

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 3: DUE THURSDAY 2 NOVEMBER, BEFORE MIDNIGHT

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@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 week’s randomly 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 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.

**Ampylobacter jejuni:** *aishab, arpun, buchok, zaklouta, katpak, soyegg*

**Clostridium:** *ielaine, alanho12, rkusko, saz, cmurphy, scampini*

**Helicobacter Pylori:** *samok, davidlin, taf, lhunting, pantea, ajuneau*

**Salmonella:** *m-scot, tejada, zkal64, s-evans, cgh, siamrut*

**Shigella:** *dian88, rachelkl, johannk, sadik, avadhany, brasin*

**Yersinia:** *tycosknr, k-chu, jszab, raffael, barnest, jskrones*

## Individual (Handworked) Exercise I3-1

*Kreyszig Problem Set 8.4* (problem 4, page 355) Diagonalize:

$$\begin{pmatrix} 3 & 2 \\ -5 & -4 \end{pmatrix}$$

## Individual Exercise I3-2

*Kreyszig Problem Set 8.4* (problem 8, page 355) Diagonalize:

$$\begin{pmatrix} -6 & -6 & 10 \\ -5 & -5 & 5 \\ -9 & -9 & 13 \end{pmatrix}$$

## Individual Exercise I3-3

*Kreyszig Problem Set 8.5* (problem 14, page 362) Determine whether

$$\begin{pmatrix} a & b + \imath c \\ b - \imath c & k \end{pmatrix}$$

is Hermitian or Skew-Hermitian; find the general quadratic form.

## Individual Exercise I3-4

Write a function that takes a vector of arbitrary length and returns a unit vector parallel to the original vector. Demonstrate that it works.

## Individual Exercise I3-5

Write a function that takes a vector in three dimensions and returns a vector representing all unit vectors normal to the original. Demonstrate that it works.

## Individual (Handworked) Exercise I3-6

*Kreyszig Problem Set 9.5* (problem 42, page 400) Show that curvature for a curve  $\vec{r}(t)$  is given by

$$\kappa(t) = \frac{\sqrt{(\dot{\vec{r}} \cdot \dot{\vec{r}})(\ddot{\vec{r}} \cdot \ddot{\vec{r}}) - (\ddot{\vec{r}} \cdot \dot{\vec{r}})^2}}{(\ddot{\vec{r}} \cdot \ddot{\vec{r}})^{(3/2)}}$$

## Individual Exercise I3-7

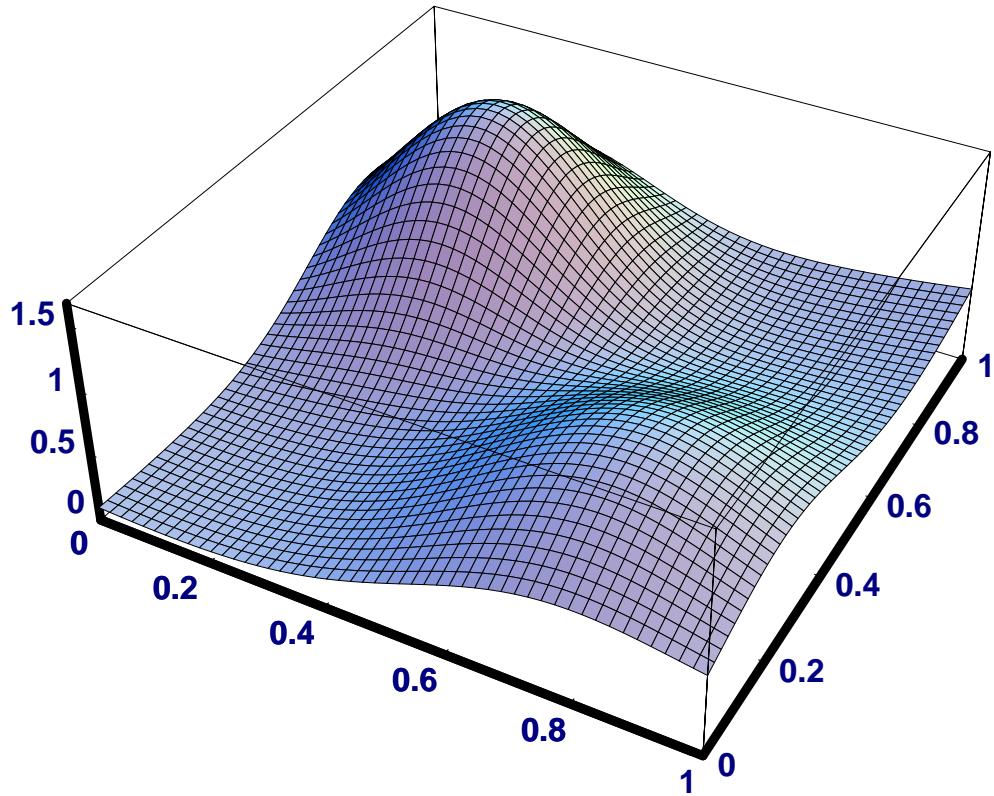
Plot the end of the unit tangent vector and the center of curvature (center of the circle of curvature, or the center of the osculating circle) for the curve given by

$$\vec{x}(t) = ((2 + \sin 2t) \cos t, (2 + \cos 2t) \sin t, \cos t + \sin t)$$

## Group Exercise G3-1

The objective of this problem is to explore and visualize how a distribution of states will evolve if state transitions are governed by local changes in energy. Students should decide what are the important *generic* physics of such an evolution and steady-states as a function of relevant parameters and present an exposition that illustrates those physics. The problem statement is purposely vague—the best solutions include elements of design and creativity as well as physical understanding.

For example, consider the following “energy landscape” where the vertical axis is potential energy as a function over the plane (for example  $E = mgh(x, y)$  or  $E = qV(x, y)$ ):



Suppose there is an initial distribution of states (i.e.,  $\rho(x, y, t = 0)dx dy$  is the number of states in a square with area  $dx dy$  with its center at  $(x, y)$  at time  $t = 0$ )

Suppose that each state at  $\vec{s} = (x, y)$  randomly samples its neighborhood and makes a transition to a new state  $\vec{s}' = (x + \Delta x, y + \Delta y)$  with the following probability (known as the Metropolis algorithm):

$$\text{probability of transition} = \begin{cases} 1 & \text{if } E(\vec{s}') \leq E(\vec{s}) \\ \exp \left[ -\frac{E(\vec{s}') - E(\vec{s})}{kT} \right] & \text{if } E(\vec{s}') > E(\vec{s}) \end{cases}$$

where  $T$  is the temperature.

Groups should develop several methods of visualization under different illustrative conditions and collect them together into a coherent exposition of such activated evolution.

STUDENTS MAY ASK FOR CLARIFICATION TO THE PROBLEM STATEMENT AND RECEIVE HINTS, BUT NO HINTS WILL BE GIVEN ABOUT THE “BEST WAY TO VISUALIZE” OR “WHAT PHYSICAL PRINCIPLES SHOULD BE DISPLAYED.” THESE ARE LEFT TO YOUR OWN CURIOSITY AND CREATIVITY.