Massachusetts Institute of Technology

Mathematical Methods for Materials Scientists and Engineers

3.016 Fall 2010

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Problem Set 4: **Out: 27 Sept.** and **Due: 4 Oct.**

Individual assigments 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 3016-psets(the symbol at)pruffle.mit.edu

For the individual problems indicated as "Handworked", you should work your solutions by hand and show your work. Print the results of software-worked solutions, and staple them to your hand-worked assignments before turning them in.

The following are this week's randomly assigned homework groups. The first member of the group is the "Jomework 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.

Bear-Claw: *ronrose, aypark, mcjasso, yhelen*

Buttermilk: *hekopp, chandrak, pmelo*

Cake: *amelanie, eogorman, eperry4*

Cruller: *ernmart, jrm90, ezuniga*

Custard: *bwee, jchenlia, changey*

Glazed: *chyan, llena, nsinatra*

Jelly: *vtrevino, viviand, m_gibson*

Malasada: *ssluo, dimitri_, ckopp*

Munchkins: *tsmickel, msee, elomeli*

Old-Fashoned: *aliciac, andy_c, spuranam*

Sprinkles: *sojung, jschein, tsarathi*

Individual (Handworked) Exercise I4-1

For matrix given below, find its form in a coordinate system after it has undergone two sequential rotations: first it is rotated by θ around the x-axis and then followed by a θ rotation around the z-axis.

$$\begin{pmatrix} 1 & 4 & -2 \\ 4 & 1 & 2 \\ -2 & 2 & -2 \end{pmatrix}$$

Compute its determinant in the initial and in the final (i.e., after both rotations) coordinate systems.

Do the same exercise for the matrix, but exchange the order of the rotations (i.e., first rotated by θ around the z-axis and then θ around the x-axis.

Individual Exercise I4-2

Purple is half blue and half red. Orange is half red and half green. Cyan is half green and half blue. Find a matrix that converts a vector given as (r, g, b) to a vector given as purple, orange, cyan (p, o, c). Find this matrix's inverse.

Here is some Mathematica code that takes a vector of numbers for red, green, and blue and draws a colored circle:

```
rgbCircle[{r_?NumberQ, g_?NumberQ, b_?NumberQ}] := Module[
  {maxval = Abs[ Max[{r, g, b}]], rs, bs, gs},
  {rs, gs, bs} = Abs[{r, g, b}]/maxval;
   Graphics[{RGBColor[rs, gs, bs], Disk[]}]
  ]

circle[{12,4,1}]
```

Write a function, `pocCircle`, that draws a circle for a purple, orange, and cyan value which uses your inverse matrix and calls the function `rgbCircle` above.

Individual Exercise I4-3

Take the function, $\xi \log \xi + (1 - \xi) \log(1 - \xi)$, and plot its real and its imaginary parts for $-2 < \xi < 2$. Do the same thing for its first and second derivatives with respect to ξ.

Individual Exercise I4-4

Plot the function $f(x, y) = \tan^{-1}(y/x)$.

Group Exercise G4-1

In this problem, the displacement field near an edge dislocation will be visualized, and its elastic field will be calculated and visualized.

Background Material

In a strained (i.e., deformed) solid, the displacement field is a vector field. This vector field represents the displacement of a point relative to its position in the unstrained (reference state).

For example, a penny expands as its temperature is increased. Each point in the penny is translated from the center proportionally to its original distance from the center; in this is a case of uniform expansion and the displacement field for uniform expansion is:

$$R_{\text{strained}}(r,\theta) = R_{\text{unstrained}}(r,\theta) + \alpha T r$$
$$\Theta_{\text{strained}}(r,\theta) = \Theta_{\text{unstrained}}(r,\theta)$$

in polar coordinates where α is the coefficient of thermal expansion. The polar displacement field is defined as:

$$\rho(r,\theta) = R_{\text{strained}}(r,\theta) - R_{\text{unstrained}}(r,\theta) = \alpha T r$$
$$\phi(r,\theta) = \Theta_{\text{strained}}(r,\theta) - \Theta_{\text{unstrained}}(r,\theta) = 0$$

In Cartesian coordinates, the displacement field is written as u being the relative displacement in the x-direction and v being the relative displacement in the y-direction.

$$(u, v) = \alpha T r\,(\cos(\theta), \sin(\theta))$$

The strains are dimensionless quantities related to derivatives of u and v with respect to x and y; the following are definitions of strains in the x-y plane for artesian displacement field.

$$\epsilon_{xx} = \frac{\partial u}{\partial x} \qquad \epsilon_{xy} = \epsilon_{yx} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \qquad \epsilon_{yy} = \frac{\partial v}{\partial y}$$

Stresses, $\underline{\sigma}$, are the generalization of applied pressure. As we will discuss later in the semester, stresses are related to forces in different directions applied to planes with particular orientations. For example, the stress σ_{yy} is related to applied forces in the y-direction applied to vertical surfaces; the stress σ_{xy} is related to applied forces in the x-direction applied to vertical surfaces. In isotropic linear elastic materials—such as a penny—the strains (expansion) are related to the applied stresses by the following expression.

$$E\epsilon_{xx} = \sigma_{xx} + \nu(\sigma_{yy} + \sigma_{zz})$$
$$E\epsilon_{yy} = \sigma_{yy} + \nu(\sigma_{zz} + \sigma_{xx})$$
$$E\epsilon_{xy} = (1+\nu)\sigma_{xy}$$

Where E is the Young's modulus, ν is the Poisson ratio. E is related to the shear modulus, G, by $E = 2G(1+\nu)$.

End of Background Material

The artesian displacement field due to an edge dislocation is given by:

$$u = \frac{b}{2\pi}\left(\tan^{-1}\frac{y}{x} + \frac{1}{2(1-\nu)}\frac{xy}{r^2}\right)$$
$$v = \frac{b}{2\pi}\left(\frac{1-2\nu}{2(1-\nu)}\log\frac{b}{r} + \frac{1}{2(1-\nu)}\frac{y^2}{r^2}\right)$$

where b is the Burger's vector (usually on the order of a lattice vector) and $r = \sqrt{x^2 + y^2}$.

1. Using b as a length, introduce dimensionless forms of the displacement fields u and v and the artesian coordinate x and y. What is the dimensionless form of the displacement field of an edge dislocation.

2. Visualize this displacement field. You will need to specify a numerical value for Poisson's ratio—for most materials $0 < \nu < 1/2$. (`VectorPlot` will be useful). Note that the field become singular as the distance becomes less than a Burger's vector. You will want to plot different regions to explain the complete behavior. Comment on the relation between your visualization and the "Burger's circuit" for an edge dislocation.

3. Compute general expressions for the strains in terms of non-dimensional coordinates. ϵ_{xx}, ϵ_{yy}, and ϵ_{xy}.

4. From these strains, compute the stresses σ_{xx}, σ_{yy}, σ_{zz}, and σ_{xy}. Using the shear modulus G which has the same units as stress, write these stresses in a non-dimensional form. Compare the computed stresses with those that appear in textbooks or other information sources.

5. Visualize the shear stress σ_{xy}, and the hydrostatic pressure $P = -(\sigma_{xx}+\sigma_{yy}+\sigma_{zz})/3$ (positive pressure is compressive, negative pressure is tensile). Linear elasticity applies at distances greater than a few Burger's vectors from the dislocation, you may wish to eliminate the inaccurate stresses near the origin from your visualization.