AMSC/CMSC 661 Scientific Computing II

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Introduction

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Welcome to AMSC/CMSC 661

- Course organization
- A motivating problem
- Classification of differential equations
- A note on linear vs nonlinear
- Pointers for success

Course organization

- The syllabus
- The homepage

A motivating problem (Chapter 29 of SCCS book)

This problem focuses on the stress induced in a rod by twisting it. We'll investigate two situations: first, when the stress is small enough that the rod behaves elastically, and second, when we pass the elastic-plastic boundary.

The physical problem: Consider a long rod made of metal, plastic, rubber, or some other homogeneous material. Attach one end to a wall and twist the other end clockwise.

What happens: This torsion (twisting) causes stresses in the rod. If the force we apply is small enough, then the rod behaves as an elastic body, and when we release it, it will return to its original state. But if we apply a lot of twisting force, we will eventually change the structure of the rod; some portion of it will behave plastically and will be permanently changed.

If the whole rod behaves elastically, or if it all behaves plastically, then modeling is relatively easy. More difficult cases occur when there is a mixture of elastic and plastic behavior.

The elastic model

We assume that the torsional force is evenly distributed throughout the rod, and that the rod has uniform cross sections.

Under these assumptions, we model the stress in any single cross section. We'll call the interior of the 2-dimensional cross section Ω and its boundary Γ.

The standard model involves the stress function $u(x, y)$ on Ω, where the quantities $-\partial u(x, y)/\partial x$ and $\partial u(x, y)/\partial y$ are the shear stress components (units = force per unit area). If we set the net force to zero at each point in the cross-section, we obtain

$$\begin{aligned} \bigtriangledown^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \equiv u_{xx} + u_{yy} &= -2G\theta \quad \text{in} \quad \Omega, \\ u &= 0 \quad \text{on} \quad \Gamma, \end{aligned}$$

where G is the shear modulus of the material (units = force per unit area) and θ (radians) is the angle of twist per unit length.

In order to guarantee existence of a smooth solution to our problem, we'll assume that the boundary Γ is smooth; in fact, in our experiments, Γ will be an ellipse.

An alternate formulation

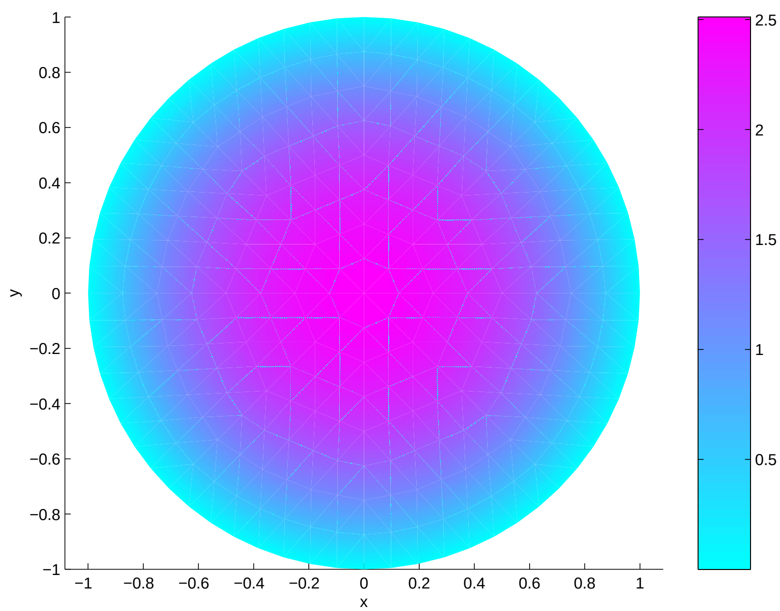
An alternate equivalent formulation is derived from minimizing an energy function

$$E(u) = \frac{1}{2} \int\int_{\Omega} |\bigtriangledown u(x, y)| dx dy - 2G\theta \int\int_{\Omega} u(x, y) dx dy \,.$$

The magnitude of the gradient $|\bigtriangledown u(x, y)| = \sqrt{(\partial u(x, y)/\partial x)^2 + (\partial u(x, y)/\partial y)^2}$ is the shear stress at the point (x, y), an important physical quantity. At any point where the shear stress exceeds the yield stress σ_0, the material becomes plastic, and our standard model is no longer valid.

For simple geometries (e.g., a circle), we can solve this problem analytically, but we'll consider a more general problem.

What the stress looks like



What if we cross the elastic boundary?

As the value of θ is increased, the maximum value of the shear stress $| \bigtriangledown u(x,y)|$ increases, eventually exceeding the yield stress of the rod, and then our model breaks down because the rod is no longer behaving elastically.

We can extend our model to this case by adding constraints: we still minimize the energy function, but we don't allow stresses larger than the yield stress:

$$\begin{aligned} \min_u \quad & E(u) \\ | \bigtriangledown u(x,y)| \quad \leq \quad & \sigma_0, \quad (x,y) \in \Omega \end{aligned}$$

$$u = 0 \text{ on } \Gamma$$

The new constraints $|\bigtriangledown u(x,y)| \leq \sigma_0$ are nonlinear, but we can reduce them to linear by a simple observation: if we start at the boundary and work our way in, we see that the constraint is equivalent to saying that $|u(x,y)|$ is bounded by σ_0 times the (shortest) distance from (x,y) to the boundary, which we denote as $d(x,y)$.

Now we have the elements in place to solve our elastoplastic torsion problem. We discretize $E(u)$ using finite elements, and we use our distance function to form the constraints, resulting in the problem

$$\begin{aligned} \min_{\mathbf{u}} 1/2\mathbf{u}^T \quad \mathbf{K} \quad \mathbf{u} - \mathbf{b}^T\mathbf{u} \\ -\sigma_0\mathbf{d} \leq \quad \mathbf{u} \quad \leq \sigma_0\mathbf{d} \end{aligned}$$

where $d_i = d(x_i, y_i)$ and the ith component of $\mathbf{u}$ approximates the solution at (x_i, y_i).

Because the matrix $\mathbf{K}$ is symmetric positive definite (due to the elliptic nature of the differential equation), the solution to the problem exists and is unique.

This problem is a quadratic programming problem. Algorithms for solving it include active set strategies and the newer interior point algorithms.

The solution

Figures 1 and 2.

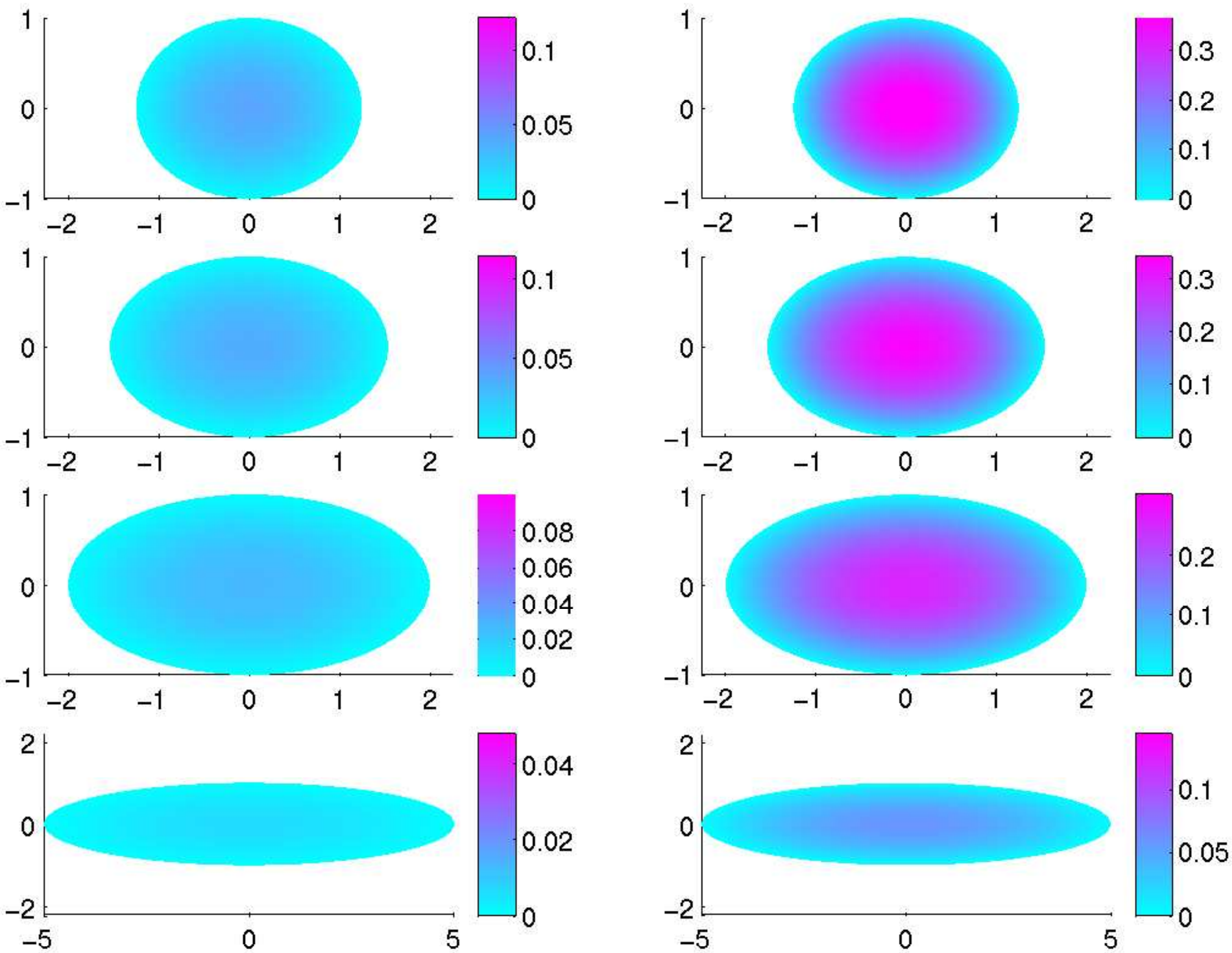
Lessons to draw from this example

- Differential equation problems arise from modeling physical systems.
- Linearization is often used to make the problem tractable.
- Most differential equations cannot be solved analytically. Instead, we use numerical methods: finite differences, finite elements, spectral methods, etc.
- Appropriate visualization of solutions is critical to physical understanding.
- Often we have constraints on the problem. The topic of constraints is covered in 660, so we will ignore this in the rest of 661.

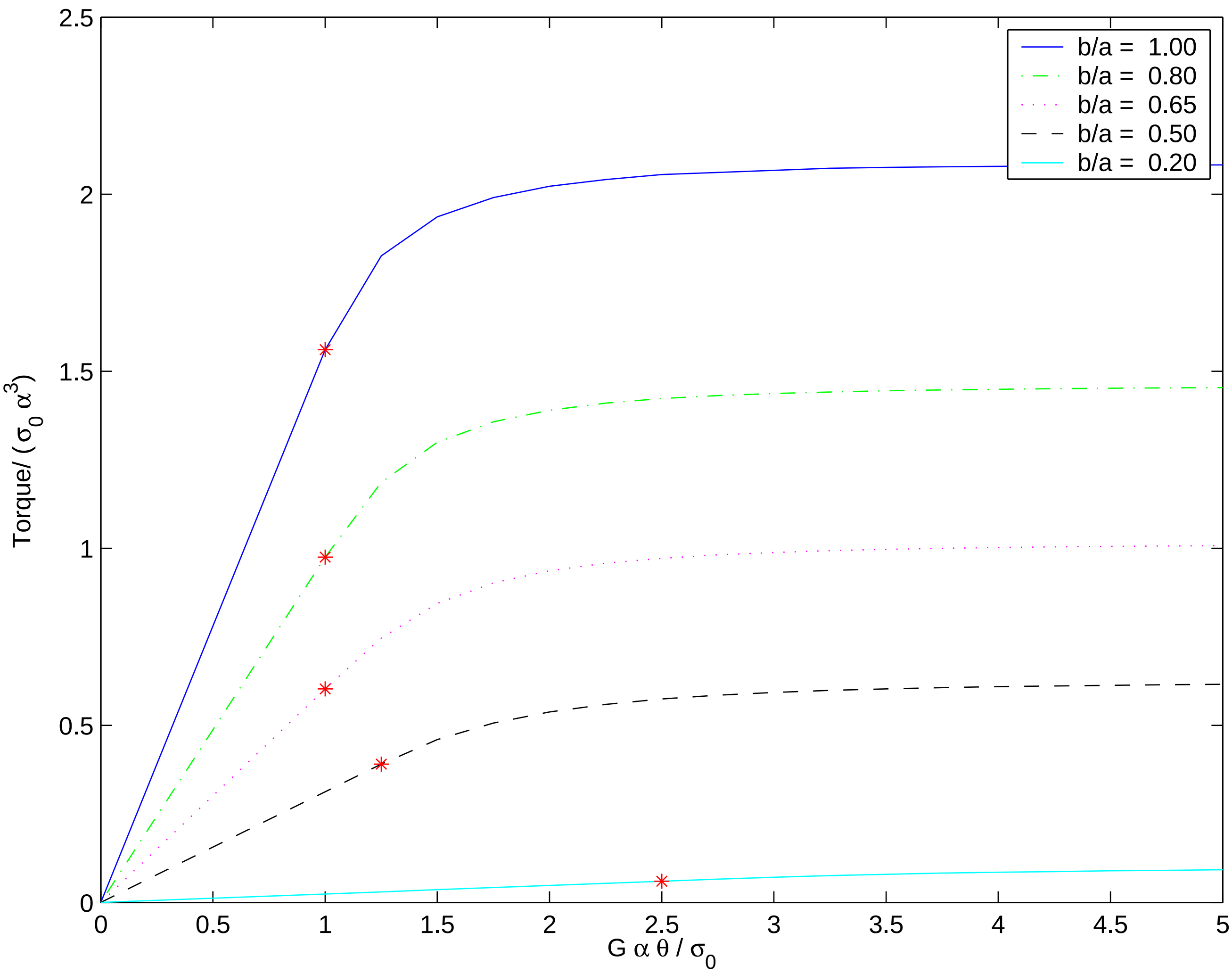
Three critical questions

The three most important questions to be answered are:

- Is the problem well-posed?



1
0
−1
−2
−1
0
1
2
0.1
0.05
0
0.3
0.2
0.1
0.08
0.06
0.04
0.02
2
−5
5



Torque/ (σ0 α3)
G α θ / σ0
b/a = 1.00
b/a = 0.80
b/a = 0.65
b/a = 0.50
b/a = 0.20
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

  - Does the solution exist?
  - Is it unique?
  - Do small changes in the data cause only small changes in the solution?

- How can we compute an approximate solution?
- How close is the computed solution to the true solution?
  We call this study error analysis.

In this course, we focus on these three questions.

Classification of differential equations (p. 4)

Consider a differential equation that is a function of two variables, x and t:

$$au_{tt} + 2bu_{xt} + cu_{xx} + \ldots = f(x,t)$$

where the dots denote terms that have fewer than 2 derivatives. We classify the differential equation depending on a, b, and c:

- elliptic if $ac - b^2 > 0$.
  Example: Poisson's equation $u_{tt} + u_{xx} = f(x,t)$.
- hyperbolic if $ac - b^2 < 0$.
  Example: the wave equation $u_{tt} - u_{xx} = f(x,t)$.
- parabolic if $ac - b^2 = 0$.
  Example: the heat equation $u_t - u_{xx} = f(x,t)$.

Note that an equation can be elliptic in part of its region and hyperbolic in another (for example).

For more than two variables, similar definitions exist, and we'll encounter them as we take up the three types in turn.

The classification of an equation determines

- what boundary information is needed for well-posedness and
- what numerical methods are appropriate.

A note on linear vs nonlinear (p. 11)

Meta-Theorem: The world is nonlinear.

In a nonlinear equation, at least one of the coefficients (a, b, c, ...) depends on u.

For example:

$$F(u) = (a(u)u')' - f(u) = 0$$

on the domain $x \in (0, 1)$, with $u(0) = u(1) = 0$.

Such equations are usually solved using a variant of Newton's method: Given a guess $u^{(0)}$, (or, in general, a current guess $u^{(k)}$), find a better guess

$$u^{(k+1)} = u^{(k)} + \delta^{(k)}$$

by solving

$$F(u^{(k)}) + F'(u^{(k)})\delta^{(k)} = 0$$

with $\delta^{(k)}(0) = \delta^{(k)}(1) = 0$.

This is a linear system of equations.

So, in 661, we will just consider linear differential equations, and count on you putting the 660 material together with 661 when you encounter nonlinear ones.

Pointers for success

- Make use of the course homepage, including the supplementary information posted there.
- Read the course notes and the textbook.
- The textbook is well organized and correct but very terse. It is best read with pencil and scratch paper, so that you can work through the details.
- Bring the textbook to class for quizzes.
- Some students find it helpful to print out the lecture notes and supplement them with their own notes taken during class.
- If you have had a course in functional analysis, it is certainly useful, but I will not assume this, and will freely gloss over the details when possible. Please forgive.
- To prepare for each quiz, make use of the hints posted after the class preceding the quiz.
- Some of the quizzes will be open book. But note that the authors are entitled to fair compensation for their work, so buy a copy of the textbook. Reproductions of pages from the textbook will not be permitted during quizzes.
- Discretization and visualization is quite important but rather difficult for differential equations. That is why we make use of the sophisticated tools in MATLAB rather than writing our own code from scratch. MATLAB can be annoying, though, so be patient with its idiosyncracies.

- Don't leave homework until the last minute. It usually helps to have a day or two to evaluate your results before doing your final write-up.
- Our starting point: Chapter 2, Boundary Value Problems for Ordinary Differential Equations (BVP-ODE) to illustrate main tools without multidimensional encumbrances.