SOLUTION OF MODEL EQUATIONS

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Contents

Summary

Solving the models that are developed for a range of application areas in engineering and the sciences is a common activity and one that demands a wide range of computer-based numerical techniques. Few problems are amenable to analytic solution and hence numerical computation dominates simulation systems.

There is a wide range of methods required, since the models developed cover steady state and dynamic systems and extend from simple 1 dimensional applications to complex 3D geometries.

This chapter reviews the principal methods available to modelers to solve such problems.

1. Introduction

Process modeling as a basis for design, optimization and control leads to sets of equations that range in their complexity. This complexity can range from simple linear equations that can characterize component mass balances to complex nonlinear and time varying equation systems that characterize process units, whole integrated processes or natural systems.

Few, if any real system models can be solved using analytical methods. This means that there is significant reliance on computer-based numerical methods that approximate the true solution to a specified degree of accuracy. The methods used for specific problems rely heavily on the underlying characteristics of the model equations and hence appropriate choice of the solution methods is essential for accuracy, robustness and efficiency reasons.

In the following sections a range of numerical methods are discussed that cover a wide spectrum of model equation types. These numerical methods provide the "toolbox" of modern simulation systems. Many numerical methods have been developed since the inception of computer based approaches. This chapter is selective in its choice of key approaches to the effective solution of process models. This area of modeling is vast in its scope and application.

2. Classes of Problems and Computer Methods

There are numerous classes of models that can are developed and require computer solutions. Figure 1 shows a hierarchy of equation or model types that need to often be considered in modern application. In many instances the higher level equation types and their solution methods are required to solve more complex problems at a lower level in the hierarchy. Hence the higher level techniques are vitally important in addressing the robust and efficient solution of lower level systems.

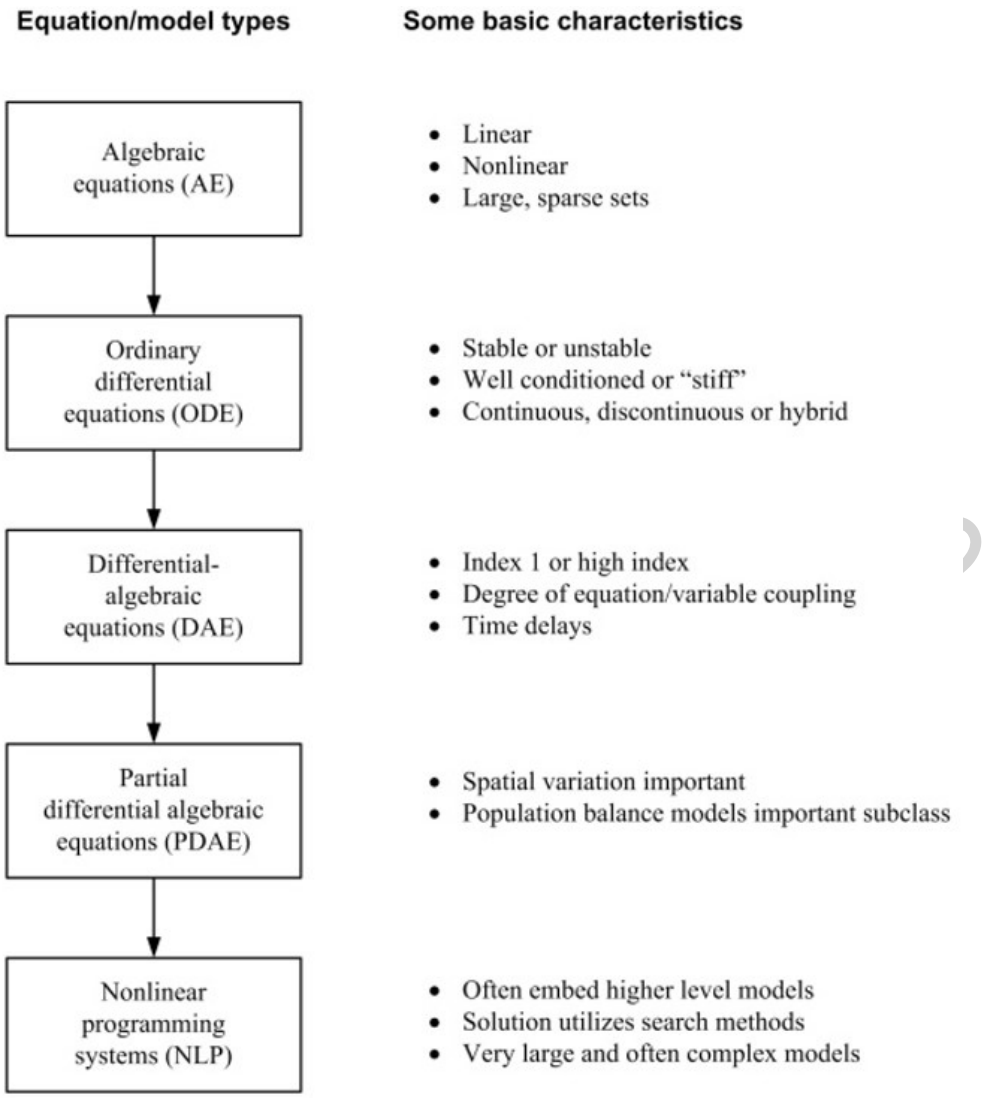

Figure 1: A hierarchy of model types, equation systems and characteristics

3. Algebraic Equation Systems

In process engineering, algebraic equations arise from many areas. These include steady state models of process systems and individual unit operations. They also form the basis of solving more complex equation systems such as time varying models of process systems. These are in the form of ordinary and partial differential equations. Without the capability of solving algebraic systems, solutions for these more complex problems are virtually impossible. There are a number of methods that can be employed including

- Iterative methods for single and multiple equation systems
- Direct methods for linear systems
- Gradient methods

The problems that arise are single equations in the form of:

$$f(x) = 0 \tag{1}$$

where f is a function of a single unknown variable x. An equation of the form $x^3 - 7x - 6 = 0$ is such an equation.

For multivariable equations involving *n* variables the form is:

$$\begin{aligned} f_1(x_1, x_2, \ldots, x_n) &= 0 \\ &\vdots \\ f_n(x_1, x_2, \ldots, x_n) &= 0 \end{aligned} \tag{2}$$

or in vector form as

$$\mathbf{f(x) = 0} \tag{3}$$

A set of equations of the form

$$\begin{aligned} x_1^2 + 2x_2 - 2 &= 0 \\ 2x_1 - 3x_2 + 5 &= 0 \end{aligned} \tag{4}$$

represents such a multivariable algebraic system in two variables, x_1 and x_2.

3.1 Iterative Methods

To solve non-linear equations there are various iterative solution methods. An iterative method essentially consists of 3 basic parts as shown in Figure 2:

a) A set of initial estimates for the solution
b) A formula for updating the approximate solution
c) A procedure for stopping the updating process.

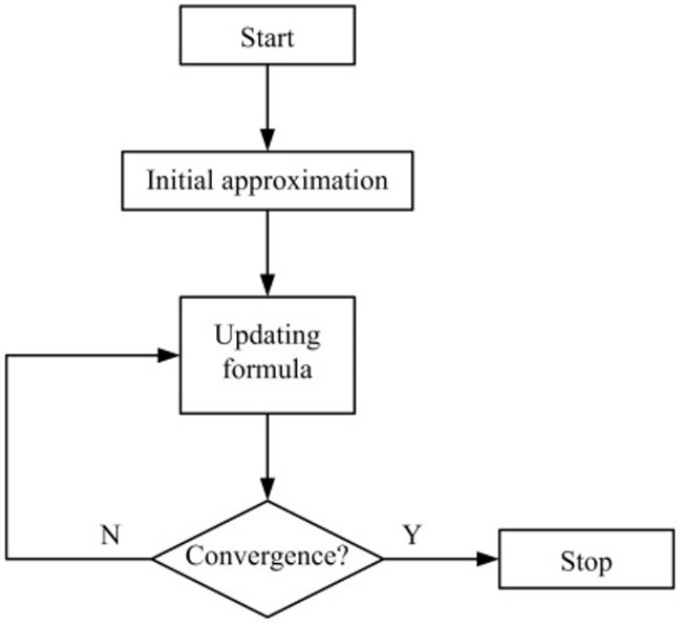

Figure 2: An iterative solution algorithm

3.1.1. One-point iteration methods

These methods only use the last computed point in obtaining the next estimate.

For the solution of $f(x)=0$, we compute a sequence $\left\{x^{(k)}\right\}$; $k=0,\ 1,\ \ldots$ which if successful converges to the solution x^*. The first approximation $x^{(0)}$ is provided. Further approximations are given by:

$$x^{(k+1)}=\phi(x^{(k)}) \qquad k=0,\ 1,\ \ldots \tag{5}$$

where $x=\phi(x)$ has the same solution as $f(x)=0$, and thus

$$x^*=\phi(x^*) \tag{6}$$

Various iteration functions ϕ can be established.

The simplest is the successive substitution or functional iterative method, where the original single equation is reformulated to provide the form given in Eq. (5). The equation $f(x)=x^3-7x-6=0$ can be easily rewritten as $\phi(x)=(x^3-6)/7=x$ and used as an iteration function. The Wegstein method is a modified method that improves convergence rate and provides an "accelerated" estimate $\hat{x}$. It can be written as:

$$\hat{x}=x^{(k)}+\frac{\left(x^{(k+1)}-x^{(k)}\right)}{(1-s)}$$

with the parameter s given by $\frac{\phi\left(x^{k+1}\right)-\phi\left(x^{k}\right)}{x^{k+1}-x^{k}}$. This technique can be extended to the solution of multivariable systems.

3.1.2. Interpolation methods for algebraic equations

Interpolation is the basis for some of the most powerful and useful solution methods for algebraic systems. The basis is the approximation of the original function by a polynomial based on the function value f and its derivatives $\frac{d^r f}{dt^r}$ or f^{r} at a particular value x. The polynomial is then solved for an estimate $x^{(k)}$, $k=1,\ 2,\ \ldots$ for the solution x^*.

The simplest approach is given by interpolating $f(x)$ and $f^1(x)$ at $x=x^{(k)}$ using the linear polynomial

$$P(x) = f(x^{(k)}) + f^1(x^{(k)})(x - x^{(k)}) \qquad (7)$$

Forcing $P(x) = 0$ and rearranging, gives a series of linear interpolations for the approximate solutions using the last solution value:

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f^1(x^{(k)})}, \quad k = 0,\ 1,\ 2,\ \ldots \qquad (8)$$

This is commonly called Newton's method and the sequence of iterates is illustrated in Figure 2.

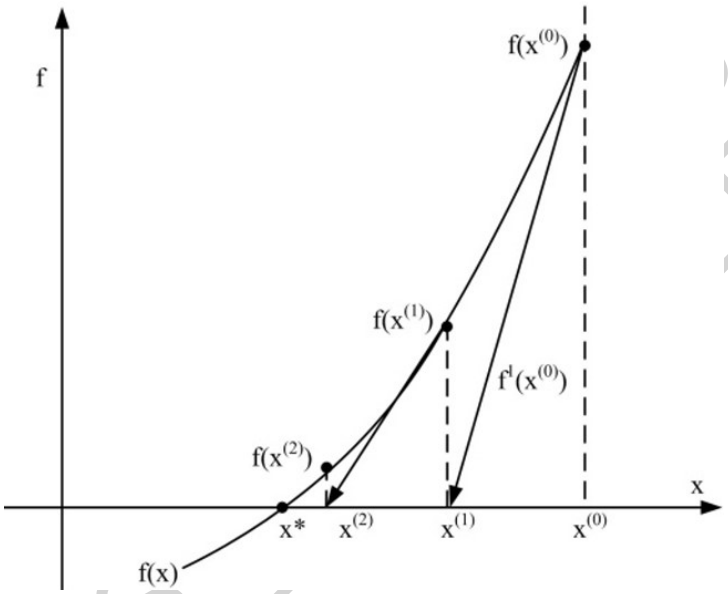

Figure 3: Newton's method for one variable

Extensions to multivariable equation systems are straightforward and lead to a large set of linear equations that are solved at each iteration. The n-dimensional Newton method is given by

$$\bar{J}^{(k)}\bar{\delta}^{(k)} = -\bar{f}^{(k)} \quad k = 0,\ 1,\ \ldots \qquad (9)$$

where $\bar{x}^{(k+1)} = \bar{x}^{(k)} + \bar{\delta}^{(k)}$

and $\bar{J}^{(k)}$ is the Jacobian matrix $\left(\frac{\partial f_i}{\partial x_j}\right)$ evaluated at $\bar{x}^{(k)}$.

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Biographical Sketch

Ian Cameron is Professor and head of Chemical Engineering at The University of Queensland, Australia where he is director of the Particle and Systems Design Centre (PSDC). He is a graduate of the University of NSW, holds a MSChE from the University of Washington and a PhD in process systems engineering from Imperial College, London.

He researches in areas of system dynamics, advanced modeling environments and risk management. His PhD was in the area of numerical methods for simulation of process systems represented by large scale differential-algebraic systems. He has continued to work on new methods for efficient solution of complex modeling problems, especially in the area of particulate systems. He has consulted widely in process systems engineering, modeling and risk management within Australia and overseas including Argentina, Turkey, Thailand and Denmark. He is the author of a widely used book on Process Modelling and Model Analysis as well as a book on Process Systems Risk Management, published by Elsevier.

He has been very active in many pedagogical developments in Chemical Engineering curriculum and teaching. He has received numerous awards for outstanding teaching and curriculum development including the 2003 Australian Prime Minister's Prize for University Teacher of the Year. He is also the recipient of the Engineers Australia A.J. Brodie Medal for excellence in Chemical Engineering. He is currently a Senior Fellow with the Carrick Institute, Australia's peak Higher Education institute.