Solutions to ODEs and PDEs: Numerical analysis using R

(Cambridge University Press, ISBN: 978-1-107-11561-3)

Graham W. Griffiths
City University, UK.

Chapter Abstracts

Chapter 1
ODE integration methods

The solution of *ordinary differential equations* (ODEs) is intrinsically bound up with the solution of *partial differential equations* (PDEs). In this chapter the basic integration methods are introduced, covering: Euler, Runge-Kutta, variable step, extrapolation, BDFs, NDFs, and Adams. Various test examples for the different integration methods are provided along with annotated code.

The *Newton* and *Levenberg-Marquardt* convergence methods are introduced with practical examples of use in *implicit* numerical integration, together with the corresponding computer code.

A discussions relating to *truncation error* and *verification of integration order* are presented with examples.

The chapter concludes with a brief discussion on *stiffness*.

All the computer code discussed in the text is available for download.

Keywords: Ordinary differential equations; ODEs; partial differential equations; PDEs; numerical integration; Euler; Runge-Kutta; variable step; extrapolation; BDFs; NDFs; Adams; Newton convergence; Levenberg-Marquardt convergence; truncation error; verification of integration order; stiffness; R language; Maple.

Chapter 2
Stability analysis of ODE integrators

To solve partial differential equations numerically, it is essential that the numerical integrator is stable. In this chapter we explore some of the theory and practical application of ODE integrator *stability analysis*. We start with a discussion on global order of accuracy, A-stable and zero-stable definitions along with the Dahlquist barrier theorems.

Using the Dahlquist test problem, we investigate the stability of various integration methods including: Runge-Kutta, variable step, BDfs, NDFs and Adams. For each method the stability regions are plotted in the complex plane to show the associated stability margins

All the associated computer code is presented and available for download.

Keywords: ODEs; Integrator stability; A-stable; zero-stable; global order of accuracy; Dahlquist barrier theorems; Dahlquist test problem; Runge-Kutta; variable step; BDFs; NDFs; Adams; R language; Maple.

Chapter 3
Solution of PDEs

The solution of PDEs is a wide subject and we confine our discussion to *initial value* and/or *boundary value* problems. These are also known as Cauchy problems. The basic concepts relating to PDEs are discussed along with *initial conditions* (ICs), the various types of *boundary condition* (BC) and PDE *classification*.

The general ideas relating to discretization methods, mesh grid, stencils, upwinding and the Courant-Friedrichs-Lewy number are introduced. This leads onto a discussion on *semi-discrete* schemes based on the *Method of Lines* (MOL), one of the major numerical schemes for solving PDEs. A good selection of 1D and 2D example MOL problems are solved. These examples, in both Cartesian and polar coordinates, have been chosen to bring out the main ideas and to show the variety of problems that can be solved using this method.

We then present a brief discussion on the following fully discrete methods: FTBS, implicit FTBS, FTCS, implicit BTCS, leapfrog, Beam-Warming, Lax-Friedrichs, Lax-Wendroff. Solutions are compared for the different methods applied to sample problems. The ideas behind finite volume methods are presented in preparation for their use in high resolution schemes which are discussed subsequently in Chapter 6.

Then follows a discussion on the interpretation of results including: verification validation and truncation errors.

Finally, two appendices are included; one giving *coefficients* for various types and order of *derivative matrices*, and the other a description of the *derivative matrix library* supplied as a download for this book.

All the associated computer code is presented and available for download.

Keywords: PDEs; ICs; BCs; Cauchy problem; discretization methods; mesh grid; stencils; upwinding; Courant-Friedrichs-Lewy number; MOL; Cartesian coordinates; polar coordinates; fully discrete methods; FTBS; implicit FTBS; FTCS; implicit BTCS; leapfrog; Beam-Warming; Lax-Friedrichs; Lax-Wendroff; finite difference; finite volume; truncation error; verification of integration order; stiffness; R language; Maple.

Chapter 4
PDE stability analysis

In selecting a scheme for the numerical solution of PDEs the analyst will generally seek to employ a method that will provide sufficient accuracy for a reasonable computational effort. One of the key requirements to achieving this goal is that the scheme is stable. This chapter discusses the concept of a system being *well posed* and ways of using this idea to investigate system stability.

The *matrix stability method* is outlined and detailed stability calculations included for semi-discrete PDE schemes. A number of examples are included that analyze PDEs and the results are presented in graphical form.

The *von Neumann* stability method is discussed with the fundamental ideas developed using Fourier transforms. Various semi-discrete and fully-discrete PDE systems are analyzed with results presented graphically.

All the associated computer code is presented and available for download.

Keywords: PDEs; stability; matrix stability method; von Neumann stability method; forward Euler; backwards Euler; BTCS; Crank-Nicholson; FTBS; implicit FTBS; FTCS; Beam-Warming; Lax-Friedrichs; Lax-Wendroff; leapfrog; first order upwind; second order upwind; advection; diffusion; convection-diffusion; heat equation; Fourier transforms; R language; Maple.

Chapter 5
Dissipation and dispersion

The numerical solution of PDEs is always subject to dissipation and/or dispersion, even in high resolution schemes. The idea of the *dispersion relation* is introduced and its relationship to *wave number* and *wave frequency*.

The accuracy of numerical schemes is discussed in relation to *numerical amplification* and *exact amplification* factors. Also, how these factors can be used to provide an indication of phase (dispersion) and amplitude (dissipation) errors.

The chapter concludes with a discussion on phase and group velocities, followed by a number of examples of calculating dissipation and dispersion errors.

All the associated computer code is presented and available for download.

Keywords: PDEs; dissipation; dispersion; dispersion relation; accuracy; numerical amplification; exact amplification; phase error; amplitude error; wave number; wave frequency; phase velocity; group velocity; R language; Maple.

Chapter 6
High resolution schemes

The numerical solution of PDEs is always subject to dissipation and/or dispersion, as discussed in Chapter 5, and high resolution schemes seek to minimize these effects. They are generally used to solve evolution problems where the solution exhibits *shocks*, *discontinuities* or *steep gradients*. This chapter introduces the *Riemann Problem* and *Godunov's method* of providing an approximate solution. A discussion follows on the principle of *Total Variation Diminishing* (TVD) and how *Godunov's order barrier* theorem places constraints on *monotonic* PDE solution methods. An introduction is then provided to two major methods that are employed widely to solve these types of problem. The first being the *flux limiter* method, where fifteen different flux limiter functions are presented. The second is the *Weighted Essentially Non-Oscilliatory* (WENO) method, where the associated weights and smoothness indicator calculations are presented. These methods are discussed within a *finite volume* and *method of lines* (MOL) framework based on the *Monotone Upstream-centered Schemes for Conservation Laws* (MUSCL) method, with the particular implementation being the *Kurganov and Tadmor central* scheme.

A variety of 1D and 2D problems are solved using the above methods and the results presented graphically. These include, advection, Burgers, Buckley-Everett, Euler equations, Sod's shock tube, Taylor-Sedov detonation, Woodward-Colella interacting blast wave and frontogenesis; all computationally demanding PDE evolution problems.

All the associated computer code is presented and available for download.

Keywords: PDEs; Riemann problem; shocks; discontinuities; steep gradients; Total variation diminishing; TVD; flux limiter, Weighted Essentially Non-Oscilliatory; WENO; monotonic; Monotone Upstream-centered Schemes for Conservation Laws; MUSCL; method of lines; MOL; advection, Burgers, Buckley-Everett, Euler equations, Sod's shock tube, Taylor-Sedov detonation, Woodward-Colella interacting blast wave and frontogenesis; R language; Maple.

Chapter 7
Meshless methods

Chapter 7 introduces the concept of *meshless methods* using *radial basis functions* (RBFs). This method is an important tool for the numerical analyst and is becoming very popular for solving otherwise difficult problems. One of the main advantages of meshless methods is that they can be used on irregular grids and therefore are applicable to problem geometries of any shape. The ideas are presented from at an introductory basic level, with examples showing how the method is used to interpolate *scattered data* and also for solving *partial differential equations.* For a number of examples, the results are compared to analytical solutions in order to demonstrate the accuracy of the results obtained. The *Halton sequence*, which produces pseudo random data, is introduced to demonstrate how the method readily handles irregular grids and/or scattered data. A number of *globally* and *compactly* supported RBFs are defined and their use illustrated with examples in 1D, 2D and 3D. This chapter also includes discussion on the use of *local* RBFs which allow the method to be used on very large problems. Local RBFs result in the system matrices becoming *sparse*, which facilitates the application of sparse matrix methods which are provided by the R package `Matrix`.

Keywords: PDEs; interpolation; meshless methods; radial basis funcrion; RBF; compactly supported RBF; CSRBF; local RBF; sparse matrix; scattered data; Halton sequence; irregular grids;

Chapter 8
Conservation Laws

This chapter introduces the concept of *conservation laws* in the context of evolutionary PDEs. Under the assumption of certain *decay conditions*, it is shown how *conserved quantities* can be identified for particular PDEs. It is then shown that conserved quantities can be used to calculate associated *constants of motion* or *invariants* . These constants of motion are very useful in numerical analysis as they can be used to provide an indication of calculation accuracy.

The ideas are discussed mainly in terms of the 1D Korteweg-de Vries (KdV) equation, where a number of the commonly known conservation laws applicable to this equation are derived. It is then shown using the *Miura* and *Gardener* transformations that, in fact, the KdV equation possesses an *infinity* of conservation laws. The discussion is extended to the 2D KdV equation, and then to the KdV equation with variable coefficients (vcKdV).

The chapter also includes conservation law discussions and example calculations in relation to the *nonlinear Schrödinger* (NLS) equation, and also to the *Boussinesq* equation.

All the associated computer code is presented and available for download.

Keywords: PDEs; conservation law; constants of motion; invariants; Korteweg-de Vries equation; KdV; vcKdV; Nonlinear Schrödinger equation; NLS; Boussinesq equation; Miura transformation; Gardener transformation; Maple.

Chapter9
Case study - Golf ball flight

The analysis of a golf ball in fight has been the subject of many theoretical investigations, with some of the earliest being published in the late 1890's. This case study provides an in-depth study of this subject with computer simulation results presented and compared to published performance data.

The various forces acting on a golf ball in flight are discussed, namely: the *drag*, *Magnus* and *gravitational* forces. The differential equations that describe the golf ball flight are then derived. The effects of *compression*, *spin*, *ambient conditions*, *wind*, *launch angle*, *bounce* and *roll* are all taken into account in the simulation calculations. The latest *coefficients* from the literature for drag and lift are used.

The results are presented graphically and compared with measured statistics for *club head speed*, *carry* and *trajectory height* for various classes of player using different golf clubs. The effect of *push, pull, fade, draw, slice* and *hook* shots are investigated, and the results discussed. The magnitude of *wind shear* at ground level is discussed and its effect on a static golf ball are investigated.

All the associated computer code is presented and available for download.

Keywords: ODEs; golf; golf ball; drag force; Magnus force; gravitational force; compression; spin; ambient conditions; wind; wind shear; launch angle; bounce; roll; drag coefficient; lift coefficient; club head speed; carry; trajectory height; push; pull; fade; draw; slice; hook; R language.

Chapter 10
Case study - Taylor-Sedov blast wave

In 1945 Sir Geoffrey Ingram Taylor was asked by the British MAUD (Military Application of Uranium Detonation) Committee to deduce information regarding the power of the first atomic *explosion* at the *Trinity site* in the *New Mexico desert*. He was able to estimate, using only public domain photographs of the blast, that the yield of the bomb was equivalent to between 16.8 and 23.7 kilo-tons of TNT. This case study discusses the subsequent seminal papers that Ingram published and traces the perceptive calculations that he made.

A systems analysis starts with a form of the *Euler equations* from which, using *similarity analysis*, certain important relationships are deduced. With the aid of a set of high speed photographs of the *detonation*, and assuming *spherical symmetry*, the underlying characteristics of the blast are gradually revealed by a sequence of thermodynamic calculations. The *thermodynamic gas laws* required to unravel this puzzle are discussed, along with *shock wave analysis* using the *Hugonoit-Rankine relations*. *Kinetic energy* and *heat energy* integrals are evaluated, leading to a full description of the *blast*. This includes blast wave speed, pressure, and temperature over time.

Closed-form *analytical solutions* to the problem, subsequently published by Sedov in 1959, are presented which provide a useful check on the accuracy of Ingram's numerical calculations. A similarity analysis is included, covering spherical, cylindrical and planar blast situations.

All the associated computer code is presented and available for download.

Keywords: ODEs; PDEs; Military Application of Uranium Detonation; MAUD; blast; explosion; detonation; Trinity site; Euler equations; similarity analysis; thermodynamic gas laws; shock wave analysis; Hugonoit-Rankine relations; blast wave speed; blast wave pressure; blast wave temperature; analytical solution; Taylor; Sedov; R language; Maple.

Chapter 11
Case study - Carbon cycle model

The *global carbon cycle* is analyzed together with a discussion on how increased concentrations in atmospheric carbon dioxide has implications for climate change. A simplified model is presented that considers four *fossil-fuel emission scenarios* based on the work of Caldeira and Wickett, and how the atmosphere and oceans respond. Air-ocean interaction is modeled using the wind-driven *gas-sea exchange* relationship due to Wanninkhof, with the subsequent dispersion of gaseous CO_2 into CO_2(aq), HCO_3^-, CO_3^{2-} and H^+ in accordance with *carbonate chemistry equilibria*. It is shown how an increasing concentration of positive hydrogen ions causes seawater acidity to rise, i.e. a fall in pH. *Seawater buffering* calculations are also introduced to demonstrate how the ability of the oceans to absorb atmospheric CO_2 reduces as seawater concentration of *dissolved inorganic carbon* increases. A discussion on *solar* and *terrestrial radiation* modeling is also included along with calculations that show how increasing CO_2 concentrations in the atmosphere can lead to increases in the Earth's surface temperature, i.e. the so-called *greenhouse effect*. All the associated computer code is presented and available for download.

Keywords: global carbon cycle; carbon dioxide; carbonate; bicarbonate; calcium carbonate; boron; carbonic acid; CO2; dissolved inorganic carbon; DIC; climate change; global warming; gas-sea exchange; solar radiation; terrestrial radiation; atmosphere; surface seawater; deep seawater; pH; fossil fuel; carbon emission scenarios; surface temperature; Revelle factor; .

Appendix
A Mathematical Aide-mémoire

Key mathematical concepts are presented in a succinct form for easy reference.

Keywords: ; Number systems; vector definitions; matrix definitions; norms; differentiation; integration; difference operators; general definitions.