
Problem 3
Consider the PDE mathematical model \(-\nabla \cdot (k \nabla u) = f\) in a two-dimensional region \(\Omega\) with smooth boundary \(\partial \Omega\), where \(k > 0\) and \(f\) are known functions of position \((x, y)\).

(a) Give an example of a physical process that might be described by this model and a corresponding physical interpretation of the PDE expression. (1 line)

(b) State the type (classification) of the PDE and comment on the dependence of the solution in the interior on specified boundary data. (2 lines)

(c) Give mathematical expressions that correspond to:
   (i) essential (Dirichlet) data:
   (ii) Neumann data:
and interpret the data physically in terms of the process being modeled. (2 lines)

(d) Use mathematical analysis to deduce a compatibility condition for the data in the case where Neumann data is specified on the entire boundary, and interpret your result physically. (about 5 lines)

(e) Apply the calculus of variations to the 'energy' functional

\[
I = \int_\Omega k \nabla u \cdot \nabla u \, dx \, dy - \int_\Omega 2fu \, dx \, dy + \frac{1}{2e} \int_{\partial \Omega} (u - g)^2 \, ds
\]

(with \(k\) and \(f\) functions of position as specified above, \(g\) a function of position on the boundary and \(0 < \epsilon << 1\) a small parameter) to determine the corresponding governing (Euler-Lagrange) partial differential equation in domain \(\Omega\) and natural boundary condition on \(\partial \Omega\). Interpret this natural boundary condition physically. Comment on the limiting behavior as the small parameter approaches zero. (6 lines)
Problem 4
Consider a boundary control problem for a temperature field \( u(x) \) in a fluid medium with thermal conductivity \( k \) occupying a domain \( \Omega \) with velocity \( v(x) \) (assumed to be independent of \( u \)):

\[
\min_{u,q} \frac{1}{2} \int_{\Omega} (u - u^*)^2 \, dx + \frac{\beta}{2} \int_{\Gamma_N} q^2 \, ds
\]
subject to \( v \cdot \nabla u - \nabla \cdot (k \nabla u) = 0 \) in \( \Omega \)
\[
k \nabla u \cdot n = q \quad \text{on} \quad \Gamma_N
\]
\[
u = 0 \quad \text{on} \quad \Gamma_D
\]

The goal is to find a heat flux \( q(s) \) on the control boundary \( \Gamma_N \) such that the temperature field \( u \) is as close (in the \( L^2(\Omega) \) sense) to a desired temperature \( u^*(x) \) as possible. The cost of the control is given by the term that includes the parameter \( \beta \).

Derive the optimality conditions for this problem, and use these conditions to derive a simple expression for the optimal \( q(s) \). Show that the optimal control problem is ill-posed if \( \beta = 0 \).
Problem 5
A homogeneous conducting body $\Omega$ is tested by being subjected to the Dirichlet boundary conditions

$$u = \lambda \cdot x \quad x \in \partial \Omega$$

where $\lambda$ is a constant vector.

(a) Show that the macroscopic temperature gradient $\mathbf{G}$, defined through volume averaging, is equal to $\lambda$.

The same body, except that now it contains a small internal void, is tested under the same boundary conditions on $\partial \Omega$.

(b) Does the macroscopic temperature gradient $\mathbf{G}$ remain equal to $\lambda$.

Address the dual problem. Namely, consider $\Omega$ subjected to the Neumann boundary conditions

$$f(x) \cdot n(x) = \mu \cdot n(x) \quad x \in \partial \Omega$$

where $\mu$ is a constant vector and $n$ is the outward normal.

(c) Show that the macroscopic flux $\mathbf{F}$ is equal to $\mu$.

(d) Will a small internal void affect $\mathbf{F}$, provided that the boundary conditions on $\partial \Omega$ remain the same.
Problem 6
In this exercise, we consider the boundary value problem

\[-\nabla \cdot [a(x/\epsilon)\nabla u_\epsilon] + c(x/\epsilon)u_\epsilon = q(x) \quad \text{in} \ \Omega ,\]
\[u_\epsilon = 0 \quad \text{on} \ \partial \Omega .\]

Assume that there exists a unique solution and that \(a(x/\epsilon) > 0\) and \(c(x/\epsilon) > 0\) are smooth and periodic in \(y = x/\epsilon\) on the unit cube, and \(q(x)\) is smooth. By differentiating the first term, we obtain

\[-a(x/\epsilon)\nabla \cdot \nabla u_\epsilon - \epsilon^{-1}(\nabla a)(x/\epsilon) \cdot \nabla u_\epsilon + c(x/\epsilon)u_\epsilon = q(x) \quad \text{in} \ \Omega .\]

More generally, we have

\[-a(x/\epsilon)\nabla \cdot \nabla u_\epsilon - \epsilon^{-1}b(x/\epsilon) \cdot \nabla u_\epsilon + c(x/\epsilon)u_\epsilon = q(x) \quad \text{in} \ \Omega ,\]

where \(b(x/\epsilon)\) is smooth and periodic in \(y = x/\epsilon\) on the unit cube. Apply formal homogenization to (4) and (2), and show that it fails unless \(b = \nabla a\). In this case, i.e., in the case of (3), find the limit function \(u_0\) and the homogenized problem it satisfies.
Problem 1. A long prismatic rubber rod with a square cross section of dimension \( a \) undergoes a motion

\[
\phi (X_1, X_2, X_3) = (\Delta (1 + \frac{X_1}{a}) (\frac{X_2}{a})^2, 0, 0)
\]

where \((X_1, X_2, X_3)\) are material coordinates, \(X_3\) along the length of the rod and \(X_1, X_2\) along the sides of the square, the origin being at a corner, \(\Delta\) being a real parameter with units of length.

a) Sketch carefully the deformed body.

b) Determine the right Cauchy-Green deformation tensor \(C\).

c) What is the displacement of point \((a, a, 0)\)?

d) Compute the Green strain component \(E_{12}\) at point \((a, a, 0)\).

Problem 2. a) Referring to problem 1, if the Cartesian components of the Cauchy stress tensor at \((a, a, 0)\) are

\[
[T_\sigma] = \begin{bmatrix}
200 & -100 & 0 \\
-100 & 300 & 0 \\
0 & 0 & 10
\end{bmatrix} \text{ GPa}
\]

what is the second Piola-Kirchhoff stress tensor at that point?

b) What is the stress vector (traction) at boundary point \((a, a, 0)\) on the surface with unit normal \((1, 1, 0) / \sqrt{2}\)?

Problem 3. a) Give a complete statement of the principle of balance of linear momentum, defining all appropriate terms.

b) State completely and precisely the Cauchy stress principle.

c) Use a) and b) to derive the local spatial (Eulerian) form of the balance of linear momentum of a continuum subject to body forces of \(b\) per unit mass.
Problem 4. Density calculation Consider a collection of \( N \) particles in two dimensions whose energy is

\[
\mathcal{E} = \frac{1}{2} \sum_{i \neq j} \phi(r_{ij})
\]  

(1)

where

\[
\phi(r) = \begin{cases} 
\phi_0 \exp(-r) \left( \frac{1}{r^3} - b \right) & \text{if } r < 1.25 \\
0 & \text{else},
\end{cases}
\]

(2)

Suppose that these particles sit in a two-dimensional triangular lattice of lattice spacing \( r = 1 \) and that \( N \) is very large. Find

1. the value of the constant \( b \) that makes \( r = 1 \) a minimum energy structure and

2. compute the energy per particle \( \mathcal{E}/N \) in the ground state.
Problem 5. Consider a 1D discrete spatial lattice random-walk model with probabilities $p$ and $q$ of a step $\alpha$ to right and left respectively for $n$ steps with time step $\Delta t$. Use this discrete model to develop a continuum PDE limit model (the Fokker-Planck equation) for $v(x,t)$, the probability that at time $t$ the ‘particle’ is located at point $x$. State the assumption on $n$ relative to $\alpha$ in the limit process.

Problem 6. (a) Apply a simple continuum conservation argument, supporting constitutive relation and appropriate modeling assumptions to obtain the following PDE model (which arises in several application classes):

$$- \nabla \cdot (k \nabla u) = f$$

in domain $\Omega$ where coefficient $k$ and source term $f$ are specified continuous functions of position. Comment on the case where Neumann (flux) data is specified on the entire boundary of the domain.

(b) Construct a corresponding weak variational form of the (above strong form) PDE problem showing how Dirichlet (essential) and Neumann (natural) data enter this weak statement. If instead $k$ has a discontinuity across a simple smooth closed contour to an interior subregion, what conditions apply on that contour and how are they addressed in the respective strong and weak statements?
Problem 7.

HOMOGENIZATION PROBLEM

In this exercise, we model a layered system in a three dimensional rectangular domain $\Omega = (0, \ell_1) \times (0, \ell_2) \times (0, \ell_3)$. At the microscale, we have the boundary value problem

$$-\nabla \cdot [a_\varepsilon(x) \nabla u_\varepsilon] = q(x) \quad \text{in } \Omega,$$

$$u_\varepsilon = 0 \quad \text{on } \partial \Omega,$$

where $a_\varepsilon(x) = a(x_1, x_2, x_3/\varepsilon)$ and $a(x_1, x_2, y)$ is smooth in $(x_1, x_2) \in (0, \ell_1) \times (0, \ell_2)$ (and thus not a problem) but varies periodically in $y \in [0, 1]$. Therefore $a_\varepsilon$ is layered in the sense that it is periodic of period $\varepsilon$ in the last variable but not in the first two variables. Assume that there exists a unique solution (i.e., $a(x_1, x_2, y) \geq \alpha > 0$). Suppose $\varepsilon$ is very small, and use formal homogenization to derive a macroscopic model for this system; that is, find the limit function $u_0$, the homogenized problem it satisfies, and the homogenized coefficient $\tilde{a}(x_1, x_2)$. [Hint: think of this as a 1-D homogenization in the third variable, with the first two variables being untreated parameters in the homogenization process.]

Problem 8.

CAM Qualifying Exam: Area C Question

Optimization of systems governed by partial differential equations

Suppose we wish to estimate the thermal conductivity $k(x)$ of a conducting medium occupying a domain $\Omega$ with boundary $\Gamma$. The conduction of heat in the medium is governed by the Poisson equation $-\nabla \cdot (k \nabla u) = 0$, where $u(x)$ is the temperature of the medium. We apply a temperature $u_\Gamma$ on $\Gamma$, and measure the heat flux $k \nabla u \cdot n$ on the boundary, where $n$ is the outward unit normal. Let $\sigma_\Gamma$ denote the measured heat flux. The goal is to estimate $k$ from the measured heat flux.

This inverse problem can be formulated as the following optimization problem:

$$\text{minimize} \quad \frac{1}{2} \int_{\Gamma} (k \nabla u \cdot n - \sigma_\Gamma)^2 \, ds + \frac{\beta}{2} \int_{\Omega} k^2 \, dx$$

subject to:

$$-\nabla \cdot (k \nabla u) = 0 \quad \text{in } \Omega,$$

$$u = u_\Gamma \quad \text{on } \Gamma,$$

where $\beta$ is a regularization parameter necessary to make the inverse problem well-posed.

Derive the optimality conditions for this problem via the method we discussed in class, i.e. by constructing the Lagrangian function and seeking its stationarity with respect to the temperature $u$, the adjoint temperature (i.e. Lagrange multiplier) $p$, and the thermal conductivity $k$. 

Area C – Pg 4
CAM AREA C PRELIMINARY EXAM (CAM 397)

Friday, May 22, 2009, 9:00 a.m. 12:00 noon

Work any 5 of the following 6 problems. Do not hand in all six!

1. [Arbogast] In this exercise, you give a formal derivation of Darcy’s Law from homogenization theory. Begin with an elementary representative cell $Y$, consisting of the solid part $Y_s$ and the fluid region $Y_f$. Let $\epsilon > 0$ and assume that the domain $\Omega$ is a union of translates of $\epsilon Y$, with fluid part $\Omega_f$ being the union of translates of $\epsilon Y_f$. The fluid obeys the Stokes equation

$$\epsilon^2 \mu \Delta v_\epsilon = \nabla p_\epsilon \quad x \in \Omega_f,$$

$$\nabla \cdot v_\epsilon = 0 \quad x \in \Omega_f,$$

$$v_\epsilon = 0 \quad x \in \partial \Omega_f,$$

where $\mu$ is the constant fluid viscosity. Formally expand both $p_\epsilon$ and $u_\epsilon$ and let $\epsilon \to 0$. You should obtain that the leading terms in the formal expansion, $u_0(x, y)$ and $p_0(x)$, satisfy a Darcy law

$$\int_{Y_f} u_0(x, y) \, dy = -\frac{1}{\mu} K \nabla_x p_0(x),$$

and also that $\nabla \cdot \int_{Y_f} u_0(x, y) \, dy = 0$. Show these facts, and also show how we can determine the permeability constant $K$.

2. [Carey] Consider steady 2D transport (e.g. of heat or species $u(x, y)$) with specified source $f(x, y)$. Let $q(x, y)$ denote the associated vector flux field.

(a) Give a contour integral relation to express the associated conservation property. Using this, determine the corresponding differential equation form of the conservation law.

(b) Introduce a constitutive relation for the flux to complete a first order mixed type PDE system mathematical model. As an alternative form, combine the system to a single second-order PDE model.

(c) Sketch a simple finite domain with examples of (i) well-posed and (ii) ill-posed boundary data for each of the models in (b).

(d) For the second model in (b) develop the compatibility condition on the data for the case of a specified flux $g(x, y)$ on the boundary.

(e) A variety of constitutive models may be possible in (b). Comment very briefly on the role of parameters in such models and how this may relate to model error and uncertainty error.

3. [Dawson] Derive the depth averaged shallow water continuity equation from the full continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial u}{\partial z} = 0.$$

Recall that $\zeta(t, x, y)$ is the elevation of the free surface above the geoid, $b(x, y)$ is the bathymetry, and $H(t, x, y) = \zeta + b$ is the total depth of the water column. Use the no-slip boundary condition at $z = -b$, and, at $z = \zeta$, the no relative normal flow condition

$$\frac{\partial \zeta}{\partial t} + u \frac{\partial \zeta}{\partial x} + v \frac{\partial \zeta}{\partial y} - w = 0.$$
4. [Denkowicz] Compute the total force on a point charge \( q \) at \((0, r)\) from a line charge distribution with a constant charge density \( q_l \) along the line \( y = 0 \). [Hint: To compute the resulting integral, use the symmetry about the \( x \)-axis and that \( \int_{-\infty}^{\infty} \frac{1}{(1 + \xi^2)^{3/2}} = 2 \).]

5. [Ghattas] Formulate an optimization problem that is governed by a state equation (this could be an optimal design, optimal control, or inverse problem). Clearly identify the (a) state variable(s) and the optimization variable(s); (b) the state equation(s) and any other constraints; and (c) the objective function. Explain the physical meaning of the optimization problem.

6. [Gonzalez] A model for the concentration \( \rho(r, t) \) of macromolecules in solution inside a spinning ultracentrifuge cell is given by the Lamm equations, where \( r \) is the radial coordinate from the axis of rotation and \( t \) is time. The system can be approximated by

\[
\frac{\partial \rho}{\partial t} + S\omega^2 r \frac{\partial \rho}{\partial r} = -2S\omega^2 \rho, \quad r > r_a, \quad t > 0.
\]

\[
S\omega^2 r \rho = 0, \quad r = r_a, \quad t > 0.
\]

\[
\rho = \rho_0, \quad r \geq r_a, \quad t = 0,
\]

where the positive constants \( \omega, \rho_0, \) and \( S \) are the angular velocity of the rotor, the initial concentration, and sedimentation coefficients of the macromolecule.

(a) Define a change of variables \( r = r(\zeta, \eta), \quad t = t(\zeta, \eta) \) by

\[
\frac{\partial r}{\partial \eta} = S\omega^2 r, \quad r(\zeta, 0) = \zeta \quad \text{and} \quad \frac{\partial t}{\partial \eta} = 1, \quad t(\zeta, 0) = 0.
\]

Solve this for \( r = r(\zeta, \eta) \) and \( t = t(\zeta, \eta) \), and invert these relations to obtain \( \zeta = \zeta(r, t) \) and \( \eta = \eta(r, t) \).

(b) Show that the PDE can be rewritten as

\[
\frac{\partial \hat{\rho}}{\partial \eta} = -2S\omega^2 \hat{\rho}.
\]

where \( \hat{\rho}(\zeta, \eta) = \rho(r, t) \). By integrating this equation, find the general solution \( \rho(r, t) \).

(c) Finally, show that the solution of the full initial-boundary value problem is given by

\[
\rho(r, t) = \begin{cases} 
0, & r < r_a e^{S\omega^2 t}, \\
\rho_0 e^{-2S\omega^2 t}, & r \geq r_a e^{S\omega^2 t}.
\end{cases}
\]
1. State completely, defining all terms, the following definitions, theorems and principles.
   (a) The Piola Transformation in Continuum Mechanics
   (b) The Cauchy Stress Principle
   (c) The Principle of Balance of Linear Momentum of continuous body
   (d) The Principle of Conservation of Energy for thermodynamical behavior of a continuum
   (e) Maxwell's Equations for Electromagnetic Fields in Vacuum
   (f) Pauli's Principle on Particle Symmetry and Spin
   (g) The Hamiltonian for the Helium atom
   (h) The Hohenberg-Kohn Theorem
   (i) The definition of pressure in Thermodynamic and Statistical Mechanics

2. The isothermal flow of an isotropic, viscous, incompressible fluid through a bounded region \( \Omega \subseteq \mathbb{R}^3 \) is characterized by a constitutive equation for Cauchy stress of the form

\[
T = -pI + \mu \left( \text{grad } \mathbf{v} + \text{grad } \mathbf{v}^T \right)
\]

where \( p = p(x,t) \) is the hydrostatic pressure, \( \mathbf{v} = \mathbf{v}(x,t) \) is the velocity field, and \( \mu \) is a positive material constant.

(a) Derive the (complete) equations of motion governing the velocity and the pressure fields at a point \((x,t) \in \Omega \times [0,t]\).

(b) If \( \Omega \) is a cube with sides aligned with the \( x_i \)-coordinate axes \( (\Omega = (0,a)^3) \) with flow entering normal to a plane perpendicular to \( x_1 \), leaving at the opposite plane, and the other sides rigid and impervious. Described an example of plausible boundary conditions on the fluid flow.

3. The particle in a box corresponds to the situation in which

\[
V(x) = \begin{cases} 
0 & \text{if } x \in [0,1] \\
\infty & \text{if otherwise}
\end{cases}
\]

with the time-independent wave function \( \Psi = 0 \) for \( x \not\in [0,1] \) and \( \Psi(0) = \Psi(1) = 0 \).

(a) Solve Schroedinger's equation for this quantum system.
(b) Calculate the first three energy levels.
(c) Sketch the corresponding wave functions (eigenstates)
(d) Find an explicit expression for the canonical partition function of this system at the limit of high temperatures (or small energy differences between the states)
4. Show that the heat capacity

\[ C = \frac{\partial \langle E \rangle}{\partial T} \]

is given in the canonical ensemble by

\[ C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{kT^2} \]

5. The kinetic of a system is described by a Master equation

\[ \frac{dP_i}{dt} = k \sum_j (P_j - P_i) \]

Show that the entropy \( S \) of the system is a non-decreasing function of time

\[ S = -\sum_i P_i \log(P_i) \]

6. We attempt to design stable structures for two protein sequences. The sequences are of the same length \( L \) and consist of two types of amino acids H (hydrophobic) and P (polar). The first sequence includes only H residues, the second includes an equal mixture of H and P. Which of the sequences is likely to have lower energy? Which of the sequences is more likely to have a unique structure?
1. Definitions, Principles, Theorem
   Give a complete statement of the following terms, principles, and theorems.
   Define all relevant terms
   1. The Green-St. Venant strain tensor
   2. The Cauchy Stress Principle (both parts)
   3. The Piola Transformation Theorem
   4. The (first) Piola-Kirchhoff stress tensor
   5. The Principle of Conservation of Energy (global and local forms, current configuration)
   6. The Hamiltonian for a system of $M$ atomic Nuclei of mass $M_K$ and charge $Z_K e$ ($K=1,2,\ldots,M$) and $N$ electrons of mass $m$
   7. The Hohenberg-Kohn Theorem
   8. The ergodic hypothesis
   9. The ideal gas law relating pressure, volume and temperature.
   10. The Liouville Theorem.
   11. The partition function in the canonical ensemble.
   12. The free energy of a rigid rotor with a moment of inertia $I$ at the high temperature limit
   13. The entropy in canonical ensemble.
   14. The $H$ theorem
   15. Cytosol
2. True/False Questions and Short Questions

1. What is the maximum number of electrons in energy shell 2?
2. True or False: The wavefunction for a system containing three electrons must be such that \( \psi(x_1, x_2, x_3) = -\psi(x_1, x_3, x_2) \) with \( x_i = (r_i, \sigma_i) \) being the position pair of electron \( i \).
3. True or False: The Slater determinant of an appropriate system of spin orbitals, as an approximation of the wavefunction of a quantum system, exploits the property of a determinant that the sign of the determinant is changed when any pair of rows are interchanged.
4. True or False: Each atomic orbital can contain up to 8 electrons.
5. True or False: In polar bonds between atoms or molecules, the notion of electronegativity has to do with the unequal sharing of electrons in some molecules or atoms, resulting in some regions effectively acquiring a negative charge (and others positive charge).
6. True or False: A plane electromagnetic wave in vacuum travels at the speed of light.
7. True or False: The vanishing of the divergence of the magnetic field \( \mathbf{B} \) is a consequence of the assumption of the non-existence of a magnetic monopole.
8. How many s, p, and d orbitals exist in each of the first three shells?
9. Show that if the Hermitian operators \( \hat{Q} \) and \( \hat{M} \) share common eigenfunctions they correspond to compatible observables.
10. True or False: Each spatial orbital can accommodate up to two electrons with paired spins of magnitude \( \hbar / 2 \)
11. True or False: Classical phase space volume element shrink to size \( \hbar \) as the system move
12. True or False: If the density matrix operator commutes with the Hamiltonian, then the system is in equilibrium.
13. True or False: The \( H \) function of Boltzmann is a monotonic increasing function of time.
14. True or False: The golgi apparatus is the organelle of the cell where lipid synthesis is taking place.
15. True or False: Most ion transport into and out of cell is of cations.
16. True or False: The main driving force for protein folding is hydrogen bonding.
17. Assume a solution of strong electrolytes of mono-valent ions with concentrations \( c \) and \( c \). What is the ionic strength of the solution?
18. \( N \) non-interacting particles have energy levels \( \pm \epsilon \) (each). Write down the canonical partition function at temperature \( \beta^{-1} \).
19. True or False: The factor \( \hbar^N \) in front of the "semi"-classical partition function is because of the uncertainty principle.
20. True or False: The chemical potential determines the average number of particles in an open system.
Problems and Derivations

1. Derive the Navier-Stokes equations for an isotropic, incompressible, viscous, Newtonian fluid. Start with the principles of conservation of Mass and Linear Momentum and use the constitutive equation for an isotropic homogeneous, incompressible viscous fluid: \( \mathbf{T} = -\rho \mathbf{I} + 2\mu \mathbf{D} \)

2. a. Confirm that the time-independent wave function for a single particle-in-a-box, subjected to a potential,

\[
V(x) = \begin{cases} 
0 & 0 \leq x \leq a \\ 
\infty & \text{elsewhere} 
\end{cases},
\]

is

\[
\psi_n(x) = \begin{cases} 
\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) & 0 \leq x \leq a \\ 
0 & \text{elsewhere} 
\end{cases}
\]

b. What is the probability density of the position of the particle at \( x = a / 2 \) for the second energy level \( (n=2) \)?

c. What is the ground state energy?

d. A trial wavefunction is \( \phi(x) = \frac{1}{2} B x (x - a) \) for \( 0 \leq x \leq a \).

What is \( B \)? Show that the expected value of the energy of this state is slightly larger than that of c)

e. Find an expression for the partition function of \( N \) identical particles in the box of mass \( m \) at the limit of high temperature, \( T \).

f. Determine the heat capacity of the system described in e).

3. Derive an expression for the second virial coefficient of a dilute non-ideal gas of \( N \) identical atoms. Assume pair interaction potential of the type \( u_{ij} \equiv u(|\mathbf{r}_i - \mathbf{r}_j|) \) and use the fugacity \( 1 - \exp(-\beta u_{ij}) \) to derive the expression

\[
B(T) = -2\pi \int_0^\infty \left[ \exp(-\beta u(r)) - 1 \right] r^2 dr.
\]
1. Consider a one dimensional motion defined in terms of spatial coordinate $x$,

$$X = x + x^{1/2}t$$  \hspace{1cm} (0.1)

- Define velocity and acceleration for a general 3D motion.

Both velocity and acceleration are defined using material coordinates. If $x = x(X, t)$ then

$$v := \frac{\partial x}{\partial t}(X, t), \quad a := \frac{\partial^2 x}{\partial t^2}(X, t)$$

- Compute the velocity and acceleration for the deformation above. Hint: you are working with Euler coordinates and not Lagrange coordinates.

One cannot invert explicitly for $x$ here so we have to use the Implicit Function Theorem. Assume that $x$ in (0.1) is a function of $X, t$, and differentiate both sides in $t$ to obtain,

$$0 = v + \frac{1}{2}x^{-\frac{1}{2}}vt + x^{\frac{1}{2}}$$

Solving for $v$, we get

$$v = -\frac{x^{1/2}}{1 + 0.5x^{-1/2}t} = -\frac{2x}{2x^{1/2} + t}$$

With velocity $v$ now known in terms of spatial coordinate $x$, $v = v(x, t) = v(x(X, t), t)$, we use the chain formula to compute the acceleration,

$$a = \frac{\partial v}{\partial x} + \frac{\partial v}{\partial t} = -2\left(\frac{x^{1/2} + t}{(2x^{1/2} + t)^2}\right)v + \frac{2x}{(2x^{1/2} + t)^2}$$  \hspace{1cm} (0.2)

- Define velocity gradient for a general 3D motion.

Velocity gradient is defined in spatial coordinates, $v = v(x, t)$,

$$L_{ij} := \frac{\partial v_i}{\partial x_j}$$

- Compute the velocity gradient for the discussed 1D example.

See formula (0.2).

- Define the deformation gradient and derive the correspondence between the velocity gradient and the deformation gradient.
Deformation gradient is defined in material coordinates, \( x = x(X, t) \),

\[
F_{ij} := \frac{\partial x_i}{\partial X_j}
\]

Changing the order of differentiation, we have

\[
\frac{\partial}{\partial t} \left( \frac{\partial x_i}{\partial X_j}(X_k, t) \right) = \frac{\partial}{\partial X_j} \frac{\partial x_i}{\partial t} = \frac{\partial v_i}{\partial X_j}
\]

With \( v_i = v_i(x_k, t) \),

\[
\frac{\partial v_i}{\partial X_j} = \frac{\partial v_i}{\partial x_k} \frac{\partial x_k}{\partial X_j}
\]

or \( \dot{F} = LF \).

- Illustrate the relation with the 1D example.

Use the Implicit Function Theorem and (0.1) to compute the deformation gradient in terms of spatial coordinates,

\[
F = \frac{\partial x}{\partial X} = \frac{1}{1 + 0.5x^{-1/2}t}
\]

Then

\[
\dot{F} = LF = \left( -2 \frac{x^{1/2} + t}{(2x^{1/2} + t)^2} \right) \left( \frac{1}{1 + 0.5x^{-1/2}t} \right)
\]
2. Electrostatics exercise.

- Recall Coulomb’s law and compute the total force exerted on a point charge \( q \) located at \((x, 0, 0)\) by a charge with constant charge density \( q_l \) distributed uniformly along the \( z \)-axis.

By symmetry argument, the \( z \) and \( y \) components of the force are zero. Using Coulomb’s law and superposition, we obtain the following formula for the \( x \)-component of the force,

\[
F_x = \frac{qql}{4\pi\varepsilon_0} \int_{-\infty}^{\infty} \frac{dz}{(x^2 + z^2)^{3/2}}
\]

Substituting \( z = x \tan \theta \), we get

\[
\int_{0}^{\infty} \frac{dz}{(x^2 + z^2)^{3/2}} = \frac{1}{x^2} \int_{0}^{\pi/2} \cos \theta \, d\theta = \frac{1}{x^2}
\]

which gives the final formula,

\[
F_x = \frac{qql}{2\pi\varepsilon_0 x}
\]

- Define the concept of electric dipole.

Dipole at \( x \) with moment \( m e \) is the limiting case of charge \(-q\) located at \( x \) and charge \( q \) located at \( x + d e \) with \( qd = m \) when \( d \to 0 \).

- Determine the total force exerted on an electric dipole directed along the \( x \) axis with moment \( p = pi \) by the line charge considered above.

Using the result above,

\[
F_x = \lim_{\epsilon \to 0} \left( \frac{qql}{2\pi\varepsilon_0 x} - \frac{qql}{2\pi\varepsilon_0 (x + \epsilon)} \right) = \lim_{\epsilon \to 0} \frac{pql}{2\pi\varepsilon_0 x (x + \epsilon)} = \frac{pql}{2\pi\varepsilon_0 x^2}
\]
3. Consider the 1D time-independent Schrödinger equation.

\[ -\frac{\hbar^2}{2m} \Psi'' + V \Psi = E \Psi \]

Consider the case of a free particle \( V = 0 \).

- Discuss the solution of the Schrödinger equation and its relation with the Fourier transform.
- Define the concept of a wave packet.
- Discuss the concept of group velocity contrasting it with phase velocity.

Look up the lecture notes and book.
4. Consider a system of $N$ non-interacting quantum-mechanical harmonic oscillators in three dimensions. Each of the masses is $m$, and the potential of one oscillator is

\[
\frac{1}{2} k [(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2]
\]

Compute the quantum canonical partition function of the system $Q(N, V, T)$ and the average thermal energy.
5. When a diatomic molecule vibrates, its moment of inertia depends to a small extent on the vibrational state. Consequently, the rotational and vibrational motions are not completely independent. Under suitable conditions, the spectrum of vibrational and rotational energies can be approximated as

\[ E_{n,l} = \hbar \omega (n + \frac{1}{2}) + \frac{\hbar^2}{2I} (l + 1) + \alpha l(l + 1)(n + \frac{1}{2}) \]

where the first two terms correspond to vibrational and rotational motions respectively, and the last term is a small correction that arises from the interdependence of vibrations and rotations. The various molecular constants satisfy

\[ \hbar \omega >> \frac{\hbar^2}{2I} >> \alpha \]

For such a gas compute the internal energy for temperatures in the range

\[ \hbar \omega > kT >> \frac{\hbar^2}{2I} \]
6. We are attempting to overlay two sets of $N$ points in three dimensions presented by vectors $R_1 = (x_1, x_2, \ldots, x_N)$ and $R_2 = (y_1, y_2, \ldots, y_N)$ ($x$ and $y$ are vectors of length 3 presenting points in 3D) such that their norm 2 distance will be minimal. Each set of points is in a (different) plane. We decide to use the Kabsch algorithm to construct the rotation matrix but we are faced with a problem. What is the problem? How can we fix it?
AREA C CoSEM QUALIFYING EXAM
Fri, May 24, 2013
CSE 389C / 389D

Solve the following six problems in 3 hours.

1. Consider a two-dimensional incompressible flow problem. You are given velocity of a fluid with density $\rho = 1$, in terms of spatial coordinates$^1$,

\[ v_1 = x_1 + x_2, \quad v_2 = x_1 - x_2 \tag{0.1} \]

(i) Verify that the flow is incompressible, and compute the corresponding acceleration $a_i(x_j, t)$.

(ii) Compute the corresponding velocity gradient $L_{ij}$ and deformation rate tensor $D_{ij}$.

(iii) Assume constitutive law in the form:

\[ T_{ij} = 2\mu D_{ij} \tag{0.2} \]

where $\mu = 1$, recall equations of motion, and use them to compute the corresponding volume forces that produce the motion.

---

$^1$No dependence in time, the flow is stationary.
2. Magnetostatics.

(i) Define magnetic vector potential $A$ in terms of current vector $J$.

(ii) Consider scenario depicted in Fig. 1. A horizontal circular loop of radius $a$ with center at the origin is carrying current $I$. Recall that the magnetic vector potential at a point $x$ is given by the formula:

$$A = \frac{\mu_0 I a^2 \sin \psi}{4|x|^2} e_\theta + \text{higher order terms in } a$$  \hspace{1cm} (0.3)

where $e_r, e_\theta, e_\psi$ denote the unit vectors of spherical system of coordinates.

(iii) Define the concept of a magnetic dipole. Introducing vector $M = \pi a^2 I e_z$, and passing to the limit with $a \to 0$ keeping $M = \pi a^2 I$ constant, derive the formula for the vector potential of the magnetic dipole:

$$A = \mu_0 M \times \nabla_x \left( \frac{1}{4\pi |x - y|} \right)$$  \hspace{1cm} (0.4)
3. Define the concept of *incompatible observables* and state and prove the *Uncertainty Principle*. Consider the 1D, single particle case only.

4. We consider a system of $N$ particles of mass $m$ (each) enclosed in a volume $V$ and in temperature $T$.
   
   (i) For a system in the canonical ensemble define the pressure as a function of the free energy and the volume.
   
   (ii) Derive the pressure for an ideal gas.
   
   (iii) For a dilute interacting gas write the second virial coefficient.
   
   (iv) Write an expression for the pressure in terms of the pair correlation function $g(r)$ for isotropic monoatomic fluid.

5. We consider the quantum density of $N$ particles with coordinate vector $X$ and Hamiltonian $H = K + V$ where $K$ is the kinetic energy and $V$ is the potential.
   
   (i) Define the quantum partition function in the canonical ensemble.
   
   (ii) What is the expectation value (average) of the kinetic energy for the case $V = 0$ and temperature $T$?
   
   (iii) What are the fluctuations (standard deviation) of the kinetic energy for the same case as in (ii)?

6. (i) State the ergodic hypothesis in the microcanonical ensemble.
   
   (ii) What is the statistical-mechanic entropy in the microcanonical and canonical ensembles?
   
   (iii) Define the temperature from the microcanonical ensemble.
1. Provide short answers and brief explanations where needed for the following questions. No analysis is required. If you write more than a sentence or two, you are writing too much.

(a) A body is deformed so that every point \( X \) in the undeformed body is displaced to the point \( x = \phi(X) \). Define the following tensors:
   i. Deformation gradient tensor
   ii. Right Cauchy-Green deformation tensor
   iii. Green-St Venant strain tensor

(b) What is the Cauchy Stress principle, and how does it arise?

(c) What is material frame indifference and why is it important?

(d) For a particle with mass \( m \) in a potential field \( V \), write Schrodinger's equation for the wave function \( \Psi \).

(e) If you know the wavefunction \( \Psi \) of a particle of mass \( m \), what can you deduce about the position and momentum of the particle?

(f) What is Pauli's principle, and what does it imply about possible quantum states of groups of bosons and of fermions?

(g) What is the ergodic hypothesis and why is it important?

2. Start with the Eulerian representation of conservation of mass and momentum.

(a) For a body with initially uniform density undergoing a time-dependent, volume-preserving deformation, show that the density is constant and that the divergence of the material velocity is zero.

(b) Using the results of (a) and introducing the Newtonian viscous stress model, derive the incompressible Navier-Stokes equations.

3. Consider a particle of mass \( m \) constrained to move only along the \( x \) axis in a potential given by:

\[
V(x) = \begin{cases} 
0 & 0 \leq x \leq a \\
\infty & \text{otherwise}
\end{cases}
\]

(a) Write the Schrodinger equation (time independent) describing the motion of the particle, stating any boundary conditions the wavefunction must satisfy.
(b) Determine the energy levels and associated wave functions.

(c) What is the probability distribution of the momentum of the particle if it is in the nth quantum state.

(d) What is the expected value of the kinetic energy of the particle if it is in the nth quantum state?

4. A quantum system in the canonical ensemble has only two states with energy levels, \( E_1 \) and \( E_2 \). Write the expressions for (a) the entropy \( S \) and (b) the heat capacity \( C_V \) for this system as a function of temperature \( T \).

5. A system has \( N \) discrete states. The probability of being in a state is \( P_n \). The transition rate between any two states is proportional to the constant coefficient \( k \). (a) Write down the Master equation for this system. (b) Prove that the entropy of the system is a non-decreasing function of time. (c) Find the long time limit solution of this Master equation.

6. Define in one or two sentences: (a) the non-linear Poisson-Boltzmann equation, (b) The HP model of protein folding, (c) The Boltzmann H theorem,
Area C CSEM Preliminary Exam
Friday, May 22, 2015

1. Provide short answers and brief explanations where needed for the following questions. No analysis is required. If you write more than a sentence or two, you are writing too much.

(a) What is a (second rank) tensor?

(b) What is the difference between the Cauchy, first Piola-Kirchhoff and second Piola-Kirchhoff stress tensors. Why do we have these different stress tensors?

(c) What physical phenomena give rise to the Cauchy stress term in the momentum equation, and why do we need a constitutive relation for this term?

(d) A particle with charge \( q \) is located at point \( x \) and is traveling with velocity \( v \) in an electric field \( E \) and magnetic field \( B \). What is the force on the particle?

(e) In quantum mechanics what observable is represented by the operator \( \left( -\frac{\hbar^2}{2m} \Delta \right) \)?

(f) An electron is in the spin-up quantum state relative to the \( x_3 \) direction. What is the expected value of its spin angular momentum in the \( x_3 \) direction and in the \( x_1 \) direction?

(g) What are Bosons? Give an example of one.

(h) How does the Pauli principle impact the electronic structure of atoms?

(i) What is the Born-Oppenheimer approximation and why is it useful?

2. A cube of incompressible material of dimension \( a \) is subjected to a uniaxial load in the \( x_1 \) direction, resulting in a deformation that reduces the dimension in the \( x_1 \) direction to \( \alpha^2 a \), with \( 0 < \alpha < 1 \). The material has an incompressible neo-Hookean strain energy density function:

\[
W(E) = \mu I_E,
\]

where \( E \) is the strain tensor, \( I_E \) is its first invariant and \( \mu \) is the shear modulous.

(a) Determine the deformation gradient tensor \( (F) \), the right Cauchy-Green deformation tensor \( (C) \) and the Green-St. Venant strain tensor \( (E) \) in the material.

(b) How much work was required to deform the material?

(c) Because the material is incompressible, there is a degeneracy in the stress relation, so that the second Piola-Kirchhoff stress is given by

\[
S = \frac{\partial W}{\partial E} + pF^{-1}F^{-T}
\]

where \( p \) can be determined from boundary conditions, in this case on the unloaded sides. Determine \( S \).

(d) What is the total load force.
3. Consider a particle of mass $m$ constrained to move in one dimension $x$, in a potential given by $V = m\omega^2 x^2 / 2$.

(a) Write Schrödinger’s equation for the particle.

(b) The ground-state wave function is given by

$$\psi(x) = ae^{-x^2/2\alpha^2}$$

where $\alpha^2 = \hbar / m\omega$. What is the ground state energy?

(c) In some quantum state, the wavefunction is given by:

$$\psi(x) \propto \begin{cases} 
(\alpha - |x|) / \alpha^2 & -\alpha \leq x \leq \alpha \\
0 & \text{otherwise}
\end{cases}$$

What are $\langle x \rangle$ and $\langle E \rangle$, the expected values of the position and energy of the particle.

(d) For the same quantum state as in (c), what is the probability that the particle will be observed with $x \geq \alpha / 2$?

4. Provide short answers to the following.

(a) In class, we used the Lagrange multipliers $\alpha$ and $\beta$ while maximizing the number of microstates for a set of occupation numbers. What are the constraints that correspond to the multipliers, $\alpha$ and $\beta$?

(b) Why is it important to introduce the concept of ensembles to find the partition function of a high temperature (classical) gas?

(c) What are the macroscopic variables in the micro-Canonical ensemble? What are the primary statistical quantities related to this ensemble? What is maximized in equilibrium? Just state these quantities.

(d) Repeat part (c) for the grand Canonical ensemble.

(e) For the 1D classical single-particle partition function, $q_{\text{class}} = 1 / h \int \int \exp(-H(x,p)) \, dx \, dp$, how is the $(1/h)$ justified from quantum mechanics?

(f) For the classical system partition function, $Q_{\text{class}} = 1 / N!(q_{\text{class}})^N$, how is the $(1/N!)$ justified from quantum mechanics?

(g) In the canonical ensemble, energy and entropy are balanced at equilibrium. Given that $-kT \ln Q = A$, how is temperature defined by functions of $S$ and $E$ at equilibrium?

(h) Starting from the definition $\mu = [\partial A(N,V,T)/\partial N]_{V,T}$ derive an expression for the chemical potential in terms of the single particle partition function, $q$, and the number of particles, $N$, in the high temperature, low density (classical) limit.

(i) What is the Metropolis acceptance probability for a Monte Carlo trial move for which the potential energy would change by $\Delta E$? Sketch this probability as a function of $\Delta E$.

(j) In the many-body expansion of a potential energy surface, give an example of a physical phenomenon that is an intrinsically 3-body term.
5. In the $N, V, T$ canonical ensemble, the energy of the system fluctuates around an average (most likely) thermodynamic value. Starting from the partition function

$$Q(N, V, T) = \sum_E \exp(-E/kT)\Omega(N, V, E)$$

(a) What is the probability, $p(E)$, of finding the system with energy $E$?

(b) Using the maximum term method, how can the canonical partition function be written in terms of the most probable energy?

(c) Write down a Taylor expansion for the function, $\ln p(E)$, expanded about the most probable energy, $\langle E \rangle$. Write the expansion to second order.

(d) Using the fact that the linear term in the Taylor expansion vanishes at a maximum, derive an expression for the temperature in terms of the entropy at equilibrium. Compare to question 4(g).

6. The following questions relate to a system (shown above) that has one ground state and three excited states with energy $\epsilon$ above the ground state.

(a) Write down the partition function of this system. Make sure to substitute the values of the energy for the states given above [do not leave your answer in summation notation].

(b) What is the high ($T \to \infty$) and low ($T \to 0$) temperature limits of the partition function? Show that these values correspond to the number of thermally accessible states in each limit.

(c) Evaluate and sketch the probability of finding the particle in any of the excited states as a function of temperature. Explicitly calculate and indicate the high and low temperature limits of this probability on your graph.

(d) At what temperature is it equally likely to find the particle in an excited state (any of them) as in the ground state? Mark this value on your plot in (c).