Project 3

Due on Monday, Apr 16

1 Introduction

The *Frank-Kamanetskii* equations are a simple model of ignition in a combustible material. The basic equations[1] for the evolution of (scaled) temperature in this case are

$$\frac{\partial \Theta}{\partial t} = \nabla^2 \Theta + \lambda \exp\left(\frac{\Theta}{1+\eta\Theta}\right), \tag{1}$$

subject to zero temperature boundary conditions. You may recognize that this looks almost like the ordinary heat equation, with the exception of the exponential term on the right-hand side that corresponds to heating from an exothermic reaction. Such reactions generate heat, *and* the hotter it gets, the faster the reaction. If the heat diffuses away sufficiently fast, the temperature will eventually approach an equilibrium; otherwise, there is a "thermal explosion," and the temperature grows without bound[2].

Our mission in this project is to understand the blow-up phenomenon in the context of a one-dimensional slab geometry. In this geometry, an equilibrium state corresponds to a solution to the differential equation

$$\frac{d^2\Theta}{dz^2} + \lambda \exp\left(\frac{\Theta}{1+\eta\Theta}\right) = 0 \tag{2}$$

subject to $\Theta(\pm 1) = 0$. At $\eta = 0$, solutions to this equation only exist for sufficiently small λ. This is illustrated in Figure 1, which shows the relationship between the maximum temperature $\Theta_0 = \Theta(0)$ for equilibrium solutions as a function of λ. Up to a critical parameter value (about 0.88), there are two equilibria[3]; beyond that critical value, there are no equilibrium solutions, and thermal explosion is inevitable. We would like to see how this behavior changes as a function of η, the constant that models rate limiting in the runaway reaction. Of course, at the same time we have a great excuse to play with interesting numerical methods!

[1] Actually, I think the original Frank-Kamanetskii equations had $\eta = 0$.

[2] At least, the temperature grows without bound according to this equation. In practice, effects that are not modeled in the equations come in to play – such as things actually starting to physically explode.

[3] The lower-temperature equilibrium is physical — the other is unstable.

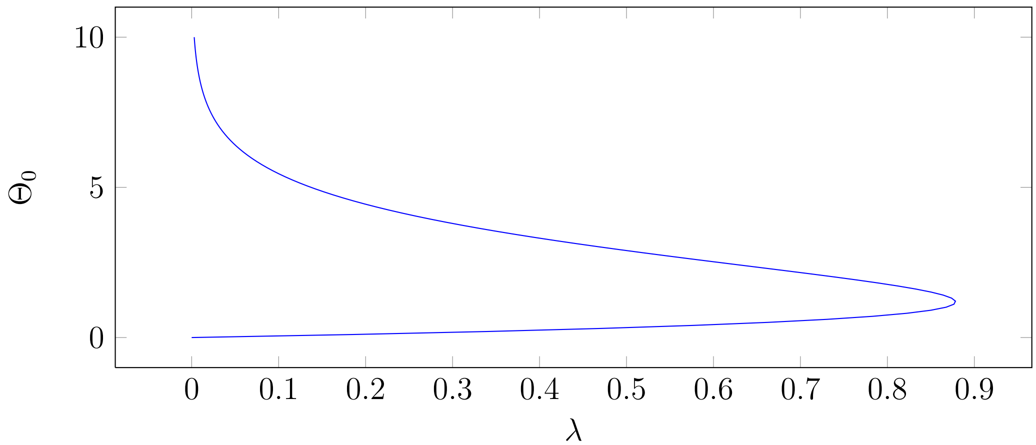

Figure 1: Maximum equilibrium temperature versus F-K parameter λ for a model of thermal explosion in an infinite slab ($\eta = 0$).

2 Basic computation

2.1 Discretization

Your first task is to write a code capable of reproducing Figure 1. To do this, you will need to repeatedly solve the boundary value problem (2). In order to solve the boundary value problem, you will need to *discretize* the derivative operator; that is, approximate

$$\frac{d^2\Theta}{dz^2} + \lambda \exp\left(\frac{\Theta}{1+\eta\Theta}\right) = 0,$$

together with the zero boundary conditions, by

$$(L\hat{\Theta})_i + \lambda \exp\left(\frac{\hat{\Theta}_i}{1+\eta\hat{\Theta}_i}\right) = 0, \tag{3}$$

where $\hat{\Theta}$ is a vector such that $\hat{\Theta}_i$ approximates $\Theta(z_i)$, where $\{z_i\}$ are the mesh points.

The conventional first-course approach to discretizing the problem would be the second-order stencil discretization of the Laplacian (as described in the book in Chapter 4, where the model problem was described); that is, take

$$(Lu)_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}.$$

To see how to efficiently form the L matrix in this case, I recommend looking at the MATLAB help page for `spdiags` — forming this matrix (modulo the scaling by h^2) is one of the examples. If you feel like being a bit more adventurous, I recommend using a *Chebyshev collocation* approximation to the derivative, as described toward the end of Chapter 14. If you take this approach, you may find it helpful to use Trefethen's `cheb` routine:

http://people.maths.ox.ac.uk/trefethen/cheb.m

2.2 Solution strategy

The most obvious approach to producing Figure 1 is to sweep over different values of λ, and for each value of λ to use Newton iteration in order to try to solve for $\hat{\Theta}$ in (3). Sadly, it is not that easy to convince Newton to converge, particularly as we get close to the critical value for λ; and even if we can get Newton to converge to *one* equilibrium, it is unclear how we should coax it into finding *both* the equilibria.

A better approach is to sweep over different values of $\hat{\Theta}_{\mathrm{mid}}$ corresponding to the point $z_{\mathrm{mid}} = 0$, and to treat λ as an unknown. That is, solve (3) together with the equation

$$\hat{\Theta}_{\mathrm{mid}} = \Theta_0,$$

treating the components of $\hat{\Theta}$ and the parameter λ as unknowns. You can iterate on this new system of equations using Newton's method. I recommend a *continuation* approach: starting at $\Theta_0 = 0$ (for which the solution is $\hat{\Theta} = 0$ and $\lambda = 0$), gradually increase Θ_0, at each step using the solution with the previous value of Θ_0 as a starting point for a new Newton iteration.

2.3 Deliverable

For the first part of the assignment, you should generate a MATLAB code with the interface

```
% Compute theta vs lambda for a range of theta values between 0 and
% thetamax.

function [theta, lambda] = p3sweep(thetamax, eta)
```

The call `[t,l] = p3sweep(10,0); plot(l,t)` should produce something like Figure 1. You should also make sure `p3sweep` works correctly for $\eta = 0.1, 0.2, 0.3$.

3 Behavior of the critical parameter

For $\eta = 0$, there is a critical value of λ (around 0.88) beyond which there is no stable equilibrium, and blow-up is guaranteed. If we plot λ as a function of Θ_0 (flip the axes in Figure 1), then this is the place where λ has a maximum with respect to Θ_0. In the language of bifurcation theory, this is an example of a *turning point*. For *small* values of η, this qualitative behavior remains the same: the branch of stable equilibria disappears past a certain critical value of λ (though for $\eta > 0$, there is a second, higher-temperature stable equilibrium branch). Once η becomes sufficiently large, this turning point vanishes, and there is no longer a critical value of λ.

Our goal for the second part of the assignment is to investigate the behavior of $\lambda_{\text{crit}}(\eta)$, i.e. the critical parameter viewed as a function of η.

3.1 Computing the critical parameter

Given η, a simple strategy to find $\lambda_{\text{crit}}(\eta)$ is this:

1. Use `p3sweep` to compute λ as a function of Θ_0 at a set of sample values of Θ_0 in a reasonable range – say, $0 \leq \Theta_0 \leq 8$.

2. Find the *local* maximum sample value of λ on the interior of the sampled range. Be careful here: for larger values of η, there is likely to be no local maximum; and even if there is, the *global* maximum is may be at the edge of the sampled range ($\Theta_0 = 8$).

3. Unless you use a very large number of sample points, steps 1–2 will only give you $\lambda_{\text{crit}}(\eta)$ to a couple digits of accuracy. To improve the accuracy, fit a low-degree polynomial to the points near the (local) max sample value — I used a quadratic. Use the maximum value of this quadratic interpolant in order to get an improved estimate of $\lambda_{\text{crit}}(\eta)$ and the corresponding value of Θ_0 (call it $\Theta_{\text{crit}}(\eta)$).

You can get a visual check of the calculation above by ploting λ versus Θ_0 and marking $(\lambda_{\text{crit}}, \Theta_{\text{crit}})$ with a big dot, for several values of η. It is illuminating to plot the locus of $(\lambda_{\text{crit}}(\eta), \Theta_{\text{crit}}(\eta))$ for η ranging from zero up to the point η_* where the turning point disappears. Take a look for yourself — what does the plot of λ versus Θ_0 look like at η_*?

3.2 Deliverables

For the second part of the assignment, you should generate a MATLAB code with the interface

```
% Use the output from p3sweep to find the critical value for lambda,
% improving the answer a bit by quadratic interpolation. If
% there is no critical value, return tcrit = [] and lcrit = [].

function [tcrit, lcrit] = p3critical(eta)
```

You should also generate a short report that includes (on a single figure) plots of Θ_0 against λ for $\eta = 0$ and $\eta = \eta_*$, and a plot of the curve traced out by $(\lambda_{\text{crit}}(\eta), \Theta_{\text{crit}}(\eta))$ for $0 \leq \eta \leq \eta_*$. Also give numbers for η_*, $\lambda_{\text{crit}}(\eta_*)$, and $\Theta_{\text{crit}}(\eta_*)$. Comment on the approximations that went into your computations[4]. How many digits do you think are probably correct, and why? Note that I'm *not* asking for a formal error analysis here — experimental evidence and convergence plots are just fine.

Notes

1. This assignment is a guided tour of some of the very basic concepts of *numerical bifurcation analysis*. If you are interested in reading further, I recommend *From Equilibrium to Chaos: Practical Bifurcation and Stability Analysis* (Seydel). For a more advanced perspective, I like the book *Numerical Methods for Bifurcations of Dynamical Equilibria* (Govaerts).

2. If you do some plots, you may notice that $\lambda_{\text{crit}}(\eta)$ and η are functions of $\Theta_{\text{crit}}(\eta)$, and η_* corresponds to a maximum of these functions. You may wish to use this observation to improve the accuracy of your estimates for η_*, $\lambda_{\text{crit}}(\eta_*)$, and $\Theta_{\text{crit}}(\eta_*)$.

3. No explosions were created in the making of this assignment.

[4] I want comments on the approximations in the numerics, not in the physics. The latter is interesting, too, but is a topic for a different course.