

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

**Mathematical Methods  
for Materials Scientists and Engineers**

3.016 Fall 2006

W. Craig Carter

Department of Materials Science and Engineering  
Massachusetts Institute of Technology  
77 Massachusetts Ave.  
Cambridge, MA 02139

PROBLEM SET 4: DUE FRIDAY 8 DEC, BEFORE 7PM

INDIVIDUAL ASSIGNMENTS SHOULD BE A COMBINATION OF YOUR HAND-WORKED SOLUTIONS AND OTHER PRINTED MATERIAL—THEY SHOULD BE PLACED IN THE MAILBOX OUTSIDE PROF. CARTER’S DOOR. EMAIL GROUP ASSIGNMENTS TO MINGTANG(THE SYMBOL AT)MIT.EDU

For the individual problems so-indicated, you should work your solutions by hand and show your work. If not indicated, you may use and print the results of software-worked solutions.

The following are this sets’s assigned homework groups. The first member of the group is the “Homework Jefe” who will be in charge of setting up work meetings and have responsibility for turning in the group’s homework notebook. If some some reason, the first member in the list is incapacitated, recalcitrant, or otherwise unavailable, then the second member should take that position. *Attention slackers:* The Jefe should include a line at the top of your notebook listing the group members that participated in the notebook’s production; only those listed will receive credit. Group names are boldfaced text.

**Acheron:** *cmurphy, soyegg, barnest, lhunting, ajuneau, samok*

**Cocytus:** *scampini,dian88 , zkal64, s\_evans, saz, pantea*

**Eriados:** *k\_chu, ielaine, aishab, sadik, buchok, m\_scot*

**Lethe:** *davidlin, katpak,jskrones, rachelkl, jszab,brasin*

**Phlegathon:** *tejada, tycosknr, raffael, alanho12, rkusko,zaklouta*

**Styx:** *johannk,arpun,siamrut,avadhany,taf,cgh*

### Individual (Handworked) Exercise I4-1

*Kreyszig Problem Set 11.2* (problem 10, page 490) Find the first few terms of the periodic series for

$$f(x) = \begin{cases} 0 & \text{if } -2 < x < 0 \\ x & \text{if } 0 < x < 2 \end{cases}$$

Also, what is the value of  $f(x = \pm 2)$  for each approximation?

### Individual (Handworked) Exercise I4-2

Show how the divergence theorem can be used, in the limit of small enclosed volumes, to derive Fick's second law in the absence of sources or sinks:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{J}$$

Now suppose that, “stuff” is being created at each point in space  $\vec{x}$  at a rate of  $\dot{\chi}(\vec{x}, t)$  per unit volume, and the flux of “stuff” follows Fick's first law:

$$\vec{J} = -D\nabla c$$

Show that

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) + \dot{\chi}$$

### Individual Exercise I4-3

With the assumption that  $D$  is independent of position and time, find the form of the above expressions in cartesian, spherical, cylindrical, and bispherical coordinate systems.

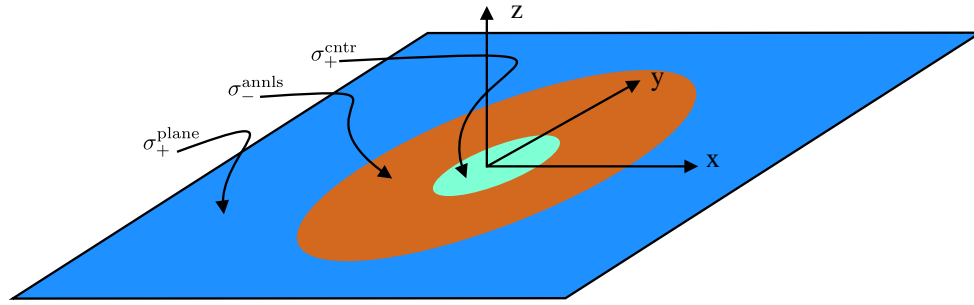
### Individual (Handworked) Exercise I4-4

Suppose very small particle's position is known to be  $x(t) = v_0 t + \pm \Delta x$  Write out a model of the particle's position in terms of a reasonable probability distribution.

The (1D) de Broglie relation is  $p = \hbar k$  where  $k = 2\pi/\lambda$ . Suppose your small localized particles is made up of distribution wavepackets of differing momenta. Use your probability distribution model and Fourier transform to  $k$ -space and find an expression for  $p$  and its uncertainty.

## Group Exercise G4-1

The objective of this problem is to design an anion trap by patterning a surface with regions of constant positive and negative charge density.



The goal is to get an anion (or say, a negatively charge macromolecule or nanoparticle) to be stably “levitated” at a predictable height above the center of the “bullseye” for subsequent “harvesting.”

By designing the radii of the circular patches and their charge densities, it is hypothesized that a stable trap configuration could be designed.

Design one and provide a convincing argument that it would be stable trap. Visualize design parameters and their effect on “trapping figures of merit.”

(This example derives from a problem set given in MIT-BE.430J/6.561J/2.795J/10.539J/HST.544J)

This is a model for how, for certain kinds of solid tumors, cells at the center of a spherical tumors can become starved for oxygen and die.

First, a model for the oxygen concentration in a single healthy cell is to be derived. Model the cell as a sphere of radius  $r_o$  and a spatially uniform oxygen diffusivity of  $D$ . The rate of consumption per unit volume,  $-\dot{\chi}$ , within a cell can be modeled as spatially uniform and approximately independent of oxygen concentration. Let the concentration of oxygen in the surrounding blood and thus surface of cell be  $C_o$ .

1. Find an expression for the steady-state concentration of oxygen in a cell. A steady-state concentration is the time-independent distribution that “sets” in after times  $t \gg r_o^2/D$
2. If typical data are  $D = 10^{-5} \text{ cm}^2/\text{s}$ ,  $\dot{\chi} = 0.015 \text{ moles}/(\text{s m}^3)$ ,  $C_o = 0.06 \text{ moles}/\text{m}^3$ , find an estimate for the maximum possible cell size.
3. Suppose a typical cell ( $r_o = 10 \mu\text{m}$ ) becomes completely depleted in oxygen and dies and the oxygen consumption rate goes to zero. If all other constants are unaffected, calculate the time required for the oxygen concentration at the center of the cell to reach half its steady-state value.
4. Now consider a spherical mass of an aggregate cells such as would be found in a tumor and treat the continuum properties if the aggregate as that of a single cell. At what tumor size would the interior cells begin to suffocate?
5. Estimate these conditions for disk-shaped and rod-shaped tumors.