TWO MODIFICATIONS TO THE SOFTWARE INTERFACE PACKAGE FOR NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

by

RICHARD LEE MORSE

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Approved by:

Richard F. Hunsinger
Major Professor

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INTRODUCTION

PDEONE is a software interface for nonlinear partial differential equations jointly developed by Dr. Richard F. Sincovec, Kansas State University and Dr. Niel K. Madsen, Lawrence Livermore Laboratory (1). It is a piece of computer software which can serve as an interface which will allow many of the recent significant developments in the field of ODE's to be applied directly to the numerical solution of PDE's.

The method being implemented by this software package is the so-called numerical method of lines (2). Roughly speaking, the method of lines can be described as follows; if one has a time dependent PDE and discretizes the spatial variables, an approximating system of ordinary differential equations results. To solve the resulting equations one uses ODE methods and obtains numerical approximations of the original PDE.

The software package is designed with user convenience as a goal. To use this package the user simply defines his system of PDE's and supplies a spatial mesh to be used for the discretization of the problem in PDEONE. Then an ODE integrator with its built-in error and stability controls may be used (3, 4, 5).

This report will discuss two recent changes to the PDE interface package developed by Sincovec and Madsen (1). The first change being the modification of the routine PDEONE to handle systems of PDE's that are coupled in the time derivative terms. Next is the addition of the routine PDEJAC to efficiently generate the Jacobian matrix needed when stiff methods are used to solve ordinary differential equations.

Chapter 2

MODIFICATION OF PDEONE AND ADDITION OF USER SUPPLIED AMATRX ROUTINE TO HANDLE COUPLED SYSTEMS OF NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

2.1. Definition of Problem

Partial differential equations may have an unlimited number of mathematical structures. Following is the structure chosen by Dr. Richard Sincovec and Dr. Niel Madsen to solve a wide class of realistic problems (1):

Let NPDE denote the number of PDE's on the interval $[a, b]$ and let

$$(2.1.1)\qquad \sum_{j=1}^{NPDE} a_{k,j} \frac{\partial u_j}{\partial t} = f_k\Bigg(t, x, u_1, u_2, \ldots, u_{NPDE}, \frac{\partial u_1}{\partial x}, \frac{\partial u_2}{\partial x}, \ldots, \frac{\partial u_{NPDE}}{\partial x}, \frac{1}{x^c}\frac{\partial}{\partial x}\left(x^c D_{k,1} \frac{\partial u_1}{\partial x}\right), \frac{1}{x^c}\frac{\partial}{\partial x}\left(x^c D_{k,2} \frac{\partial u_2}{\partial x}\right), \ldots, \frac{1}{x^c}\frac{\partial}{\partial x}\left(x^c D_{k,NPDE} \frac{\partial u_{NPDE}}{\partial x}\right)\Bigg),$$

$$a < x < b\ , \quad t > t_o\ , \quad k = 1,2,\ldots,NPDE\ ,$$

denote the coupled systems of PDE's with boundary conditions,

$$(2.1.2)\qquad \alpha_k u_k + \beta_k \frac{\partial u_k}{\partial x} = \gamma_k \quad \text{at } x = a \text{ and } b, \quad t > t_o\ , \quad k = 1,2,\ldots,NPDE,$$

and initial conditions,

(2.1.3) $u_k(t_o,x) = \phi_k(x)$, $a \leq x \geq b$, $k = 1,2,\ldots,NPDE$.

If $\beta_k \neq 0$ then α_k, β_k and γ_k may be functions of t, x, and $\vec{u} \equiv (u_1,u_2,\ldots,u_{NPDE})$. but only functions of x and t otherwise; $D_{k,j}$ and $a_{k,j}$ $(k,j = 1,2,\ldots,NPDE)$ are functions of x, t, and $\vec{u}$; and c is 0, 1, or 2 depending on whether the problem is in Cartesian, cylindrical, or spherical coordinates, respectively.

By assuming that all the coefficient functions, α_k, β_k, γ_k, $D_{k,j}$, $a_{k,j}$, f_k, and ϕ_k, are at least piecewise continuous functions of all their respective variables; problems with physical discontinuities can be defined using the software interface.

Boundary conditions for PDE's are often classified into three types: Dirichlet ($\beta_k = 0$), Neumann ($\alpha_k = 0$), or mixed ($\alpha_k \neq 0$, $\beta_k \neq 0$). The boundary condition may change with respect to time, as well as from equation to equation. Also the initial condition is not required to satisfy the boundary conditions as x approaches either a or b.

The $(a_{k,j})$ $(k,j = 1,2,\ldots,NPDE)$ matrix allows for a coupling of the time derivative of systems of parabolic PDE's and/or hyperbolic PDE's. The coupling may be nonlinear as each $a_{k,j}$ may be a function of $\vec{u}$.

Note that problem (2.1.1) - (2.1.3) is completely defined if one specifies the interval, $[a, b]$; the initial time, t_o; the vector functions $f = (f_k)$, $\alpha = (\alpha_k)$, $\beta = (\beta_k)$, $\gamma = (\gamma_k)$ $(k = 1,2,\ldots,NPDE)$; the matrix functions $D = (D_{k,j})$, $A = (a_{k,j})$ $(k,j = 1,2,\ldots,NPDE)$; and the initial conditions $\phi_k(x)$, $k = 1,2,\ldots,NPDE$. With the software interface