17.5 Automated Allocation of Mesh Points

In relaxation problems, you have to choose values for the independent variable at the mesh points. This is called *allocating* the grid or mesh. The usual procedure is to pick a plausible set of values and, if it works, to be content. If it doesn't work, increasing the number of points usually cures the problem.

If we know ahead of time where our solutions will be rapidly varying, we can put more grid points there and less elsewhere. Alternatively, we can solve the problem first on a uniform mesh and then examine the solution to see where we should add more points. We then repeat the solution with the improved grid. The object of the exercise is to allocate points in such a way as to represent the solution accurately.

It is also possible to automate the allocation of mesh points, so that it is done "dynamically" during the relaxation process. This powerful technique not only improves the accuracy of the relaxation method, but also (as we will see in the next section) allows internal singularities to be handled in quite a neat way. Here we learn how to accomplish the automatic allocation.

We want to focus attention on the independent variable x, and consider two alternative reparametrizations of it. The first, we term q; this is just the coordinate corresponding to the mesh points themselves, so that $q = 1$ at $\mathtt{k} = 1$, $q = 2$ at $\mathtt{k} = 2$, and so on. Between any two mesh points we have $\Delta q = 1$. In the change of independent variable in the ODEs from x to q,

$$\frac{d\mathbf{y}}{dx} = \mathbf{g} \tag{17.5.1}$$

becomes

$$\frac{d\mathbf{y}}{dq} = \mathbf{g}\frac{dx}{dq} \tag{17.5.2}$$

In terms of q, equation (17.5.2) as an FDE might be written

$$\mathbf{y}_k - \mathbf{y}_{k-1} - \tfrac{1}{2}\left[\left(\mathbf{g}\frac{dx}{dq}\right)_k + \left(\mathbf{g}\frac{dx}{dq}\right)_{k-1}\right] = 0 \tag{17.5.3}$$

or some related version. Note that dx/dq should accompany $\mathbf{g}$. The transformation between x and q depends only on the *Jacobian* dx/dq. Its reciprocal dq/dx is proportional to the density of mesh points.

Now, given the function $\mathbf{y}(x)$, or its approximation at the current stage of relaxation, we are supposed to have some idea of how we want to specify the density of mesh points. For example, we might want dq/dx to be larger where $\mathbf{y}$ is changing rapidly, or near to the boundaries, or both. In fact, we can probably make up a formula for what we would like dq/dx to be proportional to. The problem is that we do not know the proportionality constant. That is, the formula that we might invent would not have the correct integral over the whole range of x so as to make q vary from 1 to M, according to its definition. To solve this problem we introduce a second reparametrization $Q(q)$, where Q is a new independent variable. The relation between Q and q is taken to be *linear*, so that a mesh spacing formula for dQ/dx differs only in its unknown proportionality constant. A linear relation implies

$$\frac{d^2Q}{dq^2} = 0 \tag{17.5.4}$$

or, expressed in the usual manner as coupled first-order equations,

$$\frac{dQ(x)}{dq} = \psi \qquad \frac{d\psi}{dq} = 0 \tag{17.5.5}$$

where ψ is a new intermediate variable. We add these two equations to the set of ODEs being solved.

Completing the prescription, we add a third ODE that is just our desired mesh-density function, namely

$$\phi(x) = \frac{dQ}{dx} = \frac{dQ}{dq}\frac{dq}{dx} \tag{17.5.6}$$

where $\phi(x)$ is chosen by us. Written in terms of the mesh variable q, this equation is

$$\frac{dx}{dq} = \frac{\psi}{\phi(x)} \tag{17.5.7}$$

Notice that $\phi(x)$ should be chosen to be positive definite, so that the density of mesh points is everywhere positive. Otherwise (17.5.7) can have a zero in its denominator.

To use automated mesh spacing, you add the three ODEs (17.5.5) and (17.5.7) to your set of equations, i.e., to the array `y(j,k)`. Now x becomes a dependent variable! Q and ψ also become new dependent variables. Normally, evaluating ϕ requires little extra work since it will be composed from pieces of the g's that exist anyway. The automated procedure allows one to investigate quickly how the numerical results might be affected by various strategies for mesh spacing. (A special case occurs if the desired mesh spacing function Q can be found analytically, i.e., dQ/dx is directly integrable. Then, you need to add only two equations, those in 17.5.5, and two new variables x, ψ.)

As an example of a typical strategy for implementing this scheme, consider a system with one dependent variable $y(x)$. We could set

$$dQ = \frac{dx}{\Delta} + \frac{|d\ln y|}{\delta} \tag{17.5.8}$$

or

$$\phi(x) = \frac{dQ}{dx} = \frac{1}{\Delta} + \left|\frac{dy/dx}{y\delta}\right| \tag{17.5.9}$$

where Δ and δ are constants that we choose. The first term would give a uniform spacing in x if it alone were present. The second term forces more grid points to be used where y is changing rapidly. The constants act to make every logarithmic change in y of an amount δ about as "attractive" to a grid point as a change in x of amount Δ. You adjust the constants according to taste. Other strategies are possible, such as a logarithmic spacing in x, replacing dx in the first term with $d\ln x$.

CITED REFERENCES AND FURTHER READING:

Eggleton, P. P. 1971, *Monthly Notices of the Royal Astronomical Society*, vol. 151, pp. 351–364.

Kippenhan, R., Weigert, A., and Hofmeister, E. 1968, in *Methods in Computational Physics*, vol. 7 (New York: Academic Press), pp. 129ff.

17.6 Handling Internal Boundary Conditions or Singular Points

Singularities can occur in the interiors of two point boundary value problems. Typically, there is a point x_s at which a derivative must be evaluated by an expression of the form

$$S(x_s) = \frac{N(x_s, \mathbf{y})}{D(x_s, \mathbf{y})} \tag{17.6.1}$$

where the denominator $D(x_s, \mathbf{y}) = 0$. In physical problems with finite answers, singular points usually come with their own cure: Where $D \to 0$, there the physical solution $\mathbf{y}$ must be such as to make $N \to 0$ simultaneously, in such a way that the ratio takes on a meaningful value. This constraint on the solution $\mathbf{y}$ is often called a *regularity condition*. The condition that $D(x_s, \mathbf{y})$ satisfy some special constraint at x_s is entirely analogous to an extra boundary condition, an algebraic relation among the dependent variables that must hold at a point.

We discussed a related situation earlier, in §17.2, when we described the "fitting point method" to handle the task of integrating equations with singular behavior at the boundaries. In those problems you are unable to integrate from one side of the domain to the other.