Chapter 13

Partial Differential Equations (PDE's)

1 Scope of the Chapter

This chapter is concerned with the numerical solution of partial differential equations (PDEs). The definition of a partial differential equation problem includes not only the equation itself but also the domain of interest and appropriate subsidiary conditions. Indeed, partial differential equations are usually classified as *elliptic*, *hyperbolic* or *parabolic* according to the form of the equation and the form of the subsidiary conditions which must be assigned to produce a well-posed problem. Modules provided in this chapter are for the three-dimensional Helmholtz equation (which includes the Laplace and Poisson equations as special cases), the two-dimensional elliptic PDE and the one-dimensional parabolic PDE. This chapter does not currently include any modules for hyperbolic problems.

Modules for more general steady and time-dependent problems are planned for future releases of NAG *fl*90.

2 Available Modules

Module 13.1: `nag_pde_helm` — **Helmholtz equations**

This module contains a procedure for solving the Helmholtz equation in three dimensions.

Module 13.2: `nag_pde_ell_mg` — **Multigrid solution of elliptic partial differential equations**

This module contains *two* procedures for generation and multigrid solution of seven-diagonal systems of linear equations which arise from discretization of two-dimensional elliptic PDEs.

Module 13.3: `nag_pde_parab_1d` — **Parabolic partial differential equations in one space variable**

This module contains *four* procedures for the solution of one-dimensional parabolic PDEs, with optional scope for coupled ordinary differential equations. The module also provides procedures for the interpolation of the solution.

3 Background

3.1 Helmholtz Equation

The three-dimensional elliptic equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + \lambda u = f(x, y, z), \qquad (1)$$

where λ is a real constant, is generally referred to as *Helmholtz equation*, or in the case $\lambda > 0$ as the *reduced wave equation*. The problem is usually posed in a region V bounded by a closed surface S. Typical boundary conditions include:

Dirichlet: solution u given on S;

Neumann: derivative $\frac{\partial u}{\partial n}$ given on S, where n is the outward unit normal to S.

In practice, Dirichlet conditions will often be prescribed on part of the boundary and Neumann conditions on the remainder. Periodic boundary conditions are also common for certain simple regions V.

For the case $\lambda < 0$, a straightforward application of the Green's identity

$$\int_V (u\nabla^2 u + \text{grad}^2 u)\text{d}V = \int_S u\frac{\partial u}{\partial n}\text{d}S$$

can be used to prove uniqueness of the solution of (1) with any combination of Dirichlet and Neumann boundary conditions in a bounded region V. For $\lambda = 0$ the solution can be proved to be unique provided a Dirichlet condition is given for at least one point on S; the solution of the *pure* Neumann problem is unique only to within an arbitrary additive constant.

For the reduced wave equation ($\lambda > 0$) there are no corresponding uniqueness theorems for bounded regions. The equation commonly arises in the theory of acoustic and electromagnetic scattering, when solutions of the form $u(x,y,z)e^{i\omega t}$ are sought for the wave equation

$$c^2\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right)-\frac{\partial^2\phi}{\partial t^2}=0.$$

This results in equation (1), where λ is given by $(\omega/c)^2$.

3.2 Elliptic Equation

A two-dimension second order linear partial differential equation is of the form

$$\alpha(x,y)\frac{\partial^2 U}{\partial x^2}+\beta(x,y)\frac{\partial^2 U}{\partial x\partial y}+\gamma(x,y)\frac{\partial^2 U}{\partial y^2}+\delta(x,y)\frac{\partial U}{\partial x}+\epsilon(x,y)\frac{\partial U}{\partial y}+\phi(x,y)U=\psi(x,y) \tag{2}$$

subject to boundary conditions of the form

$$a(x,y)U+b(x,y)\frac{\partial U}{\partial n}=c(x,y),$$

where $\frac{\partial U}{\partial n}$ denotes the outward pointing normal derivative on the boundary. Equation (2) is said to be elliptic if

$$4\alpha(x,y)\gamma(x,y)\geq\beta^2(x,y)$$

for all points in the domain where the equation (2) is defined.

Under the ellipticity assumption and for regular data, uniqueness of the solution of (2) can be proved via Green's identity.

3.3 Parabolic Equation

A one-dimensional parabolic partial differential equation is of the form

$$\sum_{j=1}^{n}P_{i,j}(x,t,U,\frac{\partial U}{\partial x},V)\frac{\partial U_j}{\partial t}+Q_i(x,t,U,\frac{\partial U}{\partial x},V,\dot{V})=x^{-m}\frac{\partial}{\partial x}(x^mR_i(x,t,U,\frac{\partial U}{\partial x},V)), \tag{3}$$

where $i=1,2,\ldots,n$, $a\leq x\leq b$ and $t\geq t_0$. The parameter m allows the user to handle different coordinate systems easily (Cartesian, cylindrical polars and spherical polars). Coupled differential algebraic systems can also optionally be included. This extended functionality allows for the solution of more complex and more general problems, e.g., periodic boundary conditions and integro-differential equations.