Notes on a 1D Finite-Difference Steady-state Heat Solver

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1 Motivation

While we require a time-dependent heat solver to simulate the temperature response of tissue exposed to laser energy, it is often the case that a steady-state heat solver would be beneficial. A steady-state heat solver is a solver that computes the steady-state temperature distribution, which is the solution to the heat equation that does not change with time. The steady-state solution is the temperature distribution that the time-dependent temperature distribution tends to for long times, so it is possible in principle to obtain the steady-state solution by running a time-dependent solver for a long time. However, this is often impractical.
In the context of simulating the thermo-optical response of tissue, there are to instances in which having a steady-state heat solver would be useful. First, when simulating the exposure of a tissue with a surface boundary and blood perfusion (such as skin), it is important to determine the initial temperature distribution in the tissue before simulating a laser exposure. Heat is lost at the surface boundary, which will lead to a temperature gradient in the tissue. This temperature gradient would just be linear if not for blood perfusion, which can be modeled as a temperature dependent source term. Therefore, in order to accurately simulate skin exposures, it is necessary to first determine the initial temperature distribution in tissue, which amounts to finding the steady-state solution without a laser source term. Without a steady-state solver, this requires running a time-dependent heat solver for a long period of time until the temperature distribution ceases (or nearly ceases) to change. Depending on the model configuration, this can be very time consuming. A steady-state heat solver would allow this to initial temperature to be quickly determined.

While not nearly as critical, a steady-state solver could also be used to determine the maximum temperature that would be reached for a given exposure. This would allow the simulated temperature to the actual exposure to be compared to this maximum temperature, or even provide a method for determining when a time-dependent simulation can be terminated by deciding if it has reached steady-state.

2 Model

The 1D, steady-state heat equation is

$$\frac{\partial}{\partial x}\left[\kappa\left(x\right)\frac{\partial}{\partial x}\nu\left(x\right)\right] = -A\left(x\right) \tag{1}$$

We proceed in the usual way, first we chain rule the left-hand side and then finite-differencing the derivatives

$$\frac{\partial}{\partial x}\left[\kappa\left(x\right)\frac{\partial}{\partial x}\nu\left(x\right)\right] = \kappa\left(x\right)\frac{\partial^2}{\partial x^2}\nu\left(x\right) + \frac{\partial}{\partial x}\kappa\left(x\right)\frac{\partial}{\partial x}\nu\left(x\right) \tag{2}$$

Let

$$\begin{array}{lllll} \delta_x f_i \equiv & \frac{\Delta x_{i-}}{\Delta x_{i+}\Delta x_i} f_{i-1}+ & \frac{\Delta x_{i+}-\Delta x_{i-}}{\Delta x_{i+}\Delta x_{i-}} f_i+ & \frac{-\Delta x_{i+}}{\Delta x_i \Delta x_{i-}} f_{i+1} \\ \delta_x^2 f_i \equiv & \frac{2}{\Delta x_{i+}\Delta x_i} f_{i-1}+ & \frac{-2}{\Delta x_{i+}\Delta x_{i-}} f_i+ & \frac{2}{\Delta x_i \Delta x_{i-}} f_{i+1} \end{array} \tag{3}$$

The finite difference representation of 1 is

$$\kappa_i \delta_x^2 \nu_i + \delta_x \kappa_i \delta_x \nu_i = -A_i \tag{4}$$

We may at times need to implement a ”source term” that depends on the temperature. This wouldn’t really be a source term in the strict definition, but if we consider a source term as anything that adds or removes energy from the system, then we could consider something like energy transfer due to blood perfusion, which depends on the temperature, a source term.
We will only consider source terms that have at most a linear dependence on temperature. In general, this will include all source terms of the form,

$$A_i = B_i \nu + C_i. \tag{5}$$

With this generalization, we have

$$\kappa_i \delta_x^2 \nu_i + \delta_x \kappa_i \delta_x \nu_i = -B_i \nu_i - C_i, \tag{6}$$

which, when expanded becomes

$$\frac{2\kappa_i}{\Delta x_{i+}\Delta x_i}\nu_{i-1}+\frac{-2\kappa_i}{\Delta x_{i+}\Delta x_{i-}}\nu_i+\frac{2\kappa_i}{\Delta x_i\Delta x_{i-}}\nu_{i+1}+\frac{\Delta x_{i-}\delta_x\kappa_i}{\Delta x_{i+}\Delta x_i}\nu_{i-1}+\frac{(\Delta x_{i+}-\Delta x_{i-})\,\delta_x\kappa_i}{\Delta x_{i+}\Delta x_{i-}}\nu_i+\frac{-\Delta x_{i+}\delta_x\kappa_i}{\Delta x_i\Delta x_{i-}}\nu_{i+1}=-B_i\nu_i-C_i. \tag{7}$$

Now, if we define three constants,

$$a_i \equiv \frac{2\kappa_i}{\Delta x_{i+}\Delta x_i}+\frac{\Delta x_{i-}\delta_x\kappa_i}{\Delta x_{i+}\Delta x_i} \tag{8}$$

$$b_i \equiv \frac{-2\kappa_i}{\Delta x_{i+}\Delta x_{i-}}+\frac{(\Delta x_{i+}-\Delta x_{i-})\,\delta_x\kappa_i}{\Delta x_{i+}\Delta x_{i-}}+B_i \tag{9}$$

$$c_i \equiv \frac{2\kappa_i}{\Delta x_i\Delta x_{i-}}+\frac{-\Delta x_{i+}\delta_x\kappa_i}{\Delta x_i\Delta x_{i-}} \tag{10}$$

we can write this in a simplified form,

$$a_i\nu_{i-1}+b_i\nu_i+c_i\nu_{i+1}=C_i \tag{11}$$

To specify a unique solution, we must specify two boundary conditions; one each for the min and max coordinates. These boundary conditions are required to handle the cases at $i = 0$ and $i = N-1$ points. For example, at $i = 0$, equation 11 is

$$a_0\nu_{-1}+b_0\nu_0+c_0\nu_1=C_i \tag{12}$$

This equation refers to the tempature at $i = -1$, which is not known. To handle this, we use a boundary condition.
In practice, we will either specify the temperature, or its derivative at the boundary.

$$\nu=\alpha \tag{13}$$

$$\frac{\partial\nu}{\partial x}=\beta(\nu) \tag{14}$$

$$\tag{15}$$

The first type, Dirichlet boundary conditions, are simple enough to implement. At the $i = 0$ and $i = N-1$, the temperatures on the other side of the boundary that are not known in equation 11 are directly given by the boundary conditions. At $i = 0$, we have

$$\alpha+b_0\nu_0+c_0\nu_1=C_0 \tag{16}$$

Defining a new constant

$$C_0' \equiv C_0 - \alpha \tag{17}$$

we can write a new version of the equation 12 at the boundary.

$$b_0 v_0 + c_0 v_1 = C_0' \tag{18}$$

The $i = N - 1$ boundary is almost identical

$$a_0 v_{N-2} + b_0 v_{N-1} = C_{N-1}' \tag{19}$$

where C' is defined the same as before.
The second type of boundary condition, Nuemann, are only slightly more difficult to implement. First, we finite-difference the derivative,

$$\frac{v_{i+1} - v_{i-1}}{x_{i+1} - x_{i-1}} = \beta(v_i) \tag{20}$$

$$\tag{21}$$

Now, for $i = 0$, we can write the v_{i-1}, which is not known, in terms of the things we do know.

$$v_{-1} = v_1 - \Delta x \beta(v_0) \tag{22}$$

and also for $i = N - 1$,

$$v_N = v_{N-2} + \Delta x \beta(v_{N-1}) \tag{23}$$

Using these, we can replace the unknown terms in the finite-difference equation. For the $i = 0$ case, 11 is

$$a_0 \left[v_1 - \Delta x \beta(v_0)\right] + b_0 v_0 + c_0 v_1 = C \tag{24}$$

As before, we can define a set of ”primed” constants,

$$c_0' \equiv c_0 + a_0 \tag{25}$$

$$C_0' \equiv C + a_0 \Delta x \beta(v_0) \tag{26}$$

so that we have

$$b_0 v_0 + c_0' v_1 = C_0' \tag{27}$$

For the $i = N - 1$ case we have

$$a'_{N-1} \equiv a_{N-1} + c_{N-1} \tag{28}$$
$$C'_{N-1} \equiv C_{N-1} - c_{N-1}\Delta x \beta\left(v_{N-1}\right) \tag{29}$$

and

$$a'_{N-1}v_{N-2} + b_{N-1}v_{N-1} = C'_{N-1} \tag{30}$$

Now, to solve the heat equation, we are going to use a ”relaxation” method. We note that, for the solution, the temperature at any point is related to its two neighbors, 11 is

$$v_i = \frac{C_i - a_i v_{i-1} - c_i v_{i+1}}{b_i} \tag{31}$$

At the two boundaries we have

$$v_0 = \frac{C'_0 - c'_0 v_1}{b_0} \tag{32}$$

and

$$v_{N-1} = \frac{C'_{N-1} - a'_{N-1}v_{N-2}}{b_{N-1}} \tag{33}$$

The relaxation method works by looping through all points and recalculating its value using equations 31 - 33. We do this until the temperature ”stops” changing. Of course, we will have to define some sort of metric to define when then temperature stops changing.

3 Analytic Solutions

In the following, we will develop a few analytic solution to the steady-state heat equation that can be used to validate a numerical heat solver.

3.1 Single slab with heat convection at one surface

Consider a single, homogeneous slab of material, with a sink boundary condition on one end, and a convective boundary condition at the other. We will have the heat equation,

$$k\frac{\partial^2}{\partial x^2}v(x) = 0, \tag{34}$$

with the following boundary conditions,

$$v(0) = 0, \tag{35}$$

$$k \frac{\partial}{\partial x} v(x)\bigg|_{x=X} = -h_e \left(v - v_\infty\right). \tag{36}$$

The solution will be a straight line, but the slope will depend on the convection at the surface,

$$v(x) = mx + b \tag{37}$$

$$v(0) = 0 \rightarrow b = 0 \tag{38}$$

$$v(x) = mx \tag{39}$$

$$k\frac{\partial}{\partial x}v(x) = km = -h\left(mX - v_\infty\right) \rightarrow m = \frac{hv_\infty}{k + hX} \tag{40}$$

So, we have

$$v(x) = \frac{hv_\infty}{k + hX}x \tag{41}$$