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A robust false transient method of lines for elliptic partial differential equations

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HIGHLIGHTS

- ▸ A more robust method of solving elliptic PDEs is developed and discussed.
- ▸ A comparison of the false transient and the proposed method is explained.
- ▸ Several engineering/transport examples are considered.
- ▸ Linear solutions are described using matrix algebra and matrix exponentials.
- ▸ Nonlinear problems are solved, including unstable steady state solutions.

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ABSTRACT

Elliptic partial differential equations (PDEs) are frequently used to model a variety of engineering phenomena, such as steady-state heat conduction in a solid, or reaction-diffusion type problems. However, computing a solution can sometimes be difficult or inefficient using standard solvers. Techniques have been developed, including the method of lines (Schiesser, 1991), which can solve parabolic PDEs using well developed numerical solvers, but are not directly applicable to elliptic PDEs. The method of false transients overcomes this limitation by arbitrarily introducing a pseudo time derivative to modify the elliptic PDE to a parabolic PDE. However, this technique diverges for certain problems, such as when the solution is an unstable equilibrium point. A Jacobian-based perturbation approach is presented as an alternative for situations when the standard false-transient method fails. Two examples are shown to demonstrate the robustness of the proposed method over the false transient method.

1. Introduction

A wide variety of partial differential equations arise when describing engineering systems. For examples, variations on Laplace's equation arise frequently in problems of transport phenomena (Bird et al., 2006). In order to solve such a wide range of problems, several numerical methods have been developed to solve partial differential equations. The choice of method is dependent on the desired accuracy, as well as concerns about the stability and robustness of the system, while maintaining computational efficiency. Furthermore, these characteristics are dependent on the form of the partial differential equation to be solved, i.e. elliptic, parabolic, or hyperbolic. For parabolic equations such as the heat equation, several numerical methods exist that can be used to find a solution (Dehghan, 2006). For example, the method of lines is one such efficient routine in which the spatial dimensions are discretized using any of a number of techniques, such as finite difference, finite element, finite volume, or collocation methods (Berzins et al., 1989; Constantinides and Mostoufi, 1999; Cutlip and Shacham, 1998; Dehghan, 2006; Sadiku and Obiozor, 2000; Schiesser, 1991, 1994a, 1994b; Schiesser and Griffiths, 2009; Schiesser and Silebi, 1997; Taylor, 1999). This converts the partial differential equation (PDE) to an initial value problem (IVP) system of ordinary differential equations (ODE) or differential algebraic equations (DAEs). Software packages have been developed to specifically solve problems using the method of lines (Berzins et al., 1989). Alternatively, the resulting DAEs can be solved using standard efficient time integrators (Cash, 2005), including FORTRAN solvers such as DASKR or DASSL or in a computer algebra system such as Matlab (MathWorks, 2012)

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(dsolve), Maple (Maplesoft, 2012) (dsolve), Mathematica (Wolfram, 2012) (ndsolve), etc. The versatility and simplicity of the method of lines has led to its use in a wide range of engineering applications, including fracture problems (Bao et al., 2001), heat transfer (Labuzov and Potapov, 1985), solving Navier-Stokes equations (Erşahin et al., 2004) and electromagnetics (Pregla and Vietzorreck, 1995; Sadiku and Obiozor, 2000). Furthermore, Pregla and Cietzorreck used the method of lines in conjunction with the source method to handle inhomogeneous boundary conditions and discontinuities in microstrip lines and antennas (Pregla and Vietzorreck, 1995).

The solution of elliptic partial differential equations, such as Laplace's equation, is more difficult because there is not a simple way to convert the equations to an initial value problem to allow the use of the method of lines. A Newton–Raphson method, or another approach to solving a system of nonlinear equations, can be used if the system of algebraic equations resulting from the discretization is sufficiently well behaved and a reasonable initial guess is available. A semianalytical method of lines, valid for linear elliptic PDEs and certain quasilinear elliptic PDEs has been presented previously (Subramanian and White, 2004). However, a more popular choice has been the method of false transients, partially due to its ability to handle some nonlinear problems, and ease of implementation. In the false transient method the variables are discretized in the spatial or boundary value independent variables (x and y), and a pseudo time derivative is arbitrarily added to the problem statement (Mallinson and de Vahl Davis, 1973; Schiesser, 1991, 1994a; Schiesser and Griffiths, 2009; Schiesser and Silebi, 1997; White and Subramanian, 2010). The addition of this fictitious time derivative converts the elliptic PDE to a parabolic PDE and allows the solution to be determined by marching in pseudo time to a steady state condition. By doing this, the efficient IVP/DAE solvers can be applied in a matter analogous to the method of lines (Schiesser and Griffiths, 2009).

Like the method of lines, the method of false transients is used to solve a variety of engineering problems. For example, Xu, et al., used the false transient method to describe the concentration and temperature profiles of catalyst particles (Xu, 1993). This approach has also been used to numerically solve for three dimensional velocity profiles by solving the Navier-Stokes equation (Lo et al., 2005), as well as solving the convective diffusion equation for axial-diffusion problems in laminar-flow reactors (Nauman and Nigam, 2004). Other researchers have used the false transient method for analyzing mass transfer in porous media (Singh et al., 1999) or laminar film boiling (Srinivasan and Rao, 1984).

However, as shown in this paper, the system of ODE/DAEs resulting from the use of the false transient method can be unstable and may not converge to the desired (or any) solution. This problem can sometimes be rectified by modifying the form of the equations or boundary conditions using intuition and trial and error. In other cases, the system cannot be made to converge, regardless of how the problem is presented. An alternative, Jacobian-based perturbation approach is proposed in this paper, which is robust and does not suffer from the same stability issues which befall the false transient method. A similar approach has been used as a superior method for the initialization of the algebraic variables in systems of DAEs (Methekar et al., 2011).

2. Generic formulation of the false transient method and the perturbation method

Consider a general PDE of the form

$$D(\phi(\mathbf{x}))=0 \tag{1}$$

where $\phi(\mathbf{x})$ is the (continuous) dependent variable of interest, $\mathbf{x}$ is the vector of independent variables, and D is a generic linear differential operator with the form:

$$D=\sum_i\sum_j a_{ij}\frac{\partial^i}{\partial x_j^i} \tag{2}$$

Eq. (1) can be discretized using any of a number of techniques, such as finite difference, finite element, finite volume, or collocation, among others. This results in a system of algebraic equations of the form

$$\mathbf{g}(\mathbf{\Phi})=0 \tag{3}$$

where $\mathbf{\Phi}$ is the vector of the discretized dependent variables. In linear systems, Eq. (3) can be solved directly, though this is not the case in highly nonlinear problems. Both the method of false transients and the perturbation method introduce a pseudo time variable, τ, such that Eq. (3) is represented as:

$$\mathbf{g}(\mathbf{\Phi}(\tau))=0 \tag{4}$$

when using the method of false transients, this is done by introducing a first order pseudo-time derivative into Eq. (4) such that it becomes:

$$\mathbf{g}(\mathbf{\Phi}(\tau))=\frac{d\mathbf{\Phi}}{d\tau} \tag{5}$$

This allows the use of efficient time adaptive ODE solvers to be used. In order for convergence to occur, the right hand side must go to zero as τ goes to infinity:

$$\lim_{\tau\to\infty}\frac{d\mathbf{\Phi}}{d\tau}=0 \tag{6}$$

This reduces Eq. (5) to Eq. (3) and ensures that the original problem is satisfied. However, the method of false transients can fail if Eq. (6) does not hold, as can occur in an unstable system. Therefore, an alternative perturbation approach is shown here. A small perturbation parameter, ϵ, can be applied in time to Eq. (4) such that

$$\lim_{\epsilon\to 0}\mathbf{g}(\mathbf{\Phi}(\tau+\epsilon))=0 \tag{7}$$

Eq. (7) can be expanded using a Taylor series to give

$$\mathbf{g}(\mathbf{\Phi}(\tau))+\epsilon\frac{d\mathbf{g}(\mathbf{\Phi}(\tau))}{d\tau}+O(\epsilon^2)=0 \tag{8}$$

Assuming that ϵ is sufficiently small that the higher order terms can be neglected, Eq. (8) reduces to

$$\mathbf{g}(\mathbf{\Phi}(\tau))+\epsilon\frac{d\mathbf{g}(\mathbf{\Phi}(\tau))}{d\tau}=0 \tag{9}$$

The total derivative in Eq. (9) can be rewritten using the chain rule with partial derivatives

$$\mathbf{g}(\mathbf{\Phi}(\tau))+\epsilon\left[\frac{\partial\mathbf{g}}{\partial\mathbf{\Phi}}\frac{\partial\mathbf{\Phi}}{\partial\tau}+\frac{\partial\mathbf{g}}{\partial\tau}\right]=0 \tag{10}$$

Noting that $\partial\mathbf{g}/\partial\mathbf{\Phi}=\mathbf{J}$, where $\mathbf{J}$ is the Jacobian representing the algebraic system. Also, note that from Eq. (3), $\mathbf{g}$ is not a function of pseudo time directly; only indirectly through the dependent variables, $\mathbf{\Phi}$, are functions of pseudo time. Therefore, $\partial\mathbf{g}/\partial\tau=0$ above and Eq. (10), can be rearranged to give

$$\mathbf{g}(\mathbf{\Phi}(\tau))=-\epsilon\mathbf{J}\frac{\partial\mathbf{\Phi}}{\partial\tau} \tag{11}$$

Eq. (11) can be considered as an application of Davidenko's Method (Schiesser, 1994a). Note that the choice of ϵ is somewhat arbitrary, and must be chosen with consideration to the system. Ideally ϵ must be sufficiently small that the assumption that the higher order terms in Eq. (8) can be neglected is valid. Here, $\epsilon=10^{-3}$ is used throughout the remainder of this work. This choice is somewhat arbitrary as changing $\epsilon=10^{-3}$ by an order of