Numerical Simulation of Dynamic Systems XIII

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PDEs in Multiple Space Dimensions

In principle, the MOL methodology can be extended without modification to the case of PDEs in multiple space dimensions. For example, the two-dimensional heat flow problem:

$$\frac{\partial u}{\partial t} = \sigma \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

discretized using third-order accurate finite difference formulae for both the discretization in the x- and in the y-directions leads to the following ODE at point $x = x_i$ and $y = y_j$:

$$\frac{du_{i,j}}{dt} \approx \sigma \left(\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\delta y^2} \right)$$

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Yet, the problems are formidable. The first, and most frightening, problem is concerned with the sheer numbers of resulting ODEs.

Let us assume that we use 50 segments in each space dimension. Then, the *2D problem* has $50 \times 50 = 2500$ ODEs, whereas the *3D problem* has $50 \times 50 \times 50 = 125,000$ ODEs. The **A**-matrix of the 3D problem has $125,000 \times 125,000 = 15,624,000,000$ elements.

PDEs in Multiple Space Dimensions II

The second problem has to do with the distribution of the non-zero elements in the **A**-matrix. Until now, it always happened that the **A**-matrix of a single linear PDE converted by use of finite differences was *band-structured* with a narrow band width. There exist special matrix routines for very efficient handling of band-structured matrices.

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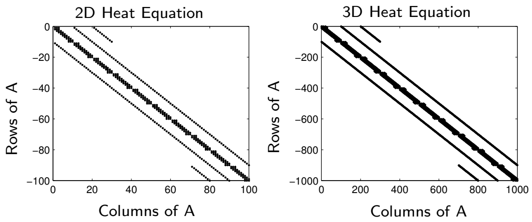

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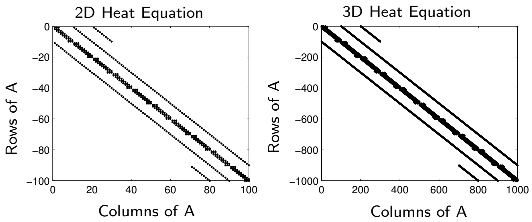

Let n be the number of segments. In the 1D case, the bandwidth was constant. In the 2D case, it grows proportional in n. In the 3D case, it grows proportional in n^2.

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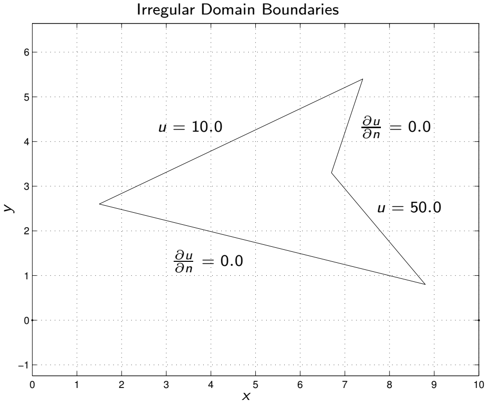
We can no longer make that assumption in the 2D and 3D cases:



PDEs in Multiple Space Dimensions IV

Let us assume that four neighboring values on grid points in x-direction for $y = y_j$ are $u_{1,j}$, $u_{2,j}$, $u_{3,j}$, and $u_{4,j}$. Let us assume further that the boundary value is known at $x = x_{1.35}$ located between x_1 and x_2.

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If we know the four solution values $u_{1,j}$, $u_{2,j}$, $u_{3,j}$, and $u_{4,j}$, we can use the *Nordsieck vector* approach to compute $u_{1.35,j}$. $u_{1.35,j}$ can be expressed as a weighted sum of $u_{1,j}$, $u_{2,j}$, $u_{3,j}$, and $u_{4,j}$.

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In reality, however, we know $u_{1.35,j}$ (*boundary value*), and $u_{2,j}$, $u_{3,j}$, and $u_{4,j}$ (*through numerical integration - internal to the domain*). What is unknown is $u_{1,j}$ (*external to the domain*).

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Thus, we need to solve the previously determined equation for the unknown $u_{1,j}$ instead for the known $u_{1.35,j}$.

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- Unfortunately, the recipes that they have come up with so far are often rather *ad hoc*. There are no good theories available yet for which techniques work best when and why.
- Consequently, there remains a formidable amount of research yet to be explored.

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Let us assume the Laplace equation is defined in a circular domain of radius $r = 1.0$ around the origin. Since the domain is circular, it is much more appropriate to formulate the problem using *polar coordinates*:

$$x = r \cdot \cos\varphi$$
$$y = r \cdot \sin\varphi$$

or:

$$r = \sqrt{x^2 + y^2}$$
$$\varphi = \arctan\left(\frac{y}{x}\right)$$

Elliptic PDEs II

We can express $u(x, y)$ as $\tilde{u}(r(x, y), \varphi(x, y))$. Thus:

$$\frac{\partial u}{\partial x} = \frac{\partial \tilde{u}}{\partial r} \cdot \frac{\partial r}{\partial x} + \frac{\partial \tilde{u}}{\partial \varphi} \cdot \frac{\partial \varphi}{\partial x}$$

or, in short–hand notation:

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Using the chain rule and the multiplication rule, we find:

$$\begin{aligned} u_{xx} + u_{yy} = {} & \left(r_x^2 + r_y^2\right) \tilde{u}_{rr} + 2\left(r_x \varphi_x + r_y \varphi_y\right) \tilde{u}_{r\varphi} + \left(\varphi_x^2 + \varphi_y^2\right) \tilde{u}_{\varphi\varphi} \\ & + \left(r_{xx} + r_{yy}\right) \tilde{u}_r + \left(\varphi_{xx} + \varphi_{yy}\right) \tilde{u}_\varphi \end{aligned}$$

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or finally:

$$\frac{\partial^2 \tilde{u}}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial \tilde{u}}{\partial r} + \frac{1}{r^2} \cdot \frac{\partial^2 \tilde{u}}{\partial \varphi^2} = 0.0$$

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- No numerical integration across time will take place at all. **We are thus in trouble with our MOL methodology.**
- We may still be able to apply the MOL approach by either differentiating along r and integrating along φ, or alternatively, by differentiating along φ and integrating along r.
- In both cases, however, we would be *lacking one initial condition*, and would instead have *one final condition too many*. This is therefore not an *initial value problem*, but rather a *boundary value problem*.

Invariant Embedding

Let us simplify the boundary condition a bit by assuming that it does not depend on time. In this case, the problem is totally *static*, i.e., the solution is not time-dependent at all. The solution consists simply of a set of u-values at the grid points.

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We can now embed this problem within another problem as follows:

$$\frac{\partial \tilde{u}}{\partial t} = \frac{\partial^2 \tilde{u}}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial \tilde{u}}{\partial r} + \frac{1}{r^2} \cdot \frac{\partial^2 \tilde{u}}{\partial \varphi^2}$$

with the boundary condition:

$$\frac{\partial \tilde{u}}{\partial r} = f(\varphi)$$

and with arbitrary initial conditions.

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- This method of solving elliptic PDEs is called *invariant embedding*.
- The price that we had to pay for this comfort is formidable. We were able to convert a *boundary value problem* into an *initial value problem* at the expense of increasing the number of dimensions by one.

Finite Element Approximations

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A differential equation is not the cause that makes physics tick, it is only one way of describing, in mathematical terms and after the fact, what happens in the process of energy exchange taking place in the physical system.

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- The technique was originally developed by civil engineers trying to determine the static stress in bridges and other building structures. However, the method has a much broader range of possible applications.

- For all practical purposes, it can be viewed as an alternative to the finite difference approaches. Thus, it can conceptually also be used for other than elliptic PDEs.

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- On the other hand, finite difference approximations always lead to *sparse matrices*. Finite element approximations do not share this property. As a consequence, although the number of equations is smaller in the finite element case, we may not be able to use sparse matrix techniques, and it is therefore not evident that the smaller system size truly leads to a more economical algorithm.

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- Also, a finite difference formulation is usually easier to derive and harder to solve than a finite element formulation.
- However, it is easier to incorporate *irregular and even non-convex domain boundaries* into a finite element description.

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- Although Ellpack represents the fruit of many man-years of research and resulted in a Fortran code with several hundreds of subroutines and many thousands of lines of code, Ellpack was unable to conquer the elliptic PDE market. Ellpack was a research tool that allowed us to quickly experiment with many different combinations of algorithms, but the resulting simulation code was too sluggish to be practically useful. After finding out, which algorithms worked on our specific problems, we then had to recode these algorithms from scratch to get software that could be used for the simulation of large-scale structures.

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- We used this tool primarily for experimenting with electronic device simulations, in particular with simulating breakdown phenomena in reverse-biased power transistors and studying the effects of total dose ionizing radiation on such devices.

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- In particular, we discussed issues with and solution methods for the class of *elliptic PDEs*.
- One quite general approach for converting *boundary value problems* to equivalent *initial value problems* is the technique of *invariant embedding*. This technique was demonstrated by embedding an elliptic PDE in two space dimensions into an equivalent parabolic PDE in two space dimensions and one time dimension.
- The presentation ended with a very brief introduction to *finite element methods*.

References

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