Week 11: Elliptic equations, non linearities and implicit methods

Solving an elliptic equation via relaxation, dealing with non linearities and use of implicit integration methods in time

Dr K Clough, Topics in Scientific computing, Autumn term 2023

Two Announcements

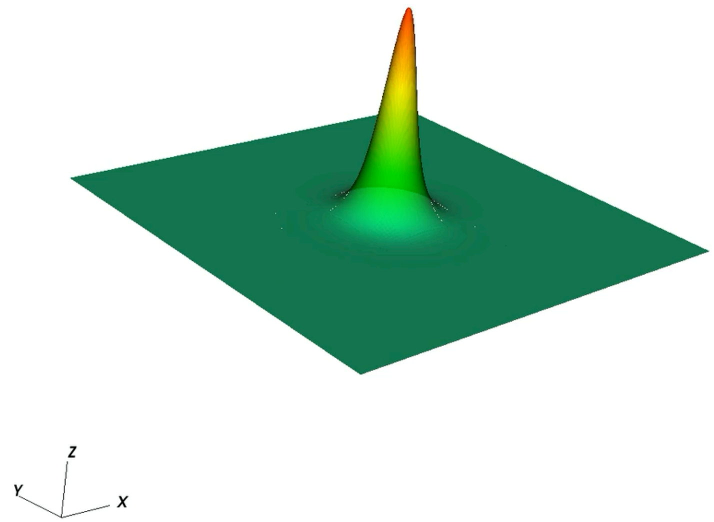
- Coursework is out!

  - Sine Gordon Breathers - oscillating solutions to a non linear wave equation

  - No help from me! Instructions should be clear - only reasonable requests for clarifications will be answered

  - I will run an online office hour after Christmas for any last minute questions

- Please provide feedback via the module evaluation TODAY!



Plan for today

1. Classification of PDEs - revision and the higher dimensional case
2. Non linearities - revision of the ODE case and extension to PDEs
3. Implicit integration methods - revision of the ODE case and extension to PDEs
4. Solving elliptic equations as a boundary value problem via relaxation, the non linear Poisson equation as an example

Classification of second order PDEs

Consider the most general second order PDE for 1 dependent variable with 2 independent variables:

$$A\frac{\partial^2 u}{\partial x^2} + 2B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + F = 0$$

The equation is classified based on the discriminant $\Delta = B^2 - 4AC$:

$\Delta < 0$ Elliptic

$\Delta = 0$ Parabolic

$\Delta > 0$ Hyperbolic

The three kinds - elliptic, parabolic, hyperbolic

1. $$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + S$$

2. $$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$$

Which is which?

3. $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

The three kinds - elliptic, parabolic, hyperbolic

1. $$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + S$$ *Parabolic - decaying and spreading out*

2. $$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$$ *Hyperbolic - wave-y*

3. $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$ *Elliptic - smooth deformation by source f*

What about higher dimensional systems?

$$\frac{\partial^2 u}{\partial t^2} - 2v\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 v}{\partial x^2} - 4\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial y^2} = f(u, v)$$

$$\frac{\partial^2 v}{\partial t^2} - v\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 v}{\partial x^2} + 3\frac{\partial^2 u}{\partial y^2} + 6\frac{\partial^2 v}{\partial y^2} = g(u, v)$$

Now have a coupled system of PDEs for 2 dependent variables (u,v), and 3 independent variables (t,x,y)…

Formulation as a matrix first order system

First consider the case with only 2 independent variables, but several dependent ones. The goal is to get the equations into a first order form so that we have something that looks like:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} = \overbrace{\begin{bmatrix} A & B \\ C & D \end{bmatrix}}^{M} \frac{\partial}{\partial x}\begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} E \\ F \end{bmatrix}$$

Formulation as a matrix first order system

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We will then be able to classify the PDE and check its well posedness by considering properties of the matrix M, specifically:

If all eigenvalues of the characteristic matrix M are purely real, the system of PDEs is hyperbolic, whereas if some are imaginary then it is elliptic.

Formulation as a matrix first order system

The goal is to get the equations into a first order form so that we have something that looks like:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \quad \boldsymbol{M} \quad \end{bmatrix} \frac{\partial}{\partial x}\begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} E \\ F \end{bmatrix}$$

If all eigenvalues of the characteristic matrix M are purely real, the system of PDEs is hyperbolic.

- If a system of PDEs is hyperbolic, and the principal matrix does not have a complete set of eigenvectors, the system is called ***weakly hyperbolic***. Such systems are ***not well posed.***
- If a system of PDEs is hyperbolic, and the principal matrix has a complete set of eigenvectors, the system is called ***strongly hyperbolic***. Such systems are ***well posed.***
- If the principal matrix of a hyperbolic system of PDEs has all of its eigenvalues distinct, then the system is called ***strictly hyperbolic*** *(includes strongly hyperbolic systems)*.
- If the principal matrix of the system of PDEs is hermitian, i.e., $M = (M^T)*$, then the system is called ***symmetric hyperbolic*** *(includes strictly hyperbolic systems)*.

The wave equation as an example

Consider trying to make the wave equation purely first order:

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$$

We define:

$$v = \frac{\partial u}{\partial t} \quad \text{and} \quad \psi = \frac{\partial u}{\partial x}$$

What system of equations do we get?

The wave equation as an example

Consider trying to make the wave equation purely first order:

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$$

We define:

$$v = \frac{\partial u}{\partial t} \quad \text{and} \quad \psi = \frac{\partial u}{\partial x}$$

Then we obtain the following system:

$$\frac{\partial v}{\partial t} = c^2 \frac{\partial \psi}{\partial x}, \qquad \frac{\partial \psi}{\partial t} = \frac{\partial^2 u}{\partial t \partial x} = \frac{\partial^2 u}{\partial x \partial t} = \frac{\partial v}{\partial x}, \qquad \frac{\partial u}{\partial t} = v$$

How to write this in matrix form?

The wave equation as an example

Then we obtain the following system:

$$\frac{\partial v}{\partial t} = c^2 \frac{\partial \psi}{\partial x}, \qquad \frac{\partial \psi}{\partial t} = \frac{\partial^2 u}{\partial t \partial x} = \frac{\partial^2 u}{\partial x \partial t} = \frac{\partial v}{\partial x}, \qquad \frac{\partial u}{\partial t} = v$$

Which we can write as:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \\ \psi \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & c^2 \\ 0 & 1 & 0 \end{bmatrix} \frac{\partial}{\partial x}\begin{bmatrix} u \\ v \\ \psi \end{bmatrix} + \begin{bmatrix} v \\ 0 \\ 0 \end{bmatrix}$$

The wave equation as an example

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \\ \psi \end{bmatrix} = \overbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & c^2 \\ 0 & 1 & 0 \end{bmatrix}}^{M} \frac{\partial}{\partial x}\begin{bmatrix} u \\ v \\ \psi \end{bmatrix} + \begin{bmatrix} v \\ 0 \\ 0 \end{bmatrix}$$

M is the characteristic matrix.

The eigenvalues are the solutions of $\det(M - \lambda I) = 0$, ie:

$$\lambda(\lambda^2 - c^2) = 0$$

What do we conclude?

The wave equation as an example

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \\ \psi \end{bmatrix} = \overbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & c^2 \\ 0 & 1 & 0 \end{bmatrix}}^{M} \frac{\partial}{\partial x}\begin{bmatrix} u \\ v \\ \psi \end{bmatrix} + \begin{bmatrix} v \\ 0 \\ 0 \end{bmatrix}$$

M is the characteristic matrix.

The eigenvalues are the solutions of $\det(M - \lambda I) = 0$

$\lambda = 0, \pm |c|$ so the equation is hyperbolic
(also strictly hyperbolic, and therefore well posed)

Note on higher numbers of independent variables

Now consider the case with d independent variables. The goal is to get the equations into a first order form so that we have something that looks like:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} = \sum_{i=1}^{i=d}\Bigg[\quad A_i \quad\Bigg]\frac{\partial}{\partial x^i}\begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} E \\ F \end{bmatrix}$$

We now construct the characteristic matrix M as follows:

$$M = \sum_{i=1}^{i=d} A_i k^i \quad \text{where } k^i \text{ is a unit vector in some norm } |k^i| = 1$$

The classification then follows as in the previous d=1 example.

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2. Non linearities - revision of the ODE case and extension to PDEs

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4. Solving elliptic equations as a boundary value problem via relaxation, the non linear Poisson equation as an example

Ordinary differential equations

What terms make this ODEs non linear?

$$\frac{d^2y}{dt^2} + \left(\frac{dy}{dt}\right)^2 + \sin(y) + y - 1 = \sin(t)$$

Ordinary differential equations

Coefficient of the derivative is another derivative of y, not a function of t, so non linear

$$\frac{d^2y}{dt^2} + \left(\frac{dy}{dt}\right)^2 + \sin(y) + y - 1 = \sin(t)$$

This term is ok - t is the independent variable!

Sinusoid can be expressed as a power series in y, that is

$\sin(y) = y - \frac{x^3}{3!}\ldots$ so is non linear

Partial differential equations

For the general PDE:

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} = \sum_{i=1}^{i=d} \begin{bmatrix} & A_i & \end{bmatrix} \frac{\partial}{\partial x^i}\begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} E \\ F \end{bmatrix}$$

The equation is:

- **Linear** if the components of A_i and E and F are just numbers or functions of the independent variables
- **Quasi linear** if the components of A_i and E and F include $\overrightarrow{u}$
- Truly **non linear** if the components of A_i and E and F include derivatives of $\overrightarrow{u}$

The three kinds - linear, quasilinear, non linear

1. $$\frac{\partial T}{\partial t} = \alpha \frac{\partial T}{\partial y} \frac{\partial^2 T}{\partial x^2} + T \frac{\partial^2 T}{\partial y^2} + sin(t)$$

2. $$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + T \frac{\partial^2 T}{\partial y^2} + sin(T) + t$$

Which is which?

3. $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial y^2} = t^3 + t$$

The three kinds - linear, quasilinear, non linear

1. $$\frac{\partial T}{\partial t} = \alpha \frac{\partial T}{\partial y} \frac{\partial^2 T}{\partial x^2} + T \frac{\partial^2 T}{\partial y^2} + sin(t)$$ *Non linear*

2. $$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + T \frac{\partial^2 T}{\partial y^2} + sin(T) + t$$ *Quasi linear*

3. $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial y^2} = t^3 + t$$ *Linear*

Recall: Well posed problems

- Theorems in mathematics guarantee the (local) well-posedness of **linear and quasi-linear*** **strongly hyperbolic*** and **parabolic** PDEs.

- Elliptic PDEs do not admit a well-posed IVP. This does not (necessarily) mean they cannot be solved, just that another method may be required.

*Now you know what these terms mean

How to implement non linear equations?

In the tutorial you will solve the quasi-linear parabolic equation:

$$\frac{\partial T}{\partial t} = -\tau \left[\frac{\partial^2 T}{\partial x^2} - e^{-\alpha T^2} \right]$$

Numerically this is simple! We just add the non linear part into time derivative that is used in solve_ivp() or any other method to integrate.

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1. ~~Classification of PDEs - revision and the higher dimensional case~~
2. ~~Non linearities - revision of the ODE case and extension to PDEs~~
3. Implicit integration methods - revision of the ODE case and extension to PDEs (including non linear ones!)
4. Solving elliptic equations as a boundary value problem via relaxation, the non linear Poisson equation as an example

Explicit versus implicit methods - ODEs

An explicit method is one where the variable we want at the next step y_{k+1} can be written explicitly in terms of quantities we know at the current step $y_k,\ t_k$, e.g.

$$y_{k+1} = y_k + h\, f(y_k, t_k) \qquad \text{“forward Euler - explicit”}$$

Implicit methods will instead result in equations where we cannot easily isolate and solve for the quantity we want,
e.g.

$$y_{k+1} = y_k + h\, f(y_{k+1}, t_{k+1}) \qquad \text{“backward Euler - implicit”}$$

How to implement implicit integration?

In the tutorial you will solve a quasi-linear parabolic equation:

$$\frac{\partial T}{\partial t} = -\tau \left[\frac{\partial^2 T}{\partial x^2} - e^{-\alpha T^2} \right]$$

Since this is non linear, we cannot easily solve for the unknown function at the next timestep.

Iterate and hope for the best…

Algorithm:

Initially use the last value as a first try:

$$T_{k+1}^{guess(0)} = T_k + h \left.\frac{\partial T}{\partial t}\right|_k$$

Now use this new guess as the value and repeat:

$$T_{k+1}^{guess(i)} = T_k + h \left.\frac{\partial T}{\partial t}\right|_{k+1}^{guess(i-1)}$$

I stop when:

$$|T_{k+1}^{guess(i)} - T_{k+1}^{guess(i-1)}| < \epsilon$$

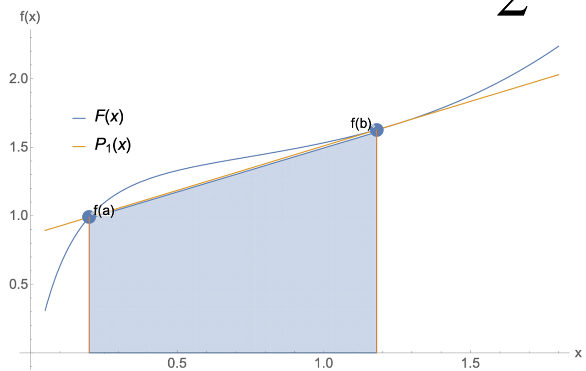
Implicit methods

In the tutorial you will use the simplest one to integrate a parabolic equation:

$$y_{k+1} = y_k + h\, f(y_{k+1}, t_{k+1})$$ *"implicit (backward) Euler method"*

In the coursework you will use the next simplest one, which is essentially the trapezoidal integration method we learned, applied to the derivatives:

$$y_{k+1} = y_k + \frac{h}{2} \left(f(y_{k+1}, t_{k+1}) + f(y_k, t_k) \right)$$ *"trapezoidal rule"*



where $f(y, t) = \dfrac{\partial y}{\partial t}$

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How do we solve elliptic equations?

In the tutorial we want to solve the quasi-linear elliptic equation:

$$\frac{\partial^2 T}{\partial x^2} = e^{-\alpha T^2}$$

subject to the boundary conditions

$T(x = 0) = 0$ and $T(x = L) = 0$

This is a boundary value problem, since we are told the values at the start and end of the interval of interest.

How can we solve this?

How do we solve elliptic equations?

What if instead we solve:

$$\frac{\partial T}{\partial t} = -\tau \left[\frac{\partial^2 T}{\partial x^2} - e^{-\alpha T^2} \right]$$ subject to the boundary conditions

$T(x=0)=0$ and $T(x=L)=0$?

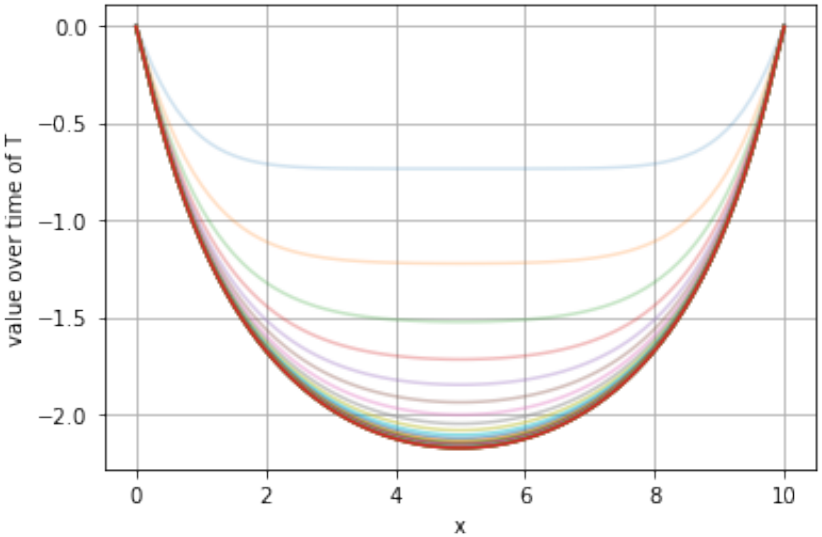
How do we know what to use as
an initial condition?

How do we solve elliptic equations?

If instead we solve:

$$\frac{\partial T}{\partial t} = -\tau\left[\frac{\partial^2 T}{\partial x^2} - e^{-\alpha T^2}\right]$$ subject to the boundary conditions

$$T(x=0) = 0 \text{ and } T(x=L) = 0$$



The solution “relaxes” into the solution ,

When $\dfrac{\partial T}{\partial t} = 0$, the original equation is solved

How do we solve elliptic equations?

If instead we solve:

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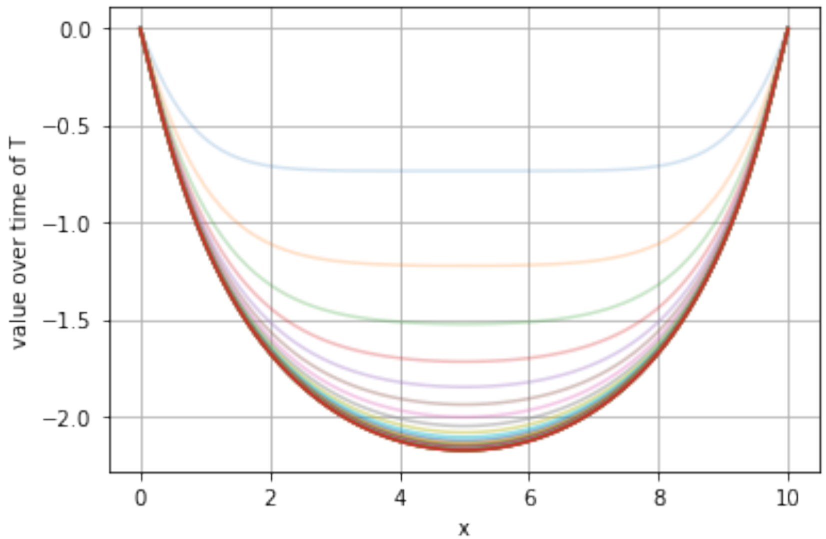


The solution “relaxes” into the solution,

When $\frac{\partial T}{\partial t} = 0$, the original equation is solved

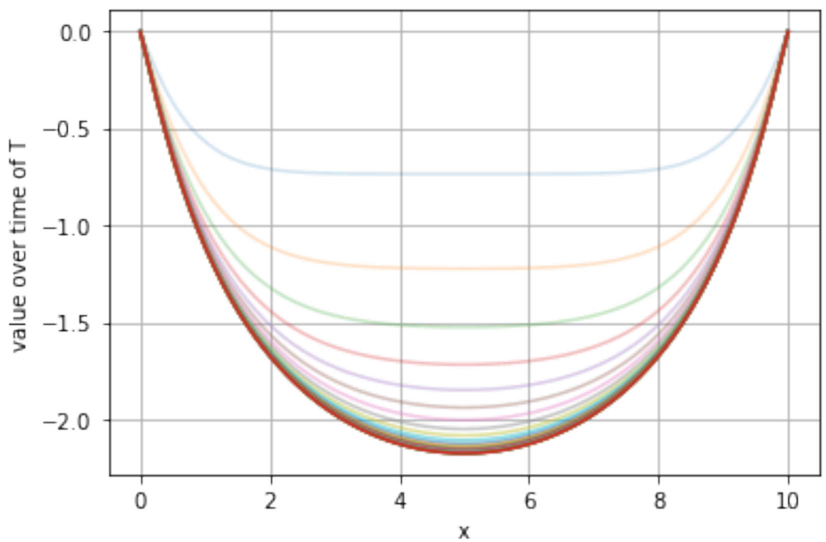
What is the role of τ?

How do we solve elliptic equations?

If instead we solve:

$$\frac{\partial T}{\partial t} = -\tau \left[\frac{\partial^2 T}{\partial x^2} - e^{-\alpha T^2} \right]$$ subject to the boundary conditions

$$T(x=0) = 0 \text{ and } T(x=L) = 0$$



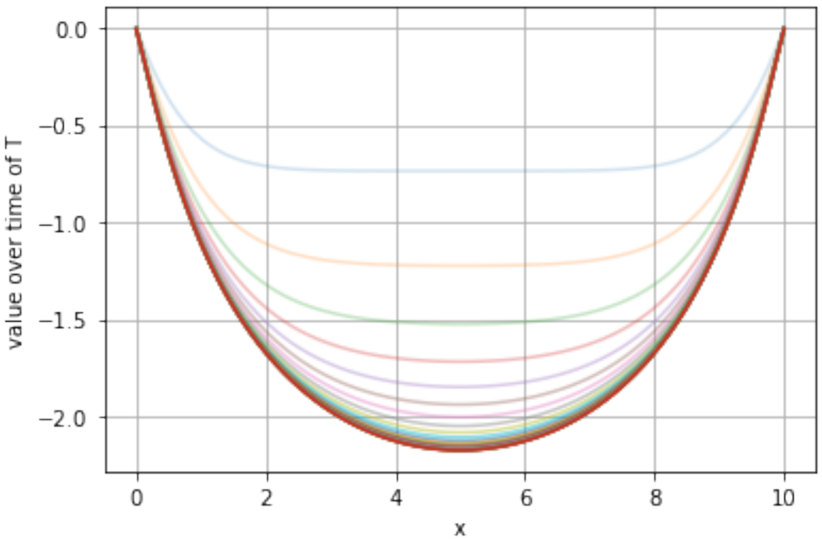
The parameter τ in an (unphysical) time parameter that controls the speed at which the solution is approached. However, by the same stability arguments as the CFL condition, it cannot be made arbitrarily large.

How do we solve elliptic equations?

If instead we solve:

$$\frac{\partial T}{\partial t} = -\tau \left[\frac{\partial^2 T}{\partial x^2} - e^{-\alpha T^2} \right]$$ subject to the boundary conditions

$T(x=0)=0$ and $T(x=L)=0$



This will work provided that the initial guess is "sufficiently close" to the actual solution.

This method is highly inefficient, but can be made more efficient using multigrid methods.

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You now know everything you need to complete the coursework, well done, and good luck!