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On 1D diffusion problems with a gradient-dependent diffusion coefficient

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In solving the 1D (flux surface averaged) transport equations for the temperatures and densities in a tokamak[1], one increasingly encounters highly nonlinear thermal conductivity and diffusivity functions, such as GLF23[2], that have a strong dependence on the temperature gradients. These arise from a subsidiary microstability based calculation in which the growth rates and hence transport coefficients are sensitive functions of these gradients [3]. When these nonlinear functions are interfaced with a standard transport framework that uses a Crank-Nicholson [4] time advancement, large non-physical oscillations and numerical instabilities can develop. Here we describe a relatively simple modification to the Crank-Nicholson method that cures this difficulty.

To illustrate the method, we start with a simple diffusion equation in cylindrical polar coordinates:

$$\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\chi\left(T'\right)\frac{\partial T}{\partial r}\right] + S \qquad (1a)$$

Now, define a new independent variable, Φ, corresponding to the area (or the toroidal magnetic flux if a uniform longitudinal magnetic field is present), that is defined as: $\Phi \equiv \pi r^2$. With this substitution, equation (1) becomes

$$\frac{\partial T}{\partial t} = 4\pi\frac{\partial}{\partial \Phi}\left[\Phi\chi\left(T'\right)\frac{\partial T}{\partial \Phi}\right] + S \qquad (1b)$$

Here we have denoted $\partial T/\partial\Phi$ by T'. Consider the unit circle so that $0 \le \Phi \le \pi$. Note that this has a steady-state solution for $\chi = 1, \quad S = 4\pi, \quad T = 1 - \Phi.$

We apply a boundary condition of T=0 at Φ=π, keep S=4π, and use the above solution as an initial condition. Now, define a function that mimics the critical gradient thermal diffusivity model GLF23:

$$\chi\left(T'\right) = \begin{cases} k\left(\left|T'\right| - T_c'\right)^{\alpha} + \chi_0 & \text{for } \left|T'\right| > T_c' \\ \chi_0 & \text{for } \left|T'\right| \le T_c' \end{cases} \qquad (2)$$

For definiteness, let χ_0*=1.0, α=0.5, k = 10,* and $T_c' = 0.5$.

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In order to finite difference Eq. (1b), we define a mesh going from 0 to 1. We make T_j a cell centered quantity, in which *j* goes from 1 to N. The temperature T_j is centered at location $\Phi_j = (j - \frac{1}{2})\Delta\Phi$. Thus, the temperature at *j=1* corresponds to a cell center located at $\Phi_1 = \frac{1}{2}\Delta\Phi$. There is no need for a ghost zone at *j=0*, since the corresponding flux where it would be used is multiplied by zero. We first try solving this with the θ-implicit method (Crank-Nicholson corresponds to θ=0.5): with s= $\Delta t / \Delta\Phi^2$

$$\begin{aligned} T_j^{n+1} &= T_j^n + s\theta\left\{\left[\Phi_{j+1/2}\chi\left(T'^n_{j+1/2}\right)\left(T_{j+1}^{n+1} - T_j^{n+1}\right)\right] - \left[\Phi_{j-1/2}\chi\left(T'^n_{j-1/2}\right)\left(T_j^{n+1} - T_{j-1}^{n+1}\right)\right]\right\} \\ &\quad + s\left(1-\theta\right)\left\{\left[\Phi_{j+1/2}\chi\left(T'^n_{j+1/2}\right)\left(T_{j+1}^n - T_j^n\right)\right] - \left[\Phi_{j-1/2}\chi\left(T'^n_{j-1/2}\right)\left(T_j^n - T_{j-1}^n\right)\right]\right\} + \Delta t S \end{aligned} \quad (3)$$

Or, in tridiagonal form,

$$\begin{aligned} &A_j T_{j+1}^{n+1} - B_j T_j^{n+1} + C_j T_{j-1}^{n+1} + D_j = 0 \\ &A_j = s\theta\Phi_{j+1/2}\chi\left(T'^n_{j+1/2}\right) \\ &C_j = s\theta\Phi_{j-1/2}\chi\left(T'^n_{j-1/2}\right) \\ &B_j = 1 + A_j + C_j \\ &D_j = T_j^n + s\left(1-\theta\right)\left\{\Phi_{j+1/2}\chi\left(T'^n_{j+1/2}\right)\left(T_{j+1}^n - T_j^n\right) - \Phi_{j-1/2}\chi\left(T'^n_{j-1/2}\right)\left(T_j^n - T_{j-1}^n\right)\right\} + \Delta t S \end{aligned} \quad (4)$$

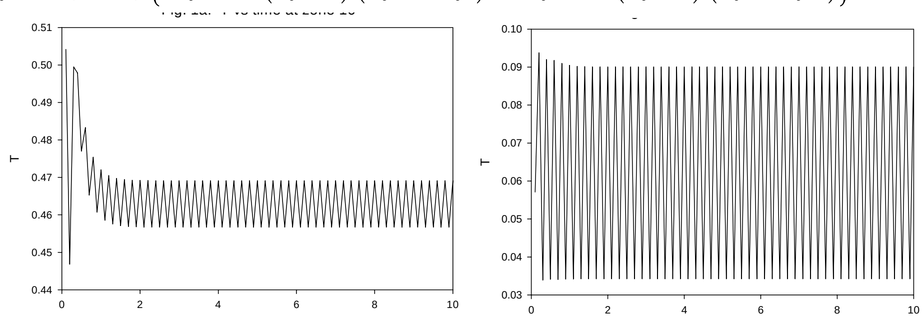

Figure 1: Initial solution of Eq. (1) using Crank-Nicholson method. Left plot is temperature vs time at zone 10, and right is temperature vs time at zone 90.

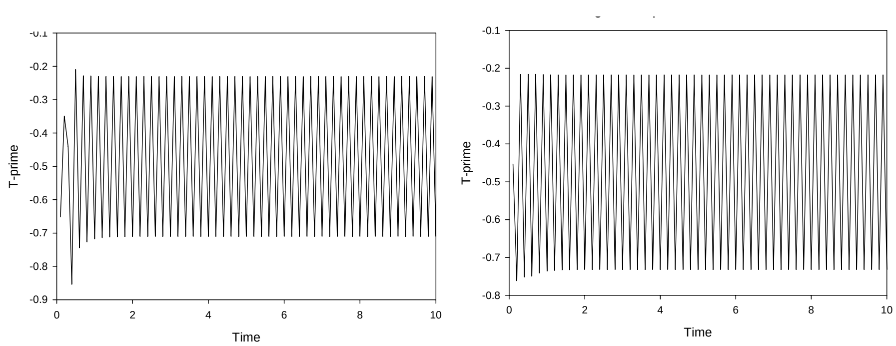

Figure 2: Initial solution of Eq. (1) using Crank-Nicholson method. Left plot is dT/dΦ at zone 10 vs time and right plot is at zone 90.

The illustrations in Figs 1 and 2 are the result of solving this with n=100 zones, with a time step Δt=0.1, implicit parameter θ=1.0 for 100 time steps. We plot the time history of the function and derivative at locations 10 and 90.

This is seen to be very noisy, with a large amplitude oscillation. In order to improve the solution, we investigate a nonlinearly implicit method that would seek to evaluate the χ functions multiplying the advanced time derivatives also at the advanced times, i.e.:

$$\begin{aligned} T_j^{n+1} = T_j^n &+ s\theta\left\{\left[\Phi_{j+1/2}\chi\left(T'^{n+1}_{j+1/2}\right)\left(T_{j+1}^{n+1} - T_j^{n+1}\right)\right] - \left[\Phi_{j-1/2}\chi\left(T'^{n+1}_{j-1/2}\right)\left(T_j^{n+1} - T_{j-1}^{n+1}\right)\right]\right\} \\ &+ s\left(1-\theta\right)\left\{\left[\Phi_{j+1/2}\chi\left(T'^{n}_{j+1/2}\right)\left(T_{j+1}^{n} - T_j^{n}\right)\right] - \left[\Phi_{j-1/2}\chi\left(T'^{n}_{j-1/2}\right)\left(T_j^{n} - T_{j-1}^{n}\right)\right]\right\} + \Delta tS \end{aligned} \tag{5}$$

We can derive a Newton's iteration to solve this by defining the modified coefficients corresponding to Newton iteration i (out of N):

$$A_j T_{j+1}^{n+i/N} - B_j T_j^{n+i/N} + C_j T_{j-1}^{n+i/N} + D_j = 0 \tag{6}$$

$$\begin{aligned} A_j &= s\theta\Phi_{j+1/2}\left[\chi\left(T'^{n+(i-1)/N}_{j+1/2}\right) + \frac{\partial\chi}{\partial T'}T'^{n+(i-1)/N}_{j+1/2}\right] \\ C_j &= s\theta\Phi_{j-1/2}\left[\chi\left(T'^{n+(i-1)/N}_{j-1/2}\right) + \frac{\partial\chi}{\partial T'}T'^{n+(i-1)/N}_{j-1/2}\right] \\ B_j &= 1 + A_j + C_j \\ D_j &= T_j^n + s\left(1-\theta\right)\left[\Phi_{j+1/2}\chi\left(T'^{n}_{j+1/2}\right)\left(T_{j+1}^{n} - T_j^{n}\right) - \Phi_{j-1/2}\chi\left(T'^{n}_{j-1/2}\right)\left(T_j^{n} - T_{j-1}^{n}\right)\right] \\ &\quad + \Delta tS + s\theta\left[\begin{aligned} &\Phi_{j+1/2}\frac{\partial\chi}{\partial T'}T'^{n+(i-1)/N}_{j+1/2}\left(T_j^{n+(i-1)/N} - T_{j+1}^{n+(i-1)/N}\right) \\ &+\Phi_{j-1/2}\frac{\partial\chi}{\partial T'}T'^{n+(i-1)/N}_{j-1/2}\left(T_j^{n+(i-1)/N} - T_{j-1}^{n+(i-1)/N}\right) \end{aligned}\right] \end{aligned} \tag{7}$$

The results of solving the equation using the coefficients in (7) with a single Newton iteration, rather than those in (4) are shown in Figures 3 and 4. We see that the solution converges to a mean result (compared to Figs 1 and 2) and without oscillations.
Note that if we apply only a single Newton iteration, we can rewrite Eq. (7) as:

$$
\begin{aligned}
T_j^{n+1} = T_j^n + s\theta & \left\{ \begin{array}{l} \Phi_{j+1/2}\left[\chi\left(T_{j+1/2}'^{n}\right) + \dfrac{\partial\chi}{\partial T'} T_{j+1/2}'^{n}\right](T_{j+1}^{n+1} - T_j^{n+1}) \\ -\Phi_{j-1/2}\left[\chi\left(T_{j-1/2}'^{n}\right) + \dfrac{\partial\chi}{\partial T'} T_{j-1/2}'^{n}\right]\left(T_j^{n+1} - T_{j-1}^{n+1}\right) \end{array} \right\} \\
+ s(1-\theta) & \left\{ \begin{array}{l} \Phi_{j+1/2}\left[\chi\left(T_{j+1/2}'^{n}\right) + \dfrac{\partial\chi}{\partial T'} T_{j+1/2}'^{n}\right]\left(T_{j+1}^{n} - T_j^{n}\right) \\ -\Phi_{j-1/2}\left[\chi\left(T_{j-1/2}'^{n}\right) + \dfrac{\partial\chi}{\partial T'} T_{j-1/2}'^{n}\right]\left(T_j^{n} - T_{j-1}^{n}\right) \end{array} \right\} \\
- s & \left[\Phi_{j+1/2} \frac{\partial\chi}{\partial T'} T_{j+1/2}'^{n}\left(T_{j+1}^{n} - T_j^{n}\right) - \Phi_{j-1/2} \frac{\partial\chi}{\partial T'} T_{j-1/2}'^{n}\left(T_j^{n} - T_{j-1}^{n}\right)\right] + \Delta t S
\end{aligned} \tag{8}
$$

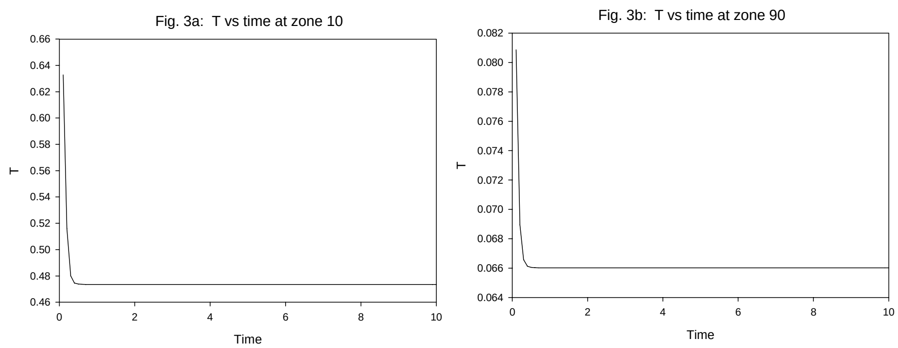

Figure 3: Temperatures at zone 10 (left) and zone 90 (right) corresponding to Figure 1 using Newton Iteration as defined by Eq. (8)

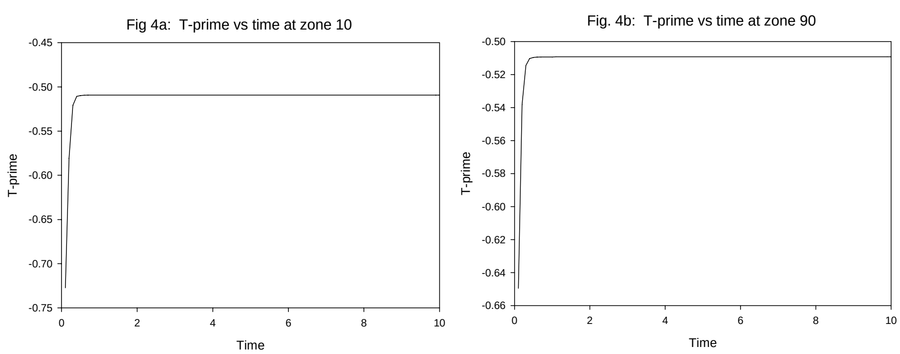

Figure 4: Temperatures derivatives at zone 10 (left) and zone 90 (right) corresponding to Figure 2 using Newton Iteration as defined by Eq. (8)

The finite difference equation (8) corresponds to the differential equation:

$$\frac{\partial T}{\partial t}=\frac{\partial}{\partial \Phi}\left\{\Phi\left[\chi\left(T'\right)+\frac{\partial \chi}{\partial T'}T'\right]\frac{\partial T}{\partial \Phi}\right\}-\frac{\partial}{\partial \Phi}\left\{\Phi\left[\frac{\partial \chi}{\partial T'}T'\right]\frac{\partial T}{\partial \Phi}\right\}+S \tag{9}$$

where the first term on the right is evaluated θ-centered in time and the second term is evaluated at the old time level. A multi-iteration Newton method is equivalent to repeating the timestep but using the most recent values of χ and $\partial\chi/\partial T'$ in (9).

We have incorporated this method in two existing production tokamak transport codes with only minor modification. Thus, in the existing numerical method in TSC [5] or in PTRANSP [6], the first term can just be treated as a modified thermal conductivity:

$$\chi\left(T'\right)\rightarrow\chi\left(T'\right)+\frac{\partial \chi}{\partial T'}T' \tag{10a}$$

and the second term can be treated as a modified source term:

$$S\rightarrow S-\frac{\partial}{\partial \Phi}\left\{\Phi\left[\frac{\partial \chi}{\partial T'}T'\right]\frac{\partial T}{\partial \Phi}\right\} \tag{10b}$$

Extending this to two temperatures T and T_e gives:

$$\begin{aligned}\frac{\partial T}{\partial t}&=\frac{\partial}{\partial \Phi}\left\{\Phi\left[\chi\left(T'\right)+\frac{\partial \chi}{\partial T'}T'\right]\frac{\partial T}{\partial \Phi}+\Phi\left[\frac{\partial \chi}{\partial T_e'}T'\right]\frac{\partial T_e}{\partial \Phi}\right\}\\&\quad-\frac{\partial}{\partial \Phi}\left\{\Phi\left[\frac{\partial \chi}{\partial T'}T'\right]\frac{\partial T}{\partial \Phi}+\Phi\left[\frac{\partial \chi}{\partial T_e'}T'\right]\frac{\partial T_e}{\partial \Phi}\right\}+S\\\frac{\partial T_e}{\partial t}&=\frac{\partial}{\partial \Phi}\left\{\Phi\left[\chi_e\left(T'\right)+\frac{\partial \chi_e}{\partial T_e'}T_e'\right]\frac{\partial T_e}{\partial \Phi}+\Phi\left[\frac{\partial \chi_e}{\partial T'}T_e'\right]\frac{\partial T}{\partial \Phi}\right\}\\&\quad-\frac{\partial}{\partial \Phi}\left\{\Phi\left[\frac{\partial \chi_e}{\partial T_e'}T_e'\right]\frac{\partial T_e}{\partial \Phi}+\Phi\left[\frac{\partial \chi}{\partial T'}T_e'\right]\frac{\partial T}{\partial \Phi}\right\}+S\end{aligned} \tag{11}$$

Here, again, the first term on the right of each equation is evaluated θ-centered in time, and the second term is evaluated at the old time level.

The algorithm presented here is a variation of an unpublished algorithm first developed by one of us for usage in transport codes employing the IFS-PPPL transport model, a precursor to the current GLF23 model. In this note we show it to be in fact a Newton iteration and hence it can be iterated each individual time step to improve robustness. Variants of this algorithm have also been briefly mentioned in Ref. [7] and [8].

Application to a JET Discharge

Here we show an example with the method implemented in the PTRANSP code (http://w3.pppl.gov/transp/) as part of the finite difference algorithm that is used to advance the electron and ion thermal transport equations. The thermal transport equations are a pair of diffusive-convective equations similar to Eq. 11 that are coupled tightly through an equipartition term that is proportional to the difference between the electron and ion temperatures. When the finite difference approximations to the transport equations are advanced in time using an implicit technique, the result is a block tridiagonal system of algebraic equations similar to Eqs. 3 and 4 that must be solved each time step.

Before the implementation of Newton's method, time smoothing was used in an effort to control the numerical artifact associated with the use of stiff transport models. The results of a simulation using time smoothing together with the GLF23 transport model are shown in the left two panels of Fig. 3, where the electron and ion thermal diffusivities are plotted as a function of normalized minor radius (electron thermal diffusivity in the bottom panel and ion thermal diffusivity in the top panel). If time smoothing (or Newton's method) were not used, the numerical artifact (ragged behavior shown in the left panels of Fig. 3) would be so severe that the simulation could not be run.

Corresponding simulation results are shown in the right panels of Fig. 3 after the implementation of Newton's method (similar to Eq. 7) with time smoothing turned off. In this simulation of a JET tokamak discharge using the GLF23 transport model, three Newton's method iterations are used to advance the finite difference equations each time step and the implicitness parameter is taken to be unity. The small remaining lack of smoothness in the diffusivity profiles can be attributed to the random Monte Carlo noise in the source terms (S in Eq. 12) and the abrupt transition to a steep gradient boundary layer that is imposed beyond $r/a > 0.95$ in these simulations.

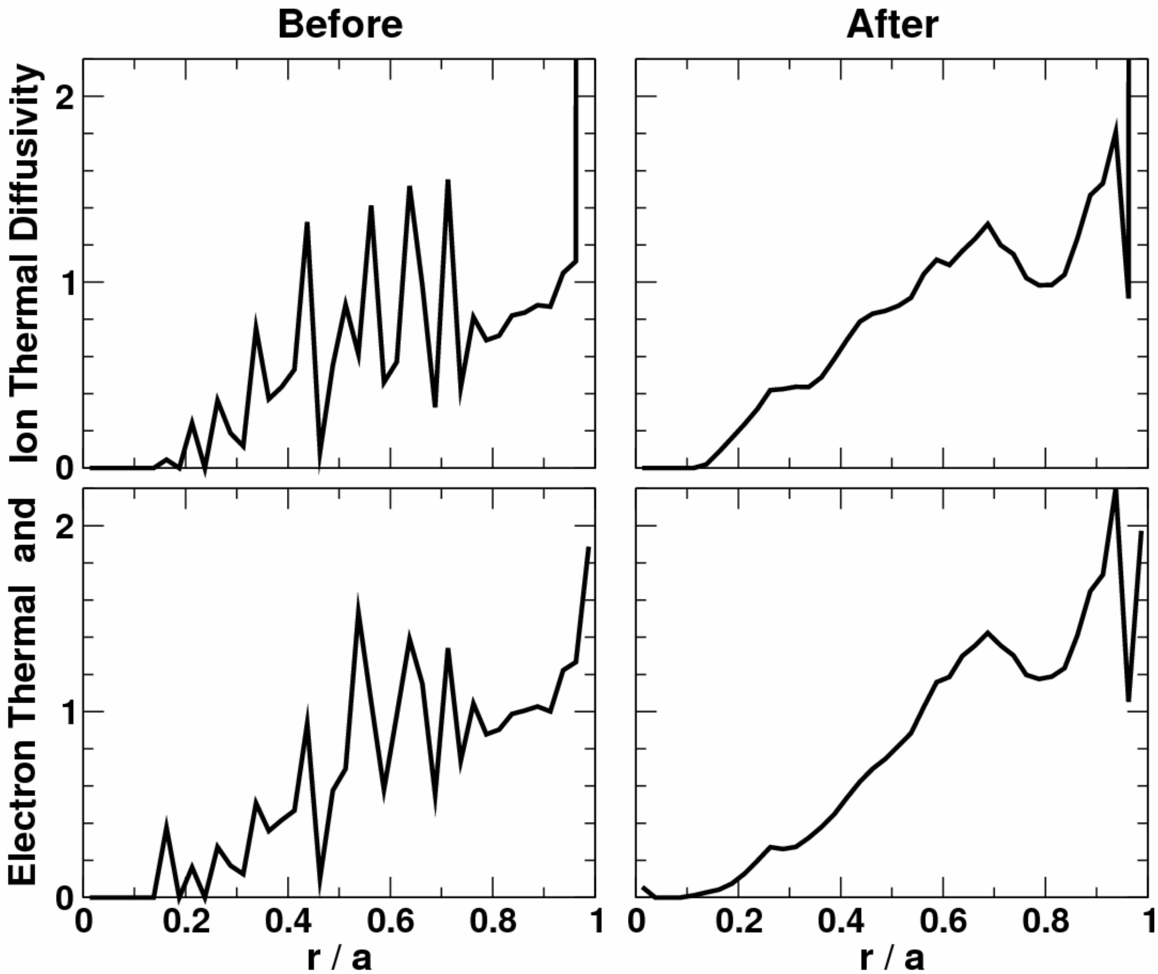

Figure 5. Electron and ion thermal diffusivity (bottom and top panels respectively) as a function of normalized minor radius, *r/a*, from a PTRANSP simulation of a JET discharge before and after Newton's method was implemented (left and right panels respectively).

Several problems were encountered in the implementation of Newton's method in the TSC and PTRANSP codes when used with the GLF23 transport model. There are some conditions, for example, that result in a negative derivative of the thermal diffusivity with respect to the temperature gradient, at least for one of the channels of transport. The negative gradient can be so large that the combination $\chi + (\partial\chi/\partial T')T'$ can be negative (such as could happen at a transport barrier bifurcation), which results in a severe numerical instability. In order to avoid this problem, the magnitude of negative values of $\partial\chi/\partial T'$ had to be limited in order to ensure that the combination $\chi + (\partial\chi/\partial T')T'$ is always positive.

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