An Investigation into the Accuracy, Stability and Parallel Performance of a Highly Stable Explicit Technique for Stiff Reaction-Transport PDEs

Al Franz

February 17, 1998

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Al Franz

**Master of Science
Thesis**

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Stiff Reaction-Transport PDEs

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of
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By
Al Franz

February 17, 1998

AN INVESTIGATION INTO THE ACCURACY, STABILITY
AND PARALLEL PERFORMANCE OF A HIGHLY STABLE
EXPLICIT TECHNIQUE FOR STIFF REACTION-TRANSPORT PDES

By

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Abstract

The numerical simulation of chemically reacting flows is a topic that has attracted a great deal of current research. At the heart of numerical reactive flow simulations are large sets of coupled, nonlinear Partial Differential Equations (PDEs). Due to the stiffness that is usually present, explicit time differencing schemes are not used despite their inherent simplicity and efficiency on parallel and vector machines, since these schemes require prohibitively small numerical stepsizes. Implicit time differencing schemes, although possessing good stability characteristics, introduce a great deal of computational overhead necessary to solve the simultaneous algebraic system at each timestep. This thesis examines an algorithm based on a preconditioned time differencing scheme. The algorithm is explicit and permits a large stable time step. An investigation of the algorithm's accuracy, stability and performance on a parallel architecture is presented.

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1 Introduction

Atmospheric chemistry deals with chemical compounds in the atmosphere, their distribution, origin, chemical transformation into other compounds, and finally, their removal from the atmospheric domain. These substances may occur as gases, liquids, or solids. The composition of the atmosphere is dominated by the gases nitrogen and oxygen in proportions that have been found invariable in time and space at altitudes up to 100 km. All other components are minor ones with many of them occurring only in traces. Atmospheric chemistry thus deals primarily with trace substances.

As an interdisciplinary field of science, atmospheric chemistry has its main roots in meteorology and chemistry, with additional ties to microbiology, plant physiology, oceanography, and geology. The full range of the subject was last treated by C. E. Junge in his 1963 monograph "Air Chemistry and Radioactivity". The extraordinarily rapid development of the field in the past two decades has added much new knowledge and insight into atmospheric processes. Most of the literature, however, addresses specifically the problems of local air pollution, whereas the natural atmosphere has received only a fragmentary treatment even though it provides the yardstick for any assessment of air pollution levels. The recognition that man has started to perturb the atmosphere on a global scale is now shifting the attention away from local toward global conditions [1].

In the laboratory, in the chemical manufacturing industry, and in many other situations, chemical reactions occur under relatively uniform conditions of temperature, pressure, and irradiation. In the atmosphere these conditions vary substantially, producing noticeable effects on composition and chemical reactions. Therefore, it is worthwhile to present some information on the gaseous medium within which this chemistry occurs.

The atmosphere is densest at the earth's surface. The density decreases rapidly with increasing altitude. Since many chemical reactions are pressure-dependent, the density structure alone implies differences in composition. Most reactions are temperature-dependent as well and thus reflect to some extent the atmospheric temperature structure.

Reactions involving solar photons are central to atmospheric chemistry. One therefore needs to know the spectrum of solar radiation in some detail. This spectrum is approximately that of a blackbody at 5900° K, crossed by numerous absorption lines. Several gases modify the solar spectrum as the radiation penetrates further into the atmosphere. O_3 , O_2 , H_2O , and CO_2 are the most important modifiers, but contributions are also made by CH_4 , N_2O , and other natural and anthropogenic gases [2]. The absorption of light, primarily by O_3 , is a major factor causing the increase in temperature with altitude in the stratosphere [3].

Of special importance to atmospheric chemistry are the photons energetic enough to dissociate photosensitive molecules, for most molecules such photons have wavelengths shorter than about 400 nm. The solar fluxes increase significantly as one moves upward from the ground toward the tropopause (the troposphere-stratosphere boundary). Similarly diatomic variations are seen at constant altitudes as one moves to different latitudes or as the seasons change. Any reactions dependent upon solar photons obviously vary in proportion to these changes.

Another important facet of atmospheric chemistry not always present in other chemical systems is atmospheric mixing. On a small scale, these motions are turbulent and serve to disperse emissions from point sources. On a larger scale, the motions are ordered and have the ability to transport emitted species far downwind and to high altitudes. The large scale mixing is not uniform over the earth. Transport along a fixed latitude band is such that emittants can circumnavigate the earth in about two weeks, as shown by volcanic eruption clouds. In the lower troposphere, typical advection velocities are of order 25 km/h, but variations due to local weather patterns are substantial. Within a single hemisphere, north-south transport occurs over a time scale of a few weeks. Transport across the equator is strongly inhibited by the convergence of opposed air flows, and requires six months to a year.

Vertical mixing is a strong function of local weather patterns also. A simplified conceptual approach often taken to describe this mixing is to assume that the flux of a species in a chosen direction is proportional to its mean gradient. This "eddy flux," due to the random motions of the atmosphere, is given by

$$\phi = -K \frac{dC}{dz}, \quad (1)$$

where C is the concentration, z is the altitude, and K is the *eddy diffusion coefficient*. The eddy coefficient is approximately constant throughout the troposphere, indicating relatively uniform mixing. The eddy coefficients at and above the tropopause are quite low, then increase as mixing again becomes reasonably efficient in the middle and upper stratosphere.

The residence times of atmospheric trace species are closely related to the mixing reflected by these eddy coefficients. Some months are required to vertically mix species emitted at the ground throughout the troposphere. Transport across the tropopause is quite slow, since mixing is inhibited by the atmospheric temperature structure. Several years are required for an average chemically inert molecule to move from the ground to the lower stratosphere.

More than 99.9% of the molecules comprising the earth's atmosphere are nitrogen (N_2), oxygen (O_2), or one of the rare gases. In addition, many trace molecules are found in the atmosphere. They are capable of influencing or controlling certain atmospheric processes, even though their total concentration is very low. Carbon dioxide, which is an important factor in the earth's radiation balance but is chemically unreactive in the troposphere, has an average (but increasing) concentration of about 330 parts per million (ppm). The most abundant of the reactive gases is methane, which comprises less than two parts per million of the tropospheric gas. Other reactive species are still less prevalent, the combined concentration of all of the reactive trace gases in the atmosphere seldom totals 10 ppm.

A most important molecule for atmospheric chemistry, especially droplet chemistry, is water vapor. The mixing ratio of water vapor in the troposphere varies by some five orders of magnitude, from a few parts per hundred in the tropics near the surface to less than one part per thousand over the poles at the surface and to a few parts per million near the tropopause. As a consequence of the mixing of the atmosphere, instantaneous water concentrations at a given altitude and location vary by about a factor of ten depending on the instantaneous vertical motion patterns.

The atmosphere is also influenced by aerosol particles, clouds and precipitation [2].

Interpretations of atmospheric behavior can be tested by comparing the predictions of a *model* of the atmosphere with results from measurements on the atmosphere itself. *Diagnostic models* are used to assess hypotheses about the physics and chemistry of atmospheres from a knowledge of present-day physical and chemical structure. *Prognostic models* are of interest in evaluating the future behavior and evolution of an atmosphere subject, for example, to changes in natural and artificial inputs of trace species. Such models can also be used to determine whether an assumed set of "starting" conditions could lead to observed present-day atmospheres.

Consider a volume element in an atmosphere small enough to be uniform with respect to all variables such as temperature, density, composition, and so on. If the rate of flux to and from that element of heat, radiation, matter, etc., from all other atmospheric elements is calculated, then the rate of change of the various physical parameters can be established. Chemical change within the volume element requires only slight modification for the local alterations in composition, and possibly in physical conditions. The *continuity equations* involved in the models are typified by the one for matter, which states that the net flow of mass into unit volume per unit time is equal to the local rate of change of density. Solution of the continuity equations for every physical and chemical parameter of interest, and for every volume element in the atmosphere, should then lead to a self-consistent model of atmospheric behavior that mimics in all respects the temporal and spatial changes in the real atmosphere. According to this view, with sufficient input information, and a fine enough

grid size for the volume elements, all meteorological as well as chemical phenomena could be simulated by the model. Such *three-dimensional models (3-D)* would be ideal for studying atmospheric chemistry. Computer-numerical solutions are naturally used in models, but the 3-D models are so demanding of computer time and memory that, at present, the chemistry has to be simplified drastically [4]. Simpler chemical models may then be more practical, e.g. the *Chapman model* of ozone distribution.

The numerical treatment of reaction-transport problems has attracted a great deal of current interest. Application areas such as combustion [5], groundwater flow [6], climate modeling [7], atmospheric science [8], and chemical oceanography [9] all rely heavily on the numerical solution of reaction-transport PDEs.

The modeling of atmospheric chemistry involves an equation with a chemical kinetics part and an advective-diffusive part. The chemical kinetics part is

$$\frac{d_i u}{dt} = {}_i R(\mathbf{u}, t) = {}_i P(\mathbf{u}, t) - {}_i \tilde{L}(\mathbf{u}, t) {}_i u - {}_i \bar{L}(\mathbf{u}, t) {}_i u^2, \quad (2)$$

where $\mathbf{u} = ({}_1 u, \dots, {}_N u)^T$ represents a vector of chemical concentrations, with ${}_i u = {}_i u(t)$ being the concentration of the i th chemical species and N being the total number of species involved. Equation (2) models the molecular reactions that change chemical species into other chemical species. The source term ${}_i R$ describes the reactions that occur between chemical species. This reaction operator is generally nonlinear and couples together the reaction equations for all species involved. ${}_i P(\mathbf{u}, t)$, ${}_i \tilde{L}(\mathbf{u}, t)$, and ${}_i \bar{L}(\mathbf{u}, t)$ are the production and loss rates. Important to note is that the production and loss rates, while functions of $\mathbf{u}$, do not depend upon the component ${}_i u$ [10] (a reaction rate depends upon the concentrations of the reactants, not the concentrations of the products [11]). Furthermore, a reaction rate at a point does not depend upon the spatial distribution of reactants, i.e. the concentration of reactants at other spatial points. Thus, equation (2) describes a system of *Ordinary Differential Equations (ODEs)*.

The advective-diffusive part

$$u_t + a u_x = D u_{xx}, \quad (3)$$

where $u = u(x, t)$, models the transport (translational movement, eddies, intermingling) of the species.

When combined, these equations take the general form

$$\frac{\partial({}_i u)}{\partial t} + a \cdot \nabla({}_i u) = D \nabla \cdot \nabla({}_i u) + {}_i R(\mathbf{u}, t), \quad i = 1, \dots, N, \quad (4)$$

where $\mathbf{u} = ({}_1 u, \dots, {}_N u)^T$ represents a vector of chemical concentrations, with ${}_i u = {}_i u(x, t)$ being the concentration of the i th chemical species. Equation (4) describes the basic conservation laws for each species (no atoms are created or destroyed in this simulation, which describes nothing lower than molecular reactions).

With the emergence of large-scale parallel platforms, full 3-D reactive flow simulations have begun to appear [12]. These 3-D simulations can consume enormous amounts of processor time [13], which can severely limit the length of the simulation that can reasonably be carried out. Thus, current research strives to develop increasingly efficient algorithms for numerically solving these reaction-transport PDE systems.

Explicit time-differencing schemes have the advantage that they are simple to implement and very efficient on parallel and vector computers. The disadvantage in using explicit schemes is the serious constraint placed upon the size of their stable timestep intervals. By contrast, implicit time-stepping schemes are often not constrained by numerical stability, but require a great deal more effort to implement. An implicit time-stepping scheme calls for the solution of a potentially nonlinear system of simultaneous algebraic equations at each timestep. This adds a great deal of overhead to the calculation and can offset the gain in efficiency due to the increase in stepsize made possible by the larger stable timestep interval.

The reaction mechanism in the reaction-transport PDE system can lead to the presence of widely disparate time scales in the modeling scenario. This situation gives rise to the phenomenon of stiffness [14], whereby the constraint on the size of explicit stable timestep intervals is exacerbated by limiting the numerical stepsize to the smallest timescale in the simulation. In this case, the use of an implicit numerical time-stepping scheme is necessary [15]. Thus, the considerable computational overhead brought about by the implicit scheme is primarily the result of the reaction operator, iR [13].

This thesis addresses a numerical method for simulating the atmospheric chemistry described by equation (4). The audience is expected to possess basic knowledge equivalent to a bachelor's degree in computer science. Knowledge of some disciplines of science is expected of such a person, e.g., calculus, linear algebra, the essentials of physics and chemistry, and the basic notions of computer science. Some principles of mathematics, physics, chemistry and parallel processing, however, occur as fundamental to the understanding of the physical problem, mathematical model, numerical method, specific algorithm and experimental results addressed by this thesis. Therefore, crucial ideas with which the reader may not be familiar are discussed in the appendices as background material. An attempt was made to order these sections so that any concept which depends upon others will be preceded by those prerequisite concepts. However, as this may not always be convenient, some ideas in this text may depend upon material to be defined thereafter.

The notation $\hat{u}$ will represent a vector $(u_1, \dots, u_q)^T$ of spatial points. $\mathbf{u}$ will represent a vector $({}_1u, \dots, {}_Nu)^T$ of chemical concentrations as described previously. Variables with hats ($\hat{y}$, $\hat{f}$, etc.) will usually denote vectors unless indicated to the contrary. The chemical production and loss rates ($iP(\mathbf{u}, t)$, $i\hat{L}(\mathbf{u}, t)$, and $i\bar{L}(\mathbf{u}, t)$) are scalar functions unless described differently. The test problem, which was used to verify the algorithm being investigated, is a simple 1-D reaction-transport problem which demonstrates many of the important difficulties seen in larger systems. Unless noted otherwise, we shall assume that, as in the test problem, the spatial discretization of $\hat{u}$ is in one dimension only (longitude, x , in units of revolution), along the earth's equator, with $0 \text{ rev} \leq x < 1 \text{ rev}$, although in general, $\hat{u}$ is discretized in latitude, longitude and altitude, as well as time. Similarly, we shall assume that $\mathbf{u} = \mathbf{u}(x, t)$ has only one spatial dimension, when in general, $\mathbf{u}$ is a function of latitude, longitude and altitude, as well as time. Time, t , will normally be in units of seconds (s).

2 History of Related Research

The chemically reactive advection-diffusion equation has its origins in the simple advection-diffusion equation

The pure advection equation takes the form

$$u_t + au_x = 0, \quad 0 \leq x \leq L, \quad 0 \leq t, \quad (5)$$

while the pure diffusion equation takes the form

$$u_t = Du_{xx}, \quad 0 \leq x \leq L, \quad 0 \leq t \quad (6)$$

An example of *Initial Conditions (IC)* for (6) are

$$u(x, 0) = \sin(\pi x/L), \quad (7)$$

and an example of *Boundary Conditions (BC)* for (6) are

$$u(0, t) = u(L, t) = 0 \quad (8)$$

Boundary conditions of various types, e.g. flux, periodic, etc. are also possible. Equation (8) is termed a *Dirichlet boundary condition* since the dependent variable u is specified at $x = 0$ and L . If the derivative of the dependent variable with respect to the boundary-value independent variable is specified, we have a *Neumann boundary condition*. E.g. [16]

$$\frac{\partial u(0, t)}{\partial x} = \frac{\partial u(L, t)}{\partial x} = 0 \quad (9)$$

Advection and diffusion can be modeled together by combining equations (5) and (6) into the advection-diffusion equation

$$u_t + au_x = Du_{xx}, \quad (10)$$

which describes the law of conservation of mass as it applies to the flow of fluids. Equation (10) is a continuity equation, i.e. it states that the mass rate of flow out of a region of space, such as a control volume, minus the mass rate of flow into the region is equal to the rate at which the fluid mass is being evacuated from the region [17].

A scheme currently under much research, for solving problems involving diffusion, is the *Preconditioned Time Differencing method (PTD)*. The multidimensional heat (diffusion) equation takes the form

$$\frac{\partial u(\hat{x}, t)}{\partial t} = \alpha \nabla \cdot \nabla u(\hat{x}, t), \quad (11)$$

where $\hat{x}$ is shorthand for the multidimensional vector $\hat{x} = (x_1, \dots, x_n)^T$ confined to some region Ω . $\hat{x} \in \Omega \subseteq \mathcal{R}^n$, $0 \leq t \leq t_{final} < \infty$ and $\alpha > 0$. With preconditioning, equation (11) with IC

$$u(\hat{x}, 0) = f(\hat{x}) \quad (12)$$

and well-posed BCs has been solved on vector and parallel computers, using an explicit difference method which is efficient and has a larger stability region than that of the classical explicit Euler schemes. The PTD method, used by Garry Rodrigue and Don Wolitzer, uses Forward Euler as predictor, Backward Euler as corrector and the over-relaxed point Jacobi method as the iterative method. Explicit methods impose severe constraints on the timestep due to stability considerations. Implicit methods on the other hand, do not have such constraints but require a system of simultaneous algebraic equations to be solved at each timestep. For pure diffusion, this system is linear since there is no nonlinear reactive term. Combining the two methods results in a method which is explicit, has a large stable timestep, and since the dominant operation in an explicit method is the matrix vector multiply, such an

operation is highly efficient on a pipeline as well as multiprocessing computer architectures [18]

The advection-diffusion equation (10) can be solved with the numerical Finite Difference Method. Specifically illustrated here is the *Finite Time Central Space method (FTCS)* [19, 20]

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = \frac{D}{(\Delta x)^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) \quad (13)$$

or

$$u_j^{n+1} = \mu(c_1 u_{j+1}^n + c_2 u_j^n + c_3 u_{j-1}^n), \quad j = 1, \dots, q \quad (14)$$

where

$$\begin{aligned} c_1 &= D - a\Delta x/2, \\ c_2 &= -2D + (\Delta x)^2/\Delta t, \\ c_3 &= D + a\Delta x/2, \\ \mu &= \Delta t/(\Delta x)^2 \end{aligned} \quad (15)$$

With the over-relaxed Jacobi preconditioner described above, the stability regions of the *Finite Time Central Space*, *Upwind Differencing (UW)*, and *Lax-Wendroff (LW)* methods have been expanded for the multidimensional diffusion equation (11), the linear advection-diffusion equation (10), and the nonlinear Burgers' equation [21]

$$u_t + uu_x = \alpha u_{xx} \quad (16)$$

FTCS, UW and LW explicit methods for solving (16), are given in stencil form by

$$u_j^{n+1} = \frac{\gamma_j^n \Delta t}{\Delta x^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) + u_j^n - \frac{u_j^n \Delta t}{2\Delta x} (u_{j+1}^n - u_{j-1}^n), \quad (17)$$

where

$$\begin{aligned} \gamma_j^n &= \alpha, & \text{FTCS,} \\ \gamma_j^n &= \alpha + u_j^n (\Delta x/2), & \text{UW,} \\ \gamma_j^n &= \alpha + (u_j^n)^2 (\Delta t/2), & \text{LW} \end{aligned} \quad (18)$$

Similarly, implicit methods are

$$u_j^{n+1} = \frac{\gamma_j^n \Delta t}{\Delta x^2} (u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + u_j^{n+1} - \frac{u_j^n \Delta t}{2\Delta x} (u_{j+1}^{n+1} - u_{j-1}^{n+1}) \quad (19)$$

The implicit methods (19) have been preconditioned and over-relaxed to produce the PTD computations reported in [21]

PTDs can be applied to advection-diffusion equations which include additional terms making the equation nonlinear. The reaction operator $_i R$ in equation (4) is generally nonlinear and couples together the reaction-transport PDEs for all species involved. Thus, a reactive flow simulation leads to a large system of coupled, nonlinear PDEs.

Equation (4) represents a conservation law for each chemical species $_i u$, if we assume that no molecules are created or destroyed, then we have equation (3) for each species. On the other hand, if we assume only that no atoms are created or destroyed, but allow molecules to react, we have equation (4).

These equations are often very stiff, placing a severe limitation on the stepsize of an explicit scheme due to stability, which forces the use of an implicit scheme. The problem with an implicit scheme, however, is that a nonlinear system must be solved at each step. Preconditioned time differencing has yielded stable, explicit methods for dealing with these otherwise unwieldy systems. Equation (4) has been solved with Jacobi and Gauss-Seidel preconditioners applied to the backward Euler method, and the Jacobi preconditioner applied to the trapezoid rule [22]

$$\hat{y}^{n+1} = \frac{1}{2} \Delta t (\hat{f}^{n+1} + \hat{f}^n) + \hat{y}^n \quad (20)$$

Equation (4) has also been solved with the Newton preconditioner applied to the backward Euler and trapezoid rules [23, 10]. An implicit scheme proposed by Stott and Harwood [24] is an Euler backward scheme in which an initial estimate of the solution is used as the first approximation in a Newton-Raphson iteration to the fully implicit solution. The Euler backward scheme may be written

$$\hat{y}^{n+1} - \hat{y}^n - \Delta t \hat{f}(\hat{y}^{n+1}) = 0 \quad (21)$$

The method chosen here to solve for y^{n+1} is to carry out a Newton-Raphson iteration given by

$$\hat{y}^{n+1,m+1} = \hat{y}^{n+1,m} + \left(I - \Delta t \left(\frac{\partial \hat{f}}{\partial \hat{y}} \right)^{n+1,m} \right)^{-1} (-\hat{y}^{n+1,m} + \Delta t \hat{f}(\hat{y}^{n+1,m}) + \hat{y}^n), \quad (22)$$

where the superscript m denotes the item evaluated at the m th iteration, I is the identity matrix and $\partial \hat{f} / \partial \hat{y}$ is the Jacobian matrix of derivatives. The initial value for the iteration, $\hat{y}^{n+1,0}$, is calculated from a linearized approximation to the implicit backward method

$$\frac{\hat{y}^{n+1,0} - \hat{y}^n}{\Delta t} = \hat{f}(\hat{y}^n) + \left(\frac{\partial \hat{f}}{\partial \hat{y}} \right)^n (\hat{y}^{n+1,0} - \hat{y}^n) \quad (23)$$

In the initial estimate to $\hat{y}^{n+1}$ (equation 23) and in each iteration step (equation 22), a matrix inversion is avoided by approximating the matrix by its diagonal. It is found that it is necessary to make only a small number of iterations (typically three) to get a very close approximation to the Euler backward solution. The method (22,23) is a *fully* implicit scheme. The method investigated in this thesis is a preconditioned scheme not a fully implicit scheme.

3 Preconditioned Time Differencing

Preconditioned time differencing (PTD) is a methodology used to construct explicit time stepping schemes with large stable timestep intervals. PTD begins with an implicit time stepping scheme and applies an iterative solution technique to the resulting simultaneous algebraic system. Rather than iterate to convergence, PTD uses a fixed number of iterations of the iterative solution technique in a classic Predictor-Corrector fashion.

Predictor-Corrector schemes can be understood as follows. Suppose that we wish to solve the standard *Initial Value Problem (IVP)* by an implicit *Linear Multistep Method (LMM)*. Then at each step we have to solve for $\hat{y}^{n+k}$ the implicit system

$$\hat{y}^{n+k} + \sum_{j=0}^{k-1} \alpha_j \hat{y}^{n+j} = h\beta_k \hat{f}(\hat{y}^{n+k}, t_{n+k}) + h \sum_{j=0}^{k-1} \beta_j \hat{f}^{n+j} \quad (24)$$

We normally do this by the fixed point iteration

$$\begin{aligned} \hat{y}^{n+k,s+1} + \sum_{j=0}^{k-1} \alpha_j \hat{y}^{n+j} &= h\beta_k \hat{f}(\hat{y}^{n+k,s}, t_{n+k}) + h \sum_{j=0}^{k-1} \beta_j \hat{f}^{n+j}, \\ \hat{y}^{n+k,0} &\text{arbitrary,} \quad s = 0, 1, \end{aligned} \quad (25)$$

which will converge to the unique solution of (24) provided that

$$h < \frac{1}{|\beta_k|L}, \quad (26)$$

where L is a Lipschitz constant of f with respect to y . For non-stiff problems, this restriction on h is not significant, in practice, considerations of accuracy put a much more restrictive constraint on h . Although (25) will converge for arbitrary $\hat{y}^{n+k,0}$, each iteration calls for one evaluation of the function f , and computation can obviously be saved if we can provide as good a guess as possible for $\hat{y}^{n+k,0}$. This is conveniently done by using a separate *explicit* LMM to provide the initial guess $\hat{y}^{n+k,0}$. We call this explicit method the *predictor* and the implicit method (24) the *corrector*, the two together comprise a *Predictor-Corrector (PC) pair* [14].

If an appropriate initial iterate is used, the implicit method's order of accuracy will be preserved [14]. In addition, the resulting time-differencing scheme typically inherits an expanded stable time step interval from the parent implicit method [22].

For illustration, consider the system of linear ODEs with constant coefficients

$$\frac{d\hat{u}}{dt} = \hat{f}(\hat{u}, t) = A\hat{u} \quad (27)$$

The implicit Euler method, applied to this ODE system, takes the form

$$\begin{aligned} \hat{u}^{n+1} &= \hat{u}^n + \Delta t \hat{f}(\hat{u}^{n+1}, t_{n+1}), \\ \hat{u}^{n+1} - \Delta t \hat{f}(\hat{u}^{n+1}, t_{n+1}) &= \hat{u}^n, \\ \hat{u}^{n+1} - \Delta t A \hat{u}^{n+1} &= \hat{u}^n, \\ (I - \Delta t A) \hat{u}^{n+1} &= \hat{u}^n \end{aligned} \quad (28)$$

and defines a system of simultaneous algebraic equations which must be solved for each timestep. An iterative method for solving this linear system defines a splitting $(I - \Delta t A) = M - N$. Substitute this splitting into (28) to get

$$\begin{aligned} (M - N) \hat{u}^{n+1} &= \hat{u}^n, \\ M \hat{u}^{n+1} &= N \hat{u}^{n+1} + \hat{u}^n \end{aligned} \quad (29)$$

Iterating $\hat{u}^{n+1}$ in (29) produces

$$M\hat{u}^{n+1,s+1} = N\hat{u}^{n+1,s} + \hat{u}^n, \quad s = 0, \dots, m \quad (30)$$

If M is chosen to be a diagonal matrix, its inverse is easy to compute. Multiplying equation (30) by M^{-1} yields

$$\hat{u}^{n+1,s+1} = M^{-1}N\hat{u}^{n+1,s} + M^{-1}\hat{u}^n, \quad s = 0, \dots, m \quad (31)$$

In a PTD method, the number of iterations m is assumed fixed. Thus, $\hat{u}^{n+1} = \hat{u}^{n+1,m}$. Depending upon the choice of preconditioner M , this will often produce an explicit scheme. For example, using the point-Jacobi preconditioner ($M = \text{diag}(I - \Delta t A)$) and one iteration ($m = 1$) gives

$$\hat{u}^{n+1} = M^{-1}N\hat{u}^{n+1,0} + M^{-1}\hat{u}^n \quad (32)$$

which (given an explicit value for the initial iterate $\hat{u}^{n+1,0}$) defines a truly explicit time stepping process.

PTD has been applied to linear and nonlinear advection-diffusion problems [18, 21] and nonlinear chemical kinetics problems [25, 10]. The main obstacle in formulating a unified algorithm for a full advection-diffusion-reaction equation is the choice of initial iterate (or predicted value). The use of an explicit time differencing method (i.e. explicit Euler) was vital in the advection-diffusion case (see [18, 21]) but was detrimental to stability in the case of chemical reactions, and led to an unstable algorithm (note the “identity predictor” used in [10] or the simple extrapolation used in [25]). Here, we investigate the combination of PTD approaches for both chemistry and transport. The proposal is to ignore the presence of chemistry during the prediction step: this will provide the necessary accuracy to the spatial derivatives while not interfering with the stability of the reaction system. This algorithm is described in the next section.

4 The Algorithm

The algorithm takes on a very clear PC flavor, the explicit Euler method is used in the predictor step (ignoring the presence of chemistry) and the Jacobi splitting is applied to the implicit Euler method for the corrector step. An overrelaxation step [18, 21] is performed after the corrector step.

To illustrate the algorithm in general terms, assume that equation (4) has been spatially discretized via the Numerical Method Of Lines [16] approach

$$\frac{\partial({}_i\ddot{u})}{\partial t} = {}_if({}_1\ddot{u}, \dots, {}_N\ddot{u}, t) = (A){}_i\hat{u} + {}_i\hat{R}({}_1\hat{u}, \dots, {}_N\hat{u}, t), \quad i = 1, \dots, N, \quad (33)$$

where A is a $q \times q$ matrix derived from the spatial discretization scheme, ${}_i\hat{R}$ is the spatial discretization of the reaction source term operator, and ${}_i\hat{u} = ({}_i u_1, \dots, {}_i u_q)^T$ is the (spatially) discretized approximation to ${}_i u(x, t)$. The notation ${}_i u_j^n$ will be used to denote the discrete numerical approximation to ${}_i u(x_j, t_n)$, i.e., the concentration of chemical species i at spatial point j and time point n . In other words, equation (33) is shorthand for the spatially discretized system of PDEs

$$\begin{pmatrix} {}_i u_1 \\ {}_i u_2 \\ \vdots \\ {}_i u_q \end{pmatrix} = A \begin{pmatrix} {}_i u_1 \\ {}_i u_2 \\ \vdots \\ {}_i u_q \end{pmatrix} + \begin{pmatrix} {}_i R_1({}_1 u_1, \dots, {}_N u_1, t) \\ {}_i R_2({}_1 u_2, \dots, {}_N u_2, t) \\ \vdots \\ {}_i R_q({}_1 u_q, \dots, {}_N u_q, t) \end{pmatrix}, \quad i = 1, \dots, N \quad (34)$$

The explicit Euler prediction step (ignoring the presence of chemistry) is given by

$${}_i\hat{u}^{n+1} = (I + \Delta t A){}_i\hat{u}^n, \quad (35)$$

so that

$${}_i\hat{u}^{n+1,0} = (I + \Delta t A){}_i\hat{u}^n \quad (36)$$

will be the predicted value

The preconditioned implicit step is derived from the implicit Euler method. Begin by applying *Backward Euler (BE)* to equation (33)

$$\begin{aligned} {}_i\hat{u}^{n+1} &= {}_i\hat{u}^n + \Delta t {}_if({}_1\hat{u}, \dots, {}_N\hat{u}, t) \\ &= {}_i\hat{u}^n + \Delta t [(A){}_i\hat{u}^{n+1} + {}_i\hat{R}({}_1\hat{u}^{n+1}, \dots, {}_N\hat{u}^{n+1}, t_{n+1})] \\ &= {}_i\hat{u}^n + \Delta t (A){}_i\hat{u}^{n+1} + \Delta t [{}_i\hat{R}({}_1\hat{u}^{n+1}, \dots, {}_N\hat{u}^{n+1}, t_{n+1})], \\ {}_i\hat{u}^{n+1} - \Delta t (A){}_i\hat{u}^{n+1} &= {}_i\hat{u}^n + \Delta t [{}_i\hat{R}({}_1\hat{u}^{n+1}, \dots, {}_N\hat{u}^{n+1}, t_{n+1})], \\ (I - \Delta t A){}_i\hat{u}^{n+1} &= {}_i\hat{u}^n + \Delta t [{}_i\hat{R}({}_1\hat{u}^{n+1}, \dots, {}_N\hat{u}^{n+1}, t_{n+1})] \end{aligned} \quad (37)$$

The Jacobi splittings (linear [21] and nonlinear [10]) can be applied to this equation to obtain

$$(M){}_i\hat{u}^{n+1,1} = (N){}_i\hat{u}^{n+1,0} + {}_i\hat{u}^n + \Delta t [{}_i\hat{R}({}_1\hat{u}^{n+1,0}, \dots, {}_i\hat{u}^{n+1,1}, \dots, {}_N\hat{u}^{n+1,0}, t_{n+1})], \quad (38)$$

where $(I - \Delta t A) = M - N$, $M = \text{diag}(I - \Delta t A)$, ${}_i\hat{u}^{n+1,0}$ denotes the predicted value of ${}_i\hat{u}^{n+1}$, and ${}_i\hat{u}^{n+1,1}$ denotes the corrected value of ${}_i\hat{u}^{n+1}$.

Chemical kinetic ODEs are used as the source terms in conservation equations and commonly take the form [26, 22] (scalar equation shown for simplicity)

$$\frac{d_i u}{dt} = {}_i R(u, t) = {}_i P(u, t) - {}_i \hat{L}(u, t) u - {}_i \bar{L}(u, t) u^2 \quad (39)$$

where ${}_i P$, ${}_i \hat{L}$, ${}_i \bar{L}$ are nonnegative quantities representing chemical production and loss rates. Important to note is that the production and loss rates, while functions of u , do not depend

on the component ${}_i u$. This allows ${}_i u^{n+1,1}$ to be computed as the solution to a quadratic equation, which is essentially an explicit process [10]

In general, the i th component equation in the PDE system will involve a nonzero term of the form ${}_i \tilde{L}(u, t) {}_i u^2$ and will therefore be nonlinear in ${}_i u$, so that (in the case of equation 38)

$$(M) {}_i \hat{u}^{n+1,1} = (N) {}_i \hat{u}^{n+1,0} + {}_i \hat{u}^n + \Delta t [({}_i \hat{P}^n) - ({}_i \tilde{L}^n)({}_i u^{n+1,1}) - ({}_i \tilde{L}^n)({}_i u^{n+1,1})^2], \quad (40)$$

where ${}_i \hat{R}(u, t)$, ${}_i \hat{P}(u, t)$, $({}_i \hat{L}^n)({}_i u^{n+1,1})$, and $({}_i \tilde{L}^n)({}_i u^{n+1,1})^2$ are vectors of length q , the cumbersome notation $({}_i \tilde{L}^n)({}_i u^{n+1,1})$ denotes

$$\begin{pmatrix} ({}_i \tilde{L}_1^n)({}_i u_1^{n+1,1}) \\ ({}_i \tilde{L}_2^n)({}_i u_2^{n+1,1}) \\ \vdots \\ ({}_i \tilde{L}_q^n)({}_i u_q^{n+1,1}) \end{pmatrix} \quad (41)$$

and $({}_i \tilde{L}^n)({}_i u^{n+1,1})^2$ denotes

$$\begin{pmatrix} ({}_i \tilde{L}_1^n)({}_i u_1^{n+1,1})^2 \\ ({}_i \tilde{L}_2^n)({}_i u_2^{n+1,1})^2 \\ \vdots \\ ({}_i \tilde{L}_q^n)({}_i u_q^{n+1,1})^2 \end{pmatrix} \quad (42)$$

Equation (40) is a set of independent *quadratic* equations, each of which can be solved for ${}_i u_j^{n+1,1}$ in terms of ${}_i u_j^{n+1,0}$ and known quantities, leading to an explicit calculation

If the PDF is linear in ${}_i u$, as our test problem will be, then

$${}_i R(u, t) = {}_i P(u, t) - {}_i \tilde{L}(u, t) {}_i u \quad (43)$$

$$(M) {}_i \hat{u}^{n+1,1} = (N) {}_i \hat{u}^{n+1,0} + {}_i \hat{u}^n + \Delta t [({}_i \hat{P}^n) - ({}_i \tilde{L}^n)({}_i u^{n+1,1})] \quad (44)$$

Since M is a diagonal matrix, its inverse is easily computable and we get a set of independent *linear* equations

The last step is to perform an overrelaxation, which is given by

$${}_i \hat{u}^{n+1} = (3/8)({}_i \hat{u}^n) + (5/8)({}_i \hat{u}^{n+1,1}) \quad (45)$$

The particular choice of overrelaxation constants comes from [18, 21] and was necessary for accuracy and stability as applied to advection-diffusion problems

Thus, the proposed algorithm takes the form

- 1 Set ${}_i \hat{u}^{n+1,0} = (I + \Delta t A) {}_i \hat{u}^n$
- 2 Solve $M {}_i \hat{u}^{n+1,1} = N {}_i \hat{u}^{n+1,0} + {}_i \hat{u}^n + \Delta t [{}_i \hat{R}({}_i \hat{u}^{n+1,0}, \quad, {}_i \hat{u}^{n+1,1}, \quad, N \hat{u}^{n+1,0}, t_{n+1})]$ for ${}_i \hat{u}^{n+1,1}$
- 3 Set ${}_i \hat{u}^{n+1} = (3/8)({}_i \hat{u}^n) + (5/8)({}_i \hat{u}^{n+1,1})$

Note that if we eliminate the reactive terms, ${}_i P^n$ and ${}_i \tilde{L}^n$, and the chemical vectorization in equation (44), we recover the linear Jacobi splitting (32) for equation (27)

5 The Test Problem

In this section, a simple reaction-transport problem is developed to study the computational performance of the algorithm from the previous section. Let ${}_1u = {}_1u(x, t)$ denote the chemical concentration of atomic oxygen (O) and let ${}_2u = {}_2u(x, t)$ denote the concentration of molecular ozone (O_3), where x is in units of revolution (**rev**) and t is in units of day (**d**) unless indicated otherwise. The concentration of molecular oxygen (O_2 , denoted by ${}_3u = \text{constant}$) is significantly larger in the earth's atmosphere than atomic oxygen or ozone and is therefore assumed to be constant in this simple numerical simulation. The Chapman model for oxygen-containing chemistry has been described elsewhere [15, 22, 23, 10]. Chapman chemistry can be modeled by a coupled system of ODEs which can, in turn, be added as a source term to a simple advective-diffusive PDE system to produce

$$\frac{\partial {}_1u}{\partial t} + a \frac{\partial {}_1u}{\partial x} = D \frac{\partial^2 {}_1u}{\partial x^2} + {}_1P - ({}_1L)({}_1u) \quad (46)$$

$$\frac{\partial {}_2u}{\partial t} + a \frac{\partial {}_2u}{\partial x} = D \frac{\partial^2 {}_2u}{\partial x^2} + {}_2P - ({}_2L)({}_2u) \quad (47)$$

where $x \in (0, 1)$ and $t \in (0, \infty)$. Periodic boundary conditions will be used (i.e. ${}_i u(0, t) = {}_i u(1, t)$) to mimic the atmosphere. The advection and diffusion parameters (a and D) are assumed constant. The chemical production and loss rates are given by

$$\begin{aligned} {}_1P &= 2(k_3)({}_3u) + (k_4)({}_2u) \\ {}_2P &= (k_1)({}_3u)({}_1u) \\ {}_1L &= (k_1)({}_3u) + (k_2)({}_2u) \\ {}_2L &= (k_2)({}_1u) + k_4 \end{aligned} \quad (48)$$

with initial conditions ${}_1u = 10^6 \text{ mol}$ and ${}_2u = 10^{12} \text{ mol}$, and with constant values ${}_3u = 3.7 \times 10^{16} \text{ mol}$, $k_1 = 1.63 \times 10^{-16} \text{ mol}^{-2} \text{ s}^{-1}$ and $k_2 = 4.66 \times 10^{-16} \text{ mol}^{-2} \text{ s}^{-1}$. The time varying rate coefficient functions (which model chemical reactions driven by the absorption of sunlight) are given by

$$k_j(x, t) = \begin{cases} \exp\left(\frac{a_j}{\cos(kx - \omega t)}\right) & \text{if } \cos(kx - \omega t) < 0 \\ 0 & \text{otherwise} \end{cases}, \quad j = 3, 4 \quad (49)$$

with $a_3 = 22.62$, $a_4 = 7.601$, $\omega = 2\pi/(86,400 \text{ s})$, $k = 2\pi/\text{rev}$, and the k_j are in units of $\text{mol}^{-1} \text{ s}^{-1}$. Note that the constant 86,400 s is one day, so that the time varying reaction rate coefficient functions (k_3 and k_4) have 24 h *period* T . These functions are also periodic in x (i.e. one and only one point in the interval experiences a sunrise/sunset at any given moment). Note also that the *wavelength* λ of these functions is one revolution, i.e. one complete circuit along the earth's equator.

This test problem, although tractable in size, carries with it many of the important difficulties seen in larger systems: it is nonlinear, it has a nonconstant Jacobian, it is sufficiently stiff, due to the chemistry. It therefore provides a reasonable initial test for any numerical technique aimed at reactive flow simulation.

6 Investigation of the Method

6.1 Introduction

This research consisted of testing the PTD method (in a C program called `reac.c`) by comparing its performance against that of the *Forward Euler (FE)* method (`euler.c`) and the *Livermore Solver for Ordinary Differential Equations (LSODE)* (`chapman.f`) on the same problem. FE was used because it is a typical explicit algorithm, against which to compare our explicit algorithm. Also, since our PTD is derived from BE, the PTD is first-order, as is FE. LSODE was used because it is a well-tested, accurate, adaptive-stepsize family of methods. Parameters used in each of the three methods were identical, except where different values were necessary, e.g. `stepsize`.

6.2 Stability

Two stability tests of PTD and FE were performed on a *Digital Equipment Corporation (DEC) Reduced Instruction Set Computer (RISC)* architecture, running the *ULTRIX 4.3 Operating System (OS)*. Data collected for PTD during these runs is presented in table (1). Data collected for FE during these runs is presented in table (2). Output values are tabulated for the spatial and temporal point where the percent error is the largest for nonzero values of ${}_1u(x, t)$, i.e. at the tabulated value of x , and $t = t_{final}$.

Test 1 used values of the advection and diffusion parameters which are reasonable for an atmospheric simulation. Parameters used were

$$\begin{aligned} a &= 10^{-4}, \\ D &= 10^{-5}, \\ q &= 100, \\ \Delta t &= 0.300 \text{ s} \quad \text{FE}, \\ \Delta t &= 5.034 \text{ s} \quad \text{PTD}, \\ t_0 &= 0.00 \text{ s}, \\ t_{final} &= 10.0 \text{ d} \end{aligned} \tag{50}$$

t_0 , t_{final} and Δt are simulation time, as opposed to real time and wall clock time. The stability of PTD evidently falls apart between $\Delta t = 5.034 \text{ s}$ and $\Delta t = 5.035 \text{ s}$. FE exhibits its instability between $\Delta t = 0.30 \text{ s}$ and $\Delta t = 0.35 \text{ s}$. This is an experimental result, not an analytical result. Note that accuracy obviously deteriorates at a much smaller Δt than stability does. A test run for $\Delta t = 5 \text{ s}$ is shown for comparison.

Test 2 used values of the advection and diffusion parameters which are much larger, to

a	D	$\Delta t/\text{s}$	t_{final}	x	${}_1u(x, t)$ (from PTD)	Percent error
10^{-4}	10^{-5}	5.000000	10 d	0.7	7.02×10^7	-30
10^{-4}	10^{-5}	5.034000	10 d	0.7	7.27×10^{11}	7.3×10^5
10^{-4}	10^{-5}	5.035000	10 d	0.7	unstable	unstable
1	1	0.000050	100 s	0.3	1.01×10^7	12
1	1	0.000051	100 s	0.3	unstable	unstable

Table 1: Stability tests of PTD

a	D	$\Delta t/s$	t_{final}	x	$u(x, t)$ (from FE)	Percent error
10^{-4}	10^{-5}	0 300000	10 d	0 7	9.96×10^7	-5.8×10^{-3}
10^{-4}	10^{-5}	0 350000	10 d	0 7	unstable	unstable
1	1	0 000049	100 s	0 3	8.99×10^6	1.2×10^{-2}
1	1	0 000050	100 s	0 3	unstable	unstable

Table 2: Stability tests of FE

exercise the sensitivity of the algorithms' stability to stepsize. Parameters used were

$$\begin{aligned}
a &= 1, \\
D &= 1, \\
q &= 100, \\
\Delta t &= 0.000049 \text{ s FE}, \\
\Delta t &= 0.000050 \text{ s PTD}, \\
t_0 &= 0.00 \text{ s}, \\
t_{final} &= 100 \text{ s}
\end{aligned} \tag{51}$$

The stability of PTD evidently disappears between $\Delta t = 0.000050 \text{ s}$ and $\Delta t = 0.000051 \text{ s}$. The stability of FE degenerates between $\Delta t = 0.000049 \text{ s}$ and $\Delta t = 0.000050 \text{ s}$. In running this test, with a very small t_{final} , both algorithms initially appeared to be stable up to a certain size Δt , but for larger t_{final} and the same Δt , they eventually exhibited their instability. Actually, they were unstable for the smaller t_{final} , the instability simply was not apparent. The moderate run of $t_{final} = 100 \text{ s}$ was chosen because it is large enough to allow any significant instability to surface, yet small enough to allow the tests to complete within a reasonable amount of wall clock time. With $a = D = 1$, we need a very small Δt , which results in very many steps, which for large t_{final} implies a very long run time. It is very interesting to note that at $t_{final} = 100 \text{ s}$, FE and PTD were both stable up to $\Delta t \approx 0.00005$, in agreement with the classical result for the *Finite Difference Method (FDM)* [20]

$$\Delta t \leq \frac{(1/q)^2}{2D} = \frac{(1/100)^2}{2 \cdot 1} = 0.00005 \text{ s} \tag{52}$$

6.3 Accuracy

The accuracy test of PTD was performed on the DEC RISC machine with the same OS. The stepsize was successively halved, from $\Delta t = 5.000000 \text{ s}$, down to $\Delta t = 0.156250 \text{ s}$, and the output values were compared against those of LSODE solving the same problem with the same parameters. The other parameters used were

$$\begin{aligned}
a &= 10^{-4}, \\
D &= 10^{-5}, \\
q &= 100, \\
t_0 &= 0.00 \text{ s}, \\
t_{final} &= 5.00 \text{ d}
\end{aligned} \tag{53}$$

With $\Delta t = 5.000000 \text{ s}$, the output values for PTD were within 19% of those for LSODE. As the stepsize decreased to $\Delta t = 0.156250 \text{ s}$, the percent error decreased below 11% of those for LSODE. It is somewhat discouraging that the accuracy is not a little better, but the difference is probably due to the PTD method not adaptively controlling its stepsize. The accuracy clearly improves slightly with decreasing stepsize (since the PTD method is first-order accurate). Data collected during these runs is presented in table (3). Output

$\Delta t/s$	t_{final}	${}_1u(x, t)$ (from PTD)	<i>Absolute error</i>	<i>Percent error</i>
5 000000	5 d	6.34×10^7	-1.51×10^7	-19.2
2 500000	5 d	6.57×10^7	-1.27×10^7	-16.2
1 250000	5 d	6.76×10^7	-1.09×10^7	-13.8
0 625000	5 d	6.88×10^7	-9.61×10^6	-12.3
0 312500	5 d	6.95×10^7	-8.88×10^6	-11.3
0 156250	5 d	6.99×10^7	-8.49×10^6	-10.8

Table 3 Comparison of PTD against LSODE for accuracy

values are tabulated for the point where the percent error is the largest for nonzero values of ${}_1u(x, t)$, i.e. at $x = 0.80$ rev, and $t = t_{final}$. The LSODE value of ${}_1u(x, t)$ at the same point is 7.84×10^7 .

6.4 Parallel Performance

The platform used for the parallel study was the Meiko CS-2 *Multi-Instruction Multi-Data* (MIMD) architecture. The CS-2 used here is a 40-Node partition, with one 90 MHz Sparc chip (capable of 180 Megaflop performance) and a local cache memory on each node. Communication is accomplished via message-passing using a multistage switching network constructed from 8 by 8 crosspoint switches. The network is configured so that the bandwidth between stages remains constant.

For the runs presented here, the parameters were

$$\begin{aligned}
 a &= 10^{-4}, \\
 D &= 10^{-5}, \\
 q &= 1000, \\
 \Delta t &= 5.00 \text{ s}, \\
 t_0 &= 0.00 \text{ s}, \\
 t_{final} &= 1.00 \text{ d}
 \end{aligned} \tag{54}$$

Although these values may seem small, the scale of the spatial domain ($x \in (0, 1)$) dictates small transport constants in order to model an "atmosphere." This type of integration would be prohibitive with a typical explicit method, since the chemistry would normally limit the maximum stepsize to only a few seconds. An application of FE to the chemical ODEs alone yields a maximum stable timestep of 0.23 s. This would require more than 21 times as many steps to reach $t_{final} = 1.00$ d as PTD and a wall clock time of over 2 h using the entire 40 *Central Processing Unit* (CPU) partition.

The spatial domain is discretized (using centered differences) into 1000 gridpoints which are divided evenly among the nodes. After each timestep, the CPUs must exchange the solution values from the boundary of their local domain before the next timestep can begin. Thus, as parallelism increases, communication overhead will increase as well. Initially, ${}_1u = 10^6$ mol and ${}_2u = 10^{12}$ mol uniformly over the entire space domain.

Figure (1) shows the wall clock time vs. the number of nodes for this problem. An interesting phenomenon is that performance does not scale well until 12-13 CPUs are used in the run. At this point, the speedup becomes superlinear, probably due to relatively low communication overhead coupled with good cache performance. This behavior can be observed further in figure (2), which depicts the relative performance vs. the number of nodes. The initial drop in this curve is due to increased message passing causing more overhead. The subsequent rise in the curve results from each node having less mesh points, each node's portion of the problem begins to fit into the node's cache. The second drop

Figure 1 Wall clock time vs number of processing nodes for sample problem

begins when the entire problem fits into cache, any further division of the problem simply results in more overhead. Data collected during these runs is presented in table (4)

Finally, the parallel performance for an increasing problem size with a constant number of spatial gridpoints per node is depicted. Figure (3) shows the wall clock time vs the number of nodes for runs using 250 spatial gridpoints per node. There is a slight increase in wall clock time with problem size, but this effect is not very pronounced. These results are quite typical for any explicit time stepping method used to numerically solve a PDE system [27]

6.5 Speed

A timing comparison of PTD and FE was performed on a Cray C90. Parameters used were

$$\begin{aligned}
 a &= 10^{-4}, \\
 D &= 10^{-5}, \\
 q &= 100, \\
 \Delta t &= 0.23 \text{ s} \quad \text{FE}, \\
 \Delta t &= 5.00 \text{ s} \quad \text{PTD}, \\
 t_0 &= 0.00 \text{ s}, \\
 t_{final} &= 5.00 \text{ d}
 \end{aligned} \tag{55}$$

The goal here was to demonstrate that the stability advantage of PTD over FE translates into faster computation. The total run time for FE was 25 min, 22 s. The total run time for PTD was 01 min, 07 s, about 1/25 of that for FE.

LSODE was not run on the Cray, as LSODE was the slowest of the three methods. Photodissociation reactions occur in the presence of sunlight and their rates of reaction change abruptly at sunset and even more abruptly at sunrise. At any given time, there is a sunrise and a sunset somewhere in the simulation. The small stepsizes taken by LSODE as a result of the sharp edges at sunrises and sunsets are a product of the dynamic error control used by LSODE, not of stiffness.

Figure 2 Relative performance vs number of processing nodes for sample problem

<i>Number of Processors</i>	<i>Wall Clock Time / s</i>
1	1476
2	1141
4	891
8	541
9	462
10	387
11	312
12	141
13	59
14	56
15	54
16	52
24	42
32	40
40	38

Table 4 Wall clock times for sample problem runs on the Meiko CS-2

Figure 3 Wall clock time vs processing nodes for 250 spatial gridpoints per processor

6.6 Output

The output of the algorithm is the concentrations of the constituent molecular species. In our test problem, the outputs are atomic oxygen and molecular ozone. Molecular oxygen is nearly constant throughout the simulation. Figure (4) shows the change in concentration of *molecular ozone* at a single point, in one day. Figure (5) shows the change in concentration of *atomic oxygen* at a single point, in one day. Figure (6) shows the concentration of atomic oxygen at *different points*, after half a day has elapsed. This wave of atomic oxygen remains pointed toward the sun as the earth turns beneath it. Figure (7) shows the concentration of atomic oxygen at different points, after *three quarters* of a day have elapsed. Notice that the wave is now at a different place on the equator. The sinusoidal in the denominator of equation (49) was chosen so that the distance along the equator is numbered from 0.00 *rev* to 1.00 *rev*, beginning at Greenwich, England, increasing to the west, and time is numbered from 0.00 *d* to 1.00 *d*, beginning at midnight. On these scales, Memphis, Tennessee is approximately at 0.25 *rev*, Midway Islands, Hawaii at 0.50 *rev*, and Gyangze, China at 0.75 *rev*. Also note that 0.25 *d* corresponds to 6 am, 0.50 *d* to noon, and 0.75 *d* to 6 pm.

Figure 4 Molecular ozone at a single gridpoint, 0.00 revolution (corresponding to Greenwich, England), over a period of one day

Figure 5 Atomic oxygen at a single gridpoint, 0.00 revolution (corresponding to Greenwich, England), over a period of one day. Note that at noon in Greenwich, England, the wave of atomic oxygen is directly overhead

Figure 6 Atomic oxygen along the equator at 0.50 day (noon) Note that at noon in Greenwich, England, the wave of atomic oxygen is directly overhead

Figure 7 Atomic oxygen along the equator at 0.75 day (6 pm) Note that at 6 pm in Greenwich, England, the wave of atomic oxygen has moved to Memphis, Tennessee

7 Conclusion

In this investigation we have seen that the stability of the Preconditioned Time Differencing method with parameter values appropriate for practical atmospheric simulations is superior to that of the explicit method, Forward Euler. In this case the timestep allowed by stability for the PTD method is about 17 times that of Forward Euler. Stability of both methods is nearly equal for large values of the advection and diffusion parameters. The accuracy of the PTD method is within 10% of the accuracy of the frequently accepted LSODE, using adaptive stepsize. On a parallel architecture, the test problem scales well for about 13–39 nodes. With a constant number of spatial gridpoints per node, the increase in wall clock time with increasing problem size is small. Moreover, the PTD method runs well on a parallel machine. Even in a non-parallel context, while running at nearly their maximum stepsize for stability, PTD requires only about 1/25 the runtime required for FE. Hence we have demonstrated stability, accuracy and speed for the PTD method in a reasonable way.

8 Appendices

Several adjunct sections are supplied here to explain prerequisite material with which the reader may not already be familiar. To see the effect of the periodic motion of the earth upon photodissociation, the relevance of heat to advection-diffusion equations, or the significance of stiff springs in differential equations, it is necessary for the non-physicist reader to have some elementary notions of traveling waves, harmonic motion, thermodynamics, and light. Before attempting to comprehend the Chapman chemical mechanism for the distribution of various oxygen species in the atmosphere, it may be prudent for the non-chemist reader to examine some simple principles of rates of reactions and photodissociation, and to be exposed to some essentials of atmospheric chemistry. As the method being discussed and investigated is very mathematical, foundations from several areas of mathematics must be thoroughly grasped before trying to follow the derivation of the method. These areas are not extremely advanced but are not frequently used by computer scientists of all disciplines. Familiarity with these fundamentals will promote the understanding of the core of this thesis. Hence these concepts are reviewed here. Appendices are also included which cover the basics of numerical methods and parallel processing.

A Physics Background

A.1 Traveling Waves

Wave motion appears in almost every branch of physics. We are all familiar with water waves. There are also sound waves, as well as light waves, radio waves, and other electromagnetic waves. One formulation of the mechanics of atoms and subatomic particles is called wave mechanics. Clearly the properties and behavior of waves are very important in physics. For our purposes we shall need an understanding of the wave properties of light and the periodic variation of the reaction rates of atmospheric gases due to solar radiation. In either case our wave is a periodic variation of some physical quantity with respect to time or a spatial dimension or both. In this subsection we confine our attention to waves in deformable elastic media. These waves, among which ordinary sound waves in air are one example, might be called *mechanical waves*. The mathematical properties of this specific type of waves applies to waves of all kinds.

Mechanical waves originate in the displacement of some portion of an elastic medium from its normal position, causing it to oscillate about an equilibrium position. Because of the elastic properties of the medium, the disturbance is transmitted from one point to the next. This disturbance, or wave, consequently progresses through the medium. It is necessary to have a material medium to transmit mechanical waves. We do not need such a medium, however, to transmit electromagnetic waves, light passing freely, for example, through the near vacuum of space from the stars.

We can distinguish different kinds of mechanical waves by considering how the motions of the particles of matter are related to the direction of propagation of the waves themselves. If the motions of the matter particles conveying the wave are perpendicular to the direction of propagation of the wave itself, we then have a *transverse* wave. For example, when a vertical string under tension is set oscillating back and forth at one end, a transverse wave travels down the string, the disturbance moves along the string but the string particles vibrate at right angles to the direction of propagation of the disturbance.

Let us consider a long string stretched in the x -direction along which a transverse wave is traveling. At some instant of time, say $t = 0$, the shape of the string can be represented by

$$y = f(x), \quad t = 0, \quad (56)$$

where y is the transverse displacement of the string at the position x . Experiment shows that as time goes on, such a wave travels along the string without changing its form, provided internal frictional losses are small enough. At some time t later the wave has traveled a distance vt to the right, where v is the magnitude of the wave velocity, assumed constant. The equation of the curve (i.e. shape of the string) at the time t is therefore

$$y = f(x - vt), \quad t = t \quad (57)$$

This gives us the same waveform about the point $x = vt$ at time t as we had about $x = 0$ at the time $t = 0$. Equation (57) is the general equation representing a wave of *any* shape *traveling to the right*. To describe a particular shape we must specify exactly what the function f is.

Let us look more carefully at this equation. If we wish to follow a particular part (or phase) of the wave as time goes on, then in the equation we look at a particular value of y (say, the top of the pulse just described). Mathematically this means we look at how x changes with t when $(x - vt)$ has some particular fixed value. We see at once that as t increases x must increase in order to keep $(x - vt)$ fixed. Hence, equation (57) does in fact represent a wave traveling to the right (increasing x as time goes on). If we wished to represent a wave *traveling to the left*, we could write

$$y = f(x + vt), \quad (58)$$

for here the position x of some fixed phase ($x + vt$) of the wave decreases as time goes on. The velocity of a particular phase of the wave is easily obtained. For a particular phase of a wave traveling to the right we require that

$$x - vt = \text{constant} \quad (59)$$

Then differentiation with respect to time gives

$$\frac{dx}{dt} - v = 0 \quad \text{or} \quad \frac{dx}{dt} = v, \quad (60)$$

so that v is really the *phase velocity* of the wave. For a wave traveling to the left we obtain $-v$, in the same way, as its phase velocity.

The general equation of a wave can be interpreted further. Note that for any fixed value of the time t the equation gives y as a function of x . This defines a curve, and this curve represents the actual shape of the string at this chosen time. It gives us a snapshot of the wave at this time. Suppose, on the other hand, we wish to focus our attention on one point of the string, that is, a fixed value of x . Then the equation gives us y as a function of the time t . This describes how the transverse position of this point on the string changes with time.

Let us now consider a particular waveform, whose importance will soon become clear. Suppose that at the time $t = 0$ we have a wavetrain along the string given by

$$y = y_m \sin \frac{2\pi}{\lambda} x \quad (61)$$

The wave shape is a sine curve. The maximum displacement y_m is the *amplitude* of the sine curve. The value of the transverse displacement y is the same at x as it is at $x + \lambda$, $x + 2\lambda$, etc. The symbol λ is called the *wavelength* of the wavetrain and represents the distance between two consecutive points in the wave having the same phase. As time goes on let the wave travel to the right with a phase velocity v . Hence, the equation of the wave at the time t is

$$y = y_m \sin \frac{2\pi}{\lambda} (x - vt) \quad (62)$$

Notice that this has the form required for a traveling wave (equation 57).

The *period* T is the time required for the wave to travel a distance of one wavelength λ , so that

$$\lambda = vT \quad (63)$$

Putting this relation into the equation of the wave, we obtain

$$y = y_m \sin 2\pi \left(\frac{x}{\lambda} - \frac{t}{T} \right) \quad (64)$$

From this form it is clear that y , at any given time, has the same value at $x + \lambda$, $x + 2\lambda$, etc., as it does at x , and that y , at any given position, has the same value at the time $t + T$, $t + 2T$, etc., as it does at the time t .

To reduce equation (64) to a more compact form, we define two quantities, the *wave number* k and the *angular frequency* ω . They are given by

$$k = \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T} \quad (65)$$

In terms of these quantities, the equation of a sine wave traveling to the right (positive x -direction) is

$$y = y_m \sin(kx - \omega t) \quad (66)$$

For a sine wave traveling to the left (negative x -direction), we have

$$y = y_m \sin(kx + \omega t) \quad (67)$$

We will sometimes have need of an inverted sine wave traveling to the right, in which case we have

$$y = -y_m \sin(kx - \omega t) = y_m \sin(\omega t - kx) \quad (68)$$

Comparing equations (63) and (65), we see that the phase velocity v of the wave is given by

$$v = \frac{\lambda}{T} = \frac{\omega}{k} \quad (69)$$

If we fix our attention on a given point of the string, say $x = \pi/k$, the displacement y in equation (68) at that point can be written as

$$y = y_m \sin(\omega t + \phi), \quad (70)$$

where ϕ is called the *phase constant*, *phase shift*, or *phase angle*, and $\phi = -\pi$ in this case. Hence, any particular element of the string undergoes what is called *simple harmonic motion (SHM)* about its equilibrium position as this wavetrain travels along the string [28]

A.2 Simple Harmonic Motion

Consider a spring attached to a wall. Let the (horizontal) axis of the spring be chosen as an x -axis, and let the origin, $x = 0$, coincide with the endpoint of the spring in its normal, unstretched state. We assume that the positive x -direction points away from the wall. In what follows we imagine that we stretch the spring so slowly that it is essentially in equilibrium at all times (acceleration $a = 0$).

If we stretch the spring so that its endpoint moves to a position x , the spring will exert a force on the agent doing the stretching given to a good approximation by

$$F = -kx, \quad (71)$$

where k is a constant called the *force constant*, or *spring modulus*, or *stiffness constant* of the spring. Equation (71) is the *force law* for springs. The direction of the force is always opposite to the displacement of the endpoint from the origin. When the spring is stretched, $x > 0$ and F is negative, when the spring is compressed, $x < 0$ and F is positive. The force exerted by the spring is a *restoring force* in that it always points toward the origin. Real springs will obey equation (71), known as *Hooke's law*, if we do not stretch them beyond a limited range. We can think of k as the magnitude of the force per unit elongation. Thus very *stiff* springs have large values of k .

A body of mass m attached to an ideal spring of force constant k and free to move over a frictionless horizontal surface is an example of a *simple harmonic oscillator*. Note that there is a position (the equilibrium position) in which the spring exerts no force on the body. If the body is displaced to the right, the force exerted by the spring on the body points to the left and is given by $F = -kx$. If the body is displaced to the left, the force points to the right and is also given by $F = -kx$. In each case the force is a *restoring force*. The motion of the oscillating mass is *simple harmonic motion (SHM)*.

Let us apply Newton's second law,

$$F = ma, \quad (72)$$

to the motion. For the force F we substitute $-kx$ and for the acceleration a we substitute d^2x/dt^2 . This gives us

$$-kx = m \frac{d^2x}{dt^2}, \quad (73)$$

or

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \quad (74)$$

Equation (74) is called the *equation of motion* of a simple harmonic oscillator [28] Equation (74) can also be written

$$m\ddot{x} + kx = 0 \quad (75)$$

A.3 Damped Harmonic Motion

In the previous section we assumed that no frictional forces act on the oscillator. If this assumption held strictly, a mass on a spring would oscillate indefinitely. Actually, the amplitude of the oscillation gradually decreases to zero as a result of friction. The motion is said to be damped by friction and is called *damped harmonic motion (DHM)*. Often the friction arises from air resistance or internal forces. The magnitude of the frictional force usually depends on the speed. In most cases of interest the frictional force is proportional to the velocity $\dot{x}$ of the body but directed opposite to it.

The equation of motion of the damped simple harmonic oscillator is given by Newton's second law of motion, $F = ma$, in which F is the sum of the restoring force $-kx$ and the damping force $-c dx/dt$ [28]. Here c is a positive constant, called the *damping constant* [29]. We obtain [28]

$$F = ma, \quad (76)$$

or

$$-kx - c\frac{dx}{dt} = m\frac{d^2x}{dt^2}, \quad (77)$$

or

$$\frac{d^2x}{dt^2} + \frac{c}{m}\frac{dx}{dt} + \frac{k}{m}x = 0 \quad (78)$$

Equation (78) can also be written

$$m\ddot{x} + c\dot{x} + kx = 0 \quad (79)$$

A.4 Thermodynamics

For processes in which heat is involved the laws relating the appropriate macroscopic quantities (which include pressure, volume, temperature, internal energy, entropy, et al.) form the basis for the science of *thermodynamics*.

The sense of touch is the simplest way to distinguish hot bodies from cold bodies. By touch we can arrange bodies in the order of their hotness, deciding that A is hotter than B , B than C , etc. We speak of this as our *temperature (T)* sense [28]. More precisely, temperature is a measure of the average internal molecular kinetic energy of an object [30]. The *kelvin (K)*, unit of thermodynamic temperature, is the fraction $1/273.16$ of the thermodynamic temperature of the triple point of water [28]. *Heat (Q)* is the energy that is transferred from one object to another because of a difference in temperature [30].

Substances differ from one another in the quantity of heat needed to produce a given rise of temperature in a given mass. The ratio of the amount of heat energy ΔQ supplied to a body to its corresponding temperature rise ΔT is called the *heat capacity (C)* of the body, i.e.

$$C = \frac{\Delta Q}{\Delta T} \quad (80)$$

The heat capacity per unit mass of a body, called *specific heat (σ)*, is characteristic of the material of which the body is composed

$$\sigma = \frac{\Delta Q}{m\Delta T} \quad (81)$$

We properly speak, on the one hand, of the heat capacity of a penny but, on the other, of the specific heat of copper

The transfer of energy arising from the temperature difference between adjacent parts of a body is called *heat conduction*. Consider a slab of material of cross-sectional area A and thickness Δx , whose faces are kept at different temperatures. We measure the heat ΔQ that flows perpendicular to the faces in a time Δt . Experiment shows that ΔQ is proportional to Δt and to the cross-sectional area A for a given temperature difference ΔT , and that ΔQ is proportional to $\Delta T/\Delta x$ for a given Δt and A , providing both ΔT and Δx are small. I.e.,

$$\frac{\Delta Q}{\Delta t} \propto \frac{\Delta T}{\Delta x}, \quad (82)$$

approximately. In the limit of a slab of infinitesimal thickness dx , across which there is a temperature difference dT , we obtain the fundamental law of heat conduction, in which the *heat flow* (H) is given by

$$H = -KA \frac{dT}{dx} \quad (83)$$

Here H is the time rate of heat transfer across the area A , dT/dx is called the *temperature gradient*, and K is a constant of proportionality called the *thermal conductivity*.

We shall also need the concept of the *density* (ρ) of a substance, which is its mass divided by its volume [28]

$$\rho = \frac{m}{V} \quad (84)$$

A.5 The Navier-Stokes Equations

A set of differential equations for the motion of a fluid can be obtained by considering the pressure, gravitational, and viscous forces acting on a fluid element. These equations are called the *Navier-Stokes equations* after L. M. Navier (1785–1836) and G. G. Stokes (1819–1903), who are credited with their development. These equations for flow of an incompressible fluid in a cartesian coordinate system are

$$\begin{aligned} \rho g_x - \frac{\partial p}{\partial x} + \nu \nabla^2 u &= \rho \frac{du}{dt}, \\ \rho g_y - \frac{\partial p}{\partial y} + \nu \nabla^2 v &= \rho \frac{dv}{dt}, \\ \rho g_z - \frac{\partial p}{\partial z} + \nu \nabla^2 w &= \rho \frac{dw}{dt}, \end{aligned} \quad (85)$$

where g is gravitational acceleration, ρ is the *mass density*, p the *pressure*, ν the *kinetic viscosity*, and $V = u\hat{i} + v\hat{j} + w\hat{k}$ the *velocity* of the fluid. It is assumed that the coordinate system is arbitrarily defined. Therefore, in the above equations ρg_x , ρg_y , and ρg_z are the gravitational forces per unit of volume in the x , y , and z direction, respectively [17]. For a rigorous derivation of equations (85), see [31].

A.6 The Advection-Diffusion Equation

Advection is defined as the *horizontal movement* of a mass of air. *Convection* is defined as the *vertical movement* of a mass of air. In a 3-D system, a fluid typically moves both horizontally and vertically, to a certain extent. Advection and convection are often used interchangeably to refer to movement of air in any direction. Thus, the advection-diffusion equation is often referred to as the convection-diffusion equation in some circles.

Diffusion is defined as the intermingling of molecules or other particles as a result of their random thermal motion. *Conduction* is defined as the transmission of energy by a

medium which does not involve movement of the medium itself. The pure diffusion equation is identical, except for dimensions, to the heat conduction equation.

The processes of mass transfer in fluids are modeled by partial differential equations (in particular, the Navier-Stokes equations). Many of our day-to-day experiences involve the process of mass transfer by convection and diffusion. As smoke pours from a tall chimney, the moving air currents *convect* or transport the smoke away at the speed of the wind, while at the same time the smoke mixes with or *diffuses* through the air, carrying it until the smoke concentration is so low that we believe the smoke is no longer there, since we cannot see it. Pollution discharged to streams and rivers is also transported and mixed in much the same way.

In the simplest, 1-D motion (x -direction only), the fluxes f_C due to convection and f_D due to diffusion of a quantity being transported across a given section x at time t are

$$f_C = au, \quad f_D = -Du_x, \quad (86)$$

where a is the speed of the main fluid (centimeters per second), u is the concentration of the transported quantity, say smoke or dye or bacteria, per unit volume (grams per cubic centimeter), and D is the diffusion coefficient (centimeters squared per second). Here f_D is given by the *Fick's rate equation* that relates the diffusive flux to the negative gradient of concentration. When the diffusion results from the random vibration of molecules in a gas or liquid, Fick's law is valid and D is often essentially a constant that can be determined experimentally. In the wind above the chimney, the diffusion is likely to result from the motion of the turbulent eddies in the wind, Fick's law and constant D are then simplifying assumptions used to gain simple, but approximate, results.

An analysis of a slice Δx thick through a 1-D stream leads to a conservation equation for the transported mass. The resulting partial differential equation is

$$u_t + au_x = Du_{xx} \quad (87)$$

and is called the 1-D *advection-diffusion equation* [19].

The 3-D *advection-diffusion equation* is

$$\frac{\partial u}{\partial t} + a \cdot \nabla u = D \nabla^2 u \quad (88)$$

For a rigorous derivation of (88), see [32].

A 6.1 Pure Convection

Suppose that the transported quantity is a red dye of strength u that diffuses slowly in water so that the dye cloud has a motion governed essentially by convection when a is fairly large. A source of dye of concentration u_0 is available at a point in a 1-D stream of constant speed a . Putting the coordinate origin at the source and turning the source on to full strength at time zero lead to a model for $u(x, t)$

$$u_t + au_x = 0, \quad 0 < x, \quad 0 < t \quad (89)$$

$$u(0, t) = u_0, \quad 0 < t \quad (90)$$

$$u(x, 0) = 0, \quad 0 \leq x \quad (91)$$

We assume that u and u_x approach zero as $x \rightarrow \infty$ for all t . Note that we have a model with a first-order partial differential equation. Equation (89) is the 1-D *pure convection equation* (a.k.a. *advection equation*) [19].

A.6.2 Pure Diffusion

Suppose, in the previous example, that the velocity of the fluid a is very slow so that diffusion dominates the convection. The model would then be modified to be, for $D > 0$,

$$u_t = Du_{xx}, \quad 0 < x, \quad 0 < t \quad (92)$$

$$u(0, t) = u_0, \quad 0 < t \quad (93)$$

$$u(x, 0) = 0, \quad 0 \leq x \quad (94)$$

$$|u(x, t)| < \infty \quad (95)$$

with u and $u_x \rightarrow 0$ as $x \rightarrow \infty$ for all t . Equation (92) is second-order and is the 1-D *diffusion equation* [19]. For a non-rigorous derivation of (92), see [33].

A.6.3 The Heat Equation

The flow of heat in a conducting solid, with certain simplifying assumptions, results in the same model employing partial differential equations as for pure diffusion (except for dimensions). The 3-D *heat equation* is

$$\frac{\partial u}{\partial t} = k \nabla^2 u, \quad (96)$$

where

$$k = \frac{K}{\rho\sigma} \quad (97)$$

is called the *thermal diffusivity*, $K(x, y, z, u)$ is the *thermal conductivity* of the solid medium, assumed constant here, ρ is the *density* of the solid (mass per unit volume), also assumed constant, and σ is the *specific heat* of the material of the solid (heat per unit mass per unit of temperature). For a rigorous derivation of (96), see [19].

A.7 Light

Light has both wave-like and particle-like properties. As a wave, it is a combination of oscillating electric and magnetic fields perpendicular to each other and to the direction of propagation. The distance between consecutive peaks is the *wavelength* λ and the number of complete cycles passing a fixed point in 1 s is the *frequency* ν . They are inversely proportional through the relationship

$$\lambda = \frac{c}{\nu}, \quad (98)$$

where c is the *velocity of light in a vacuum*.

Considered as a particle, the *energy* E of a quantum of light is

$$E = h\nu = \frac{hc}{\lambda}, \quad (99)$$

where h is *Planck's constant* [3].

B Chemistry Background

B.1 Rates of Reactions

Different chemical reactions take place at different rates. Some reactions, such as the reaction between $AgNO_3(aq)$ and $KCl(aq)$ to produce a precipitate of $AgCl(s)$, seem to occur almost instantaneously, whereas other reactions, such as the reaction between $H_2(g)$ and $N_2(g)$ to produce $NH_3(g)$, occur very slowly. The reaction rate law, which must be determined by experiment, tells us how the rate of a reaction depends on the concentration of the reactants and of other added substances, such as catalysts.

Consider the decomposition of hydrogen peroxide in aqueous solution

Because a gaseous product $O_2(g)$ forms, we can determine how its concentration increases with time by measuring the increase in pressure above the reaction mixture. Let us see how we can use this measurement to define a reaction rate.

Suppose that we know the concentration of the oxygen gas at some time to be $[O_2]_1$, and suppose we find that at some later time it is $[O_2]_2$. We can write the change in its concentration as

$$\Delta[O_2] = [O_2]_2 - [O_2]_1 \quad (101)$$

Because the concentration of the product increases with time, we know that $\Delta[O_2]$ must be positive. We can now define a *reaction rate* as the average rate at which oxygen is produced, or the change in concentration divided by the elapsed time

$$\frac{\Delta[O_2]}{\Delta t} \quad (102)$$

Note that the rate of a reaction is a positive quantity. Its units are moles per liter per second ($\text{mol L}^{-1} \text{s}^{-1}$ or M s^{-1}), or, more generally, moles per liter per unit time.

We can also define a reaction rate by examining how quickly the reactant is consumed. Now we are interested in the average number of moles per liter *reacted* per second. Because the concentration of H_2O_2 is decreasing, $\Delta[H_2O_2]$ is a negative quantity, but we can insert a minus sign to make the reaction rate positive

$$-\frac{\Delta[H_2O_2]}{\Delta t} \quad (103)$$

The relation between the two equations depends on the equation for the reaction. In this case, we know the rate at which O_2 is produced is equal to one half the rate at which H_2O_2 is consumed, because two H_2O_2 molecules react for each O_2 molecule produced. Thus, for the reaction rate R , we have

$$R = -\left(\frac{1}{2}\right) \left(\frac{\Delta[H_2O_2]}{\Delta t}\right) = \frac{\Delta[O_2]}{\Delta t} \quad (104)$$

The rate of the reaction for the decomposition of $N_2O_5(g)$ in

can be expressed as

$$R = -\left(\frac{1}{1}\right) \left(\frac{\Delta[N_2O_5]}{\Delta t}\right) = \left(\frac{1}{2}\right) \left(\frac{\Delta[NO_2]}{\Delta t}\right) = \left(\frac{1}{1/2}\right) \left(\frac{\Delta[O_2]}{\Delta t}\right) \quad (106)$$

Notice that the numerical factor in the denominator of each expression is the same as the balancing coefficient of the species in the chemical equation.

Thus, for the reaction

we define the rate to be

$$R = -\left(\frac{1}{2}\right) \left(\frac{\Delta[O_3]}{\Delta t}\right) = \left(\frac{1}{3}\right) \left(\frac{\Delta[O_2]}{\Delta t}\right) \quad (108)$$

Table (5) gives the numerical values of $[N_2O_5]$, $[NO_2]$, and $[O_2]$ that correspond to reaction (105), as a function of time at 45°C. An inspection of the data in table (5) shows that the reaction rate decreases as $[N_2O_5]$ decreases. For example, the rate of decomposition of N_2O_5 over the first 10 minutes of the reaction is

$$R = -\frac{\Delta[N_2O_5]}{\Delta t} = 3.2 \times 10^{-4} \text{ mol L}^{-1} \text{ min}^{-1} \quad (109)$$

whereas the rate over the period 10 min to 20 min is

$$R = 2.4 \times 10^{-4} \text{ mol L}^{-1} \text{ min}^{-1} \quad (110)$$

t/min	$[N_2O_5]/M$	$[NO_2]/M$	$[O_2]/M$
0	1.24×10^{-2}	0	0
10	0.92×10^{-2}	0.64×10^{-2}	0.16×10^{-2}
20	0.68×10^{-2}	1.12×10^{-2}	0.28×10^{-2}
30	0.50×10^{-2}	1.48×10^{-2}	0.37×10^{-2}
40	0.37×10^{-2}	1.74×10^{-2}	0.44×10^{-2}
50	0.27×10^{-2}	1.92×10^{-2}	0.48×10^{-2}
60	0.20×10^{-2}	2.08×10^{-2}	0.52×10^{-2}
70	0.14×10^{-2}	2.18×10^{-2}	0.55×10^{-2}
80	0.11×10^{-2}	2.26×10^{-2}	0.57×10^{-2}
90	0.08×10^{-2}	2.32×10^{-2}	0.58×10^{-2}
100	0.06×10^{-2}	2.36×10^{-2}	0.59×10^{-2}

Table 5 Concentration of $N_2O_5(g)$, $NO_2(g)$ and $O_2(g)$ as a function of time

It is important to realize that, given the initial concentrations in table (5), the concentrations of $NO_2(g)$ and $O_2(g)$ can be calculated from the concentration of $N_2O_5(g)$ at any time.

We have noted that the rate of a reaction changes as the reactants are consumed and the products are formed. This change occurs because the rates of chemical reactions usually depend on the concentrations of one or more of the reactants. The mathematical equation that gives this dependence is called the *rate law* of the reaction. Many experiments show that the rate of a reaction usually is proportional to the concentrations of the reactants raised to small integer powers. Thus, for the case of the thermal decomposition of N_2O_5 , we will assume that

$$R \propto [N_2O_5]^x \quad (111)$$

We can write this proportionality as an equation by inserting a proportionality constant

$$R = k[N_2O_5]^x \quad (112)$$

The proportionality constant k in a rate law is called the *rate constant* of the reaction.

The value of x in equation (112) must be determined *experimentally*; it is *not* necessarily the same as the balancing coefficient of N_2O_5 in the chemical equation. *There is no relation*

between the balancing coefficients in a chemical equation and the reaction rate law. For example, the rate law for the reaction

is

$$R = k[\text{H}_2\text{O}_2] \quad (114)$$

whereas the rate law for the reaction

is

$$R = k[\text{NOBr}]^2 \quad (116)$$

In practice, rate laws often are determined from data involving reaction rates at the early stage of reactions. Using the *method of initial rates*, we measure the rate of a reaction over an initial time interval that is short enough so that the concentrations of the reactants do not vary appreciably from their initial values. If we use zeros as subscripts to denote the initial values of the rate and of the various concentrations, then for any reaction described by an equation of the form

we can write

$$R_0 = k[A]_0^x[B]_0^y[C]_0^z \quad (118)$$

We can then determine the values of x , y , and z by varying the initial concentration of each reactant in turn, while keeping the other reactant concentrations constant. As a simple example, let's consider the N_2O_5 decomposition reaction, in which there is only one reactant

Suppose that we run this reaction using successively doubled concentrations of N_2O_5 , and obtain the initial-rate data in table (6). Notice that when the initial concentration, $[\text{N}_2\text{O}_5]_0$,

Run	$[\text{N}_2\text{O}_5]_0/\text{mol L}^{-1}$	$R_0/\text{mol L}^{-1} \text{ s}^{-1}$
1	0.010	0.018
2	0.020	0.036
3	0.040	0.072

Table 6 Initial rate data for reaction $\text{N}_2\text{O}_5(g) \rightarrow 2\text{NO}_2(g) + \frac{1}{2}\text{O}_2(g)$

is increased by a factor of 2, the initial rate R_0 also increases by a factor of 2. These results show that R_0 is directly proportional to $[\text{N}_2\text{O}_5]_0$, so we can write

$$R_0 = k[\text{N}_2\text{O}_5]_0 \quad (120)$$

showing that $x = 1$ in equation (118).

Extensive experimental studies show that in most cases the reaction rate law determined from initial-rate data describes the reaction rate as the reaction proceeds. Thus, we can drop the subscript zero in equation (120) to obtain the rate law

$$R = k[\text{N}_2\text{O}_5] \quad (121)$$

Because $[\text{N}_2\text{O}_5]$ is raised to the first power in equation (121), the rate law is said to be a *first-order rate law*, and the reaction is said to be a *first-order reaction*. We say that the rate law is first-order in $[\text{N}_2\text{O}_5]$.

We can determine the numerical value of the rate constant k in equation (121) by using the tabulated initial-rate data. If we substitute the fact that $R_0 = 0.072 \text{ mol L}^{-1} \text{ h}^{-1}$ when $[N_2O_5]_0 = 0.040 \text{ mol L}^{-1}$, then we obtain

$$k = \frac{R_0}{[N_2O_5]_0} = 1.8 \text{ h}^{-1} \quad (122)$$

Notice that the units of the rate constant for a first-order reaction are reciprocal time, i.e. time^{-1} .

So far we have encountered only first-order reactions. Although it will not be demonstrated here, the rate law for the reaction described by

is

$$R = k[NO_2]^2 \quad (124)$$

Because the exponent of $[NO_2]$ in the rate law is 2, we say that the reaction *rate law is second-order* with respect to NO_2 , and because $[NO_2]$ is the only concentration that appears in the rate-law expression, we say that the decomposition of $NO_2(g)$ to $NO(g)$ and $O_2(g)$ is a *second-order reaction*.

We can also determine rate laws for reactions involving more than one reactant. For example, the reaction

has the reaction rate law

$$R = k[NO_2][F_2] \quad (126)$$

with

$$k = 1.00 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1} \quad (127)$$

This rate law is first-order in both $[NO_2]$ and $[F_2]$, and we say that it is second-order overall because the sum of the exponents is two. Note that the units of k for a second-order reaction are reciprocal concentration per time, i.e. $\text{M}^{-1} \text{ s}^{-1}$.

More generally, if a reaction rate law is of the form

$$R = k[A]^x[B]^y[C]^z, \quad (128)$$

then the rate law is x -order in $[A]$, y -order in $[B]$, and z -order in $[C]$, with an overall order of $x + y + z$. [11]

B.2 Photodissociation

The principle of photochemical processes can be summarized as follows. A certain atmospheric gaseous component A absorbs a given band of solar radiation in the ultraviolet or visible spectrum. Due to the energy of the absorbed photon $h\nu$, A is changed to an excited state A^* . Because of this energy, the molecule decomposes, or reacts with another species B , or fluoresces, or undergoes quenching, or transfers its energy to another species [1]. We will consider here only the molecular decomposition or dissociation. The process may be symbolized in the following way

The last step in this sequence is termed a *primary photochemical process*. We have

$$\frac{d[A^*]}{dt} = k_a[A], \quad (130)$$

where k_a is the *absorption rate of photons*. The rate R of the primary photochemical process will be

$$R = \frac{d[D_1]}{dt} = k_a \phi [A], \quad (131)$$

where ϕ is the so-called *quantum yield*. Its value is equal to the ratio of the number of A reacted, to that of excited molecules. In photochemical reactions, the rate constant is given by the product of the absorption rate and the quantum yield [34]

B.3 The Chapman Mechanism

The Chapman mechanism for oxygen-containing chemistry has been dealt with previously [15, 22, 23, 10] and was the first attempt (in the late 1930s) to explain the ozone distribution in the stratosphere. The Chapman model assumes that oxygen-containing chemistry alone is sufficient to explain ozone distribution. In this case, only the chemistry for O , O_2 , and O_3 is included.

Let ${}_1u = {}_1u(x, t)$ denote the concentration of atomic oxygen (O) and let ${}_2u = {}_2u(x, t)$ denote the concentration of molecular ozone (O_3). The concentration of molecular oxygen (O_2 , denoted by ${}_3u = \text{constant}$) is significantly larger in the earth's atmosphere than atomic oxygen or ozone and is therefore assumed to be constant in this simple model, as with most atmospheric simulations.

The formation of the stratospheric ozone layer can be understood most simply on the basis of a reaction model composed of a minimum set of four elementary processes: (a) the attachment of oxygen atoms to molecular oxygen, leading to the formation of ozone, (b) the destruction of ozone by its reaction with oxygen atoms, (c) the dissociation of oxygen molecules by solar radiation in the wavelength region 180–240 nm, and (d) the photodissociation of ozone in the Hartley band between 200 and 300 nm. The reactions may be written

In reaction (132), M denotes as usual an inert third body, which in the atmosphere is supplied by either nitrogen or oxygen [1].

These reactions have reaction rate coefficient functions [26] k_1 , k_2 , k_3 , and k_4 respectively. The first two reactions are thermal reactions, so k_1 and k_2 can be taken as constants. The last two reactions, however, are photochemical in nature (involving the absorption of light energy — $h\nu$), and change with the rising/setting of the sun. Thus, k_3 and k_4 have diurnal cycles and vary with time.

The ordinary differential system describing the time-evolving behavior of these chemical concentrations subject to the four reactions is taken from Aro [10]

$$\frac{d_1u}{dt} = {}_1P - ({}_1L)({}_1u) \quad (136)$$

$$\frac{d_2u}{dt} = {}_2P - ({}_2L)({}_2u), \quad (137)$$

where ${}_1u$ and ${}_2u$ are in units of mol. Here, ${}_1P$ and ${}_2P$ denote rates of production and ${}_1L$ and ${}_2L$ denote rates of loss. These production/loss rates are given by

$$\begin{aligned} {}_1P &= 2(k_3)({}_3u) + (k_4)({}_2u) \\ {}_2P &= (k_1)({}_3u)({}_1u) \\ {}_1L &= (k_1)({}_3u) + (k_2)({}_2u) \\ {}_2L &= (k_2)({}_1u) + k_4 \end{aligned} \quad (138)$$

The constant values are $3u = 3.7 \times 10^{16} \text{ mol}$, $k_1 = 1.63 \times 10^{-16} \text{ mol}^{-2} \text{ s}^{-1}$, and $k_2 = 4.66 \times 10^{-16} \text{ mol}^{-2} \text{ s}^{-1}$. The time varying rate coefficient functions (which model chemical reactions driven by the absorption of sunlight) are given by

$$k_j(t) = \begin{cases} \exp\left(\frac{a_j}{\cos(-\omega t)}\right) & \text{if } \cos(-\omega t) < 0 \\ 0 & \text{otherwise} \end{cases}, \quad j = 3, 4 \quad (139)$$

with $a_3 = 22.62$, $a_4 = 7.601$, $\omega = 2\pi/(86,400 \text{ s})$, and the k_j are in units of $\text{mol}^{-1} \text{ s}^{-1}$. Note that the constant $86,400 \text{ s}$ is one day, so that the time varying reaction rate coefficient functions (k_3 and k_4) have 24 h *period* T .

C Mathematics Background

C.1 Power Series

A *power series* is a series of the form

$$c_0 + c_1(x - a) + c_2(x - a)^2 + \cdots + c_n(x - a)^n + \cdots, \quad (140)$$

in which a and the c_i , $i = 0, 1, 2, \dots$, are constants. If a particular value is given to x , we then obtain an infinite series of numbers. The special case $a = 0$ occurs frequently, in which case the series becomes

$$c_0 + c_1x + c_2x^2 + c_3x^3 + \cdots + c_nx^n + \cdots \quad (141)$$

Most often, we use the Σ -notation, writing

$$\sum_{n=0}^{\infty} c_n(x - a)^n \quad \text{and} \quad \sum_{n=0}^{\infty} c_nx^n \quad (142)$$

If a power series converges for certain values of x , we may define a function of x by setting

$$f(x) = \sum_{n=0}^{\infty} c_n(x - a)^n \quad \text{or} \quad g(x) = \sum_{n=0}^{\infty} c_nx^n \quad (143)$$

for those values of x . The majority of functions which are encountered in the principal problems of mathematics and its applications to science and technology can be represented by convergent power series (with certain exceptions for the value a) [35]. A function that can be locally represented by a power series is called an *analytic function*. The class of analytic functions is *closed* with respect to the fundamental operations of arithmetic, algebra and analysis.

C.1.1 Taylor's Series

A power series of the form

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x - a)^n \quad (144)$$

is called the *Taylor series for f about the point a* or the *expansion of f into a power series about a* [35].

C.1.2 Maclaurin Series

For the special case $a = 0$, the Taylor series (144) is

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n \quad (145)$$

The right side of (145) is called the *Maclaurin series* for f [35].

C.1.3 Taylor's Theorem with Remainder

Suppose that $f, f', f^{(2)}, \dots, f^{(n)}, f^{(n+1)}$ are all continuous on some interval containing a and b . Then there is a number ξ between a and b such that

$$f(b) = f(a) + \frac{f'(a)}{1!} (b - a) + \frac{f^{(2)}(a)}{2!} (b - a)^2 + \cdots + \frac{f^{(n)}(a)}{n!} (b - a)^n + \frac{f^{(n+1)}(\xi)}{(n+1)!} (b - a)^{n+1}$$

$$+ \frac{f^{(n)}(a)}{n!}(b-a)^n + \frac{f^{(n+1)}(\xi)(b-a)^{n+1}}{(n+1)!}, \quad (146)$$

i.e., the remainder R_n is given by the formula

$$R_n = \frac{f^{(n+1)}(\xi)(b-a)^{n+1}}{(n+1)!} \quad (147)$$

C.2 Linear Systems

Central to the study of *linear algebra* is the algebraic system known as a *vector space* $\mathbf{V}$ over a *field* $\mathbf{F}$. Although much of what follows applies to general vector spaces, for our purposes we shall need only the concept of the n -dimensional real vector space $\mathcal{R}^n$ over the field of real numbers $\mathcal{R}$, with which most computer scientists are already familiar.

A general *linear system* of m linear equations in n unknowns $x_1, \dots, x_n$ has the form

$$\begin{array}{ccccccccccc} E_1 & a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + & & + & a_{1n}x_n & = & b_1 \\ E_2 & a_{21}x_1 & + & a_{22}x_2 & + & a_{23}x_3 & + & & + & a_{2n}x_n & = & b_2 \\ E_3 & a_{31}x_1 & + & a_{32}x_2 & + & a_{33}x_3 & + & & + & a_{3n}x_n & = & b_3 \end{array} \quad (148)$$

$$E_m \quad a_{m1}x_1 \quad + \quad a_{m2}x_2 \quad + \quad a_{m3}x_3 \quad + \quad \quad + \quad a_{mn}x_n \quad = \quad b_m,$$

where the coefficients a_{ij} are real numbers and the constants b_i are also in R . Our problem is to determine all points $(x_1, x_2, x_3, \dots, x_n)^T \in \mathcal{R}^n$ whose components satisfy all the equations in system (148)

System (148) can be expressed more efficiently in terms of matrix multiplication as

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{1n} \\ a_{21} & a_{22} & a_{23} & a_{2n} \\ a_{31} & a_{32} & a_{33} & a_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & a_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_m \end{pmatrix} \quad (149)$$

If we use matrix multiplication to compute the i th entry in this column-vector equation (149), we obtain the i th equation in system (148)

Let us use the notations $\hat{x}$, $\hat{b}$, etc., to denote both n -dimensional row vectors and n -dimensional column vectors in $\mathcal{R}^n$, depending on the context. E.g. equation (149) may be written

$$A\hat{x} = \hat{b}, \quad (150)$$

where the $m \times n$ matrix $A = (a_{ij})$ is the *coefficient matrix*,

$$\hat{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} \quad (151)$$

is the *column* vector of unknowns, and

$$\hat{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_m \end{pmatrix} \quad (152)$$

is the *column* vector of constants. For our purposes, we shall say that the matrix A *maps* or *transforms* the vector $\hat{x}$ to the vector $\hat{b}$. We now face the problem of finding all column vectors $\hat{x}$ such that (150) holds [36].

C.2.1 Matrices

To simplify computations, the matrix A in (150) can be dealt with instead of the equations in (148). This gives rise to matrix methods. Although these matrix methods can be accomplished in principle, the calculation in actual practice is often so computationally intensive as to render the problem impractical or altogether impossible. An understanding of the properties of some special matrices is therefore useful in selecting or massaging a numerical method. Several types of matrices, operations and principles are described briefly here, without proof.

An $m \times n$ *matrix* (plural *matrices*) is a rectangular array of elements with m rows and n columns in which not only is the value of an element important, but also its position in the array. E.g. A in (149, 150).

A $1 \times n$ matrix $\hat{x} = (x_1, x_2, \dots, x_n)$ is called an *n-dimensional row vector*. An $n \times 1$ matrix $\hat{x} = (x_1, x_2, \dots, x_n)^T$ is called an *n-dimensional column vector*. E.g. $\hat{x}$ in (149–151).

Let A be an $m \times n$ matrix and B an $n \times r$ matrix. The *matrix product*, or *matrix-matrix product* of A and B , denoted AB , is an $m \times r$ matrix C whose entries c_{ij} are given by

$$c_{ij} = \sum_{k=1}^n a_{ik} b_{kj}, \quad \forall i = 1, 2, \dots, m, \quad \text{and} \quad \forall j = 1, 2, \dots, r \quad (153)$$

Let A be an $m \times n$ matrix and $\hat{x}$ be an n -dimensional vector. The *matrix-vector product* of A and $\hat{x}$, denoted $A\hat{x}$, is an m -dimensional column vector $\hat{b}$ whose entries b_i are given by

$$b_i = \sum_{k=1}^n a_{ik} x_k, \quad \forall i = 1, 2, \dots, m \quad (154)$$

E.g. the product $A\hat{x}$ in (149, 150).

A *square* matrix has the same number of rows as columns.

A *diagonal* matrix is a square matrix $D = (d_{ij})$ with $d_{ij} = 0$ whenever $i \neq j$. E.g.

$$A = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 20 \end{pmatrix} \quad (155)$$

The *identity matrix* of order n , $I_n = (\delta_{ij})$, is the diagonal matrix with entries

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j \end{cases} \quad (156)$$

When the size of I_n is clear, this matrix is sometimes simply written as I .

An *upper-triangular* $n \times n$ matrix $U = (u_{ij})$ has entries $u_{ij} = 0, \forall i > j$, i.e. the elements below the main diagonal are zero. We will call a matrix *strictly upper-triangular* if it is an upper-triangular matrix in which the diagonal elements are zero, i.e. the elements on and below the main diagonal are all zero. Similarly, a *lower-triangular* $n \times n$ matrix $L = (l_{ij})$ has entries $l_{ij} = 0, \forall i < j$, i.e. the elements above the main diagonal are zero. We will call a matrix *strictly lower-triangular* if it is a lower-triangular matrix in which the diagonal elements are zero, i.e. the elements on and above the main diagonal are all zero.

If $\exists$ an $n \times n$ matrix $A^{-1} \ni AA^{-1} = A^{-1}A = I$, then the matrix A^{-1} is called the *inverse* of A . It can be shown that to calculate the inverse of a general $n \times n$ matrix requires $O(n^3)$ multiplications/divisions and additions/subtractions. For the special case of

a diagonal matrix A , however, the inverse A^{-1} is obtained by simply inverting the diagonal elements, and therefore requires only n divisions. E.g. the inverse of A in equation (155) is

$$A^{-1} = \begin{pmatrix} \frac{1}{10} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{20} \end{pmatrix} \quad (157)$$

The *transpose* of an $m \times n$ matrix $A = (a_{ij})$ is the $n \times m$ matrix $A^T = (a_{ji})$.

A square matrix A is said to be *symmetric* if $A = A^T$.

The *determinant* of an $n \times n$ matrix A , denoted $\det A$ or $|A|$, is defined recursively as follows

1. If $A = (a)$ is a 1×1 matrix, then $\det A = a$.
2. If A is an $n \times n$ matrix, with $n > 1$, then the *minor* M_{ij} is the determinant of the $(n-1) \times (n-1)$ submatrix of A obtained by deleting the i th row and j th column of the matrix A , and the determinant of A is given either by

$$\det A = \sum_{j=1}^n (-1)^{i+j} a_{ij} M_{ij}, \quad \text{for any } i = 1, 2, \dots, n, \quad (158)$$

or

$$\det A = \sum_{i=1}^n (-1)^{i+j} a_{ij} M_{ij}, \quad \text{for any } j = 1, 2, \dots, n \quad (159)$$

E.g. the determinant of the matrix

$$A = \begin{pmatrix} 10 & 5 & 0 \\ 2 & 30 & -4 \\ 0 & 3 & 20 \end{pmatrix} \quad (160)$$

is 5920. It can be shown that to calculate the determinant of a general $n \times n$ matrix requires $O(n!)$ multiplications/divisions and additions/subtractions. Even for relatively small values of n , the number of calculations becomes unwieldy. The calculation of the determinant of a diagonal matrix, however, requires only n multiplications and is simply the product of the diagonal elements. E.g. the determinant of A in equation (155) is 6000.

If the linear system $A\hat{x} = \hat{b}$ has a unique solution for each n -dimensional column vector $\hat{b}$, then we say that the matrix A is *non-singular*. This is equivalent to saying that $A\hat{x} = \hat{0}$ has the unique solution $\hat{x} = \hat{0}$, or to say that the inverse A^{-1} exists, or to say that $\det A \neq 0$. Otherwise the matrix A is *singular*.

The $n \times n$ matrix A is said to be *Strictly Diagonally Dominant (SDD)* when

$$|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^n |a_{ij}|, \quad \forall i = 1, 2, \dots, n \quad (161)$$

A matrix A is *Positive Definite (PD)* if it is symmetric and if $\hat{x}^T A \hat{x} > 0$ for every n -dimensional column vector $\hat{x} \neq \hat{0}$.

An $n \times n$ matrix A is called a *band matrix* or *banded matrix* if $\exists$ integers $p, q, \exists 1 < p, q < n$, and $a_{ij} = 0$ whenever $i + p \leq j$, or $j + q \leq i$. The *bandwidth* of a band matrix is defined to be $w = p + q - 1$. E.g. the matrix A in equation (160) is a band matrix with $p = q = 2$ and bandwidth $w = 3$.

The definition of band matrices forces those matrices to concentrate all their nonzero entries about the diagonal. Two special cases of band matrices that occur often in practice

have $p = q = 2$ and $p = q = 4$. The matrix of bandwidth 3, occurring when $p = q = 2$, is encountered in connection with the study of cubic spline approximations. These matrices are called *tridiagonal*, since they have (loosely speaking) a main diagonal of width 3. The matrix A in equation (160) above is tridiagonal.

The *norm* $\|\hat{x}\|$ of a n -dimensional vector $\hat{x}$ can be defined in several ways, one of which is

$$\|\hat{x}\| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}, \quad (162)$$

which is called the l_2 norm of $\hat{x}$ [37].

C.2.2 Eigenvalue Problem

Let

$$A\hat{x} = \hat{b}, \quad (163)$$

represent an $n \times n$ linear system. A nonzero vector $\hat{x}$ is called an *eigenvector* or *characteristic vector* of A if there exists a scalar λ such that

$$A\hat{x} = \lambda\hat{x}, \quad (164)$$

i.e. A maps $\hat{x}$ into a scalar multiple of itself. The scalar λ is called the *eigenvalue* or *characteristic value* of A corresponding to $\hat{x}$ [38]. The set of eigenvalues is called the *spectrum* of A . The largest of the absolute values of the eigenvalues of A is called the *spectral radius* of A , denoted $\rho(A)$.

The problem of determining the eigenvalues and eigenvectors of a matrix is called an *eigenvalue problem*. Problems of this type occur in connection with physical and technical applications [29].

C.3 Lipschitz Condition

A function $\phi(\hat{y})$ is said to satisfy a *Lipschitz condition* in a neighborhood $N(\hat{y})$ of $\hat{y}$ if $\forall \hat{y}^* \in N(\hat{y})$,

$$\|\phi(\hat{y}) - \phi(\hat{y}^*)\| \leq L\|\hat{y} - \hat{y}^*\| \quad (165)$$

where L is called the Lipschitz constant. This condition essentially says that the magnitude of the slope of the line through $(\hat{y}, \phi(\hat{y}))$ and $(\hat{y}^*, \phi(\hat{y}^*))$ is bounded everywhere in the neighborhood [14].

C.4 Differential Equations

An equation involving one dependent variable and its derivatives with respect to one or more independent variables is called a *differential equation (DE)*. Many of the general laws of nature — in physics, chemistry, biology, and astronomy — find their most natural expression in the language of differential equations. Applications also abound in mathematics itself, especially in geometry, and in engineering, economics, and many other fields of applied science.

It is easy to understand the reason behind this broad utility of differential equations. The reader will recall that if $y = f(x)$ is a given function, then its derivative dy/dx can be interpreted as the rate of change of y with respect to x . In any natural process, the variables involved and their rates of change are connected with one another by means of the basic scientific principles that govern the process. When this connection is expressed in mathematical symbols, the result is often a differential equation.

The following example may illuminate these remarks. According to Newton's second law of motion, the acceleration a of a body of mass m is proportional to the total force F acting on it, with $1/m$ as the constant of proportionality, so that $a = F/m$ or

$$ma = F \quad (166)$$

Suppose, for instance, that a body of mass m falls freely under the influence of gravity alone. In this case the only force acting on it is mg , where g is the acceleration due to gravity. If y is the distance down to the body from some fixed height, then its acceleration is d^2y/dt^2 , and (166) becomes

$$m \frac{d^2y}{dt^2} = mg \quad (167)$$

or

$$\frac{d^2y}{dt^2} = g \quad (168)$$

If we alter the situation by assuming that air exerts a resisting force proportional to the velocity, then the total force acting on the body is $mg - k(dy/dt)$, and (166) becomes

$$m \frac{d^2y}{dt^2} = mg - k \frac{dy}{dt} \quad (169)$$

Equations (168) and (169) are the differential equations that express the essential attributes of the physical processes under consideration [39].

Various analytical methods exist for solving DEs. We shall not examine them here, since we are interested in numerical methods.

C 4.1 Ordinary Differential Equations

As further examples of differential equations, we list the following

$$\frac{dy}{dt} = -ky, \quad (170)$$

$$m \frac{d^2y}{dt^2} = -ky, \quad (171)$$

$$\frac{dy}{dx} + 2xy = e^{-x^2}, \quad (172)$$

$$\frac{d^2y}{dx^2} - 5 \frac{dy}{dx} + 6y = 0, \quad (173)$$

$$(1 - x^2) \frac{d^2y}{dx^2} - 2x \frac{dy}{dx} + p(p+1)y = 0, \quad (174)$$

$$x^2 \frac{d^2y}{dx^2} + x \frac{dy}{dx} + (x^2 - p^2)y = 0 \quad (175)$$

The dependent variable in each of these equations is y , and the independent variable is either t or x . The letters k , m , and p represent constants. An *Ordinary Differential Equation (ODE)* is one in which there is only one independent variable, so that all the derivatives occurring in it are ordinary derivatives. Each of these equations is ordinary. The *order* of a differential equation is the order of the highest derivative present. Equations (170) and (172) are first-order equations, and the others are second-order. Equations (174) and (175) are classical, and are called *Legendre's equation* and *Bessel's equation*, respectively. Each has a vast literature and a history reaching back hundreds of years [39].

The most important type of differential equation is the *linear equation*, in which the derivative of highest order is a linear function of the lower order derivatives. Thus the general first-order linear equation is

$$\frac{dy}{dx} = q(x)y + r(x), \quad (176)$$

the general second-order linear equation is

$$\frac{d^2y}{dx^2} = p(x) \frac{dy}{dx} + q(x)y + r(x), \quad (177)$$

and so on. It is understood that the coefficients on the right in these expressions, namely, $p(x)$, $q(x)$, $r(x)$, etc., are functions of x alone [39]. If $r(x) = 0$ in (176) or (177) then the ODE is *homogeneous*. Otherwise it is *inhomogeneous* [29]. The general solution of (176) is

$$y = e^{\int q(x) dx} \left(\int r(x) e^{-\int q(x) dx} dx + c \right) \quad (178)$$

The general ODE of the n th-order is

$$F \left(x, y, \frac{dy}{dx}, \frac{d^2y}{dx^2}, \dots, \frac{d^ny}{dx^n} \right) = 0, \quad (179)$$

or, using the prime notation for derivatives,

$$F(x, y, y', y'', \dots, y^{(n)}) = 0 \quad (180)$$

It is normally a simple task to verify that a given function $y = y(x)$ is a *solution* of an equation like (179). All that is necessary is to compute the derivatives of $y(x)$ and to show that $y(x)$ and these derivatives, when substituted into the equation, reduce it to an identity in x . In this way we see that

$$y = e^{2x} \quad \text{and} \quad y = e^{3x} \quad (181)$$

are both solutions of the second-order equation

$$y'' - 5y' + 6y = 0, \quad (182)$$

and, more generally, that

$$y = c_1 e^{2x} + c_2 e^{3x} \quad (183)$$

is also a solution for every choice of the constants c_1 and c_2 [39]. Equation (183) is called the *general solution* to (182).

In many engineering applications we are not interested in the general solution of a given differential equation but only in the *particular solution* $y(x)$ satisfying a given *initial condition (IC)*, say, the condition that at some point x_0 the solution $y(x)$ has a prescribed value y_0 , briefly

$$y(x_0) = y_0 \quad (184)$$

A first-order differential equation together with an initial condition is called an *Initial Value Problem (IVP)*. To solve such a problem we must find the particular solution of the equation which satisfies the given initial condition. E.g. the IVP

$$(x^2 + 1)y' + y^2 + 1 = 0, \quad y(0) = 1 \quad (185)$$

has the particular solution [29]

$$y = \frac{1-x}{1+x} \quad (186)$$

As another example, the IVP

$$\ddot{x} + 8\dot{x} + 25x = 0, \quad x(0) = x_0, \quad \dot{x}(0) = 0, \quad (187)$$

has the particular solution

$$x(t) = x_0 \left(\cos 3t + \frac{4}{3} \sin 3t \right) e^{-4t} \quad (188)$$

Notice that IVP (185) is first-order with one IC and that IVP (187) is second-order with two ICs. This is no accident. A solution of a differential equation of the order n (linear

or not) is called a *general solution* if it contains n arbitrary independent constants. Here *independence* means that the solution cannot be reduced to a form containing less than n arbitrary constants. If we assign definite values to the n constants, then the solution so obtained is called a *particular solution* of that equation [29].

Let us now seek a nontrivial solution $y(x)$ of the equation

$$y'' + \lambda y = 0 \quad (189)$$

that satisfies the *boundary conditions (BCs)*

$$y(0) = 0 \quad \text{and} \quad y(\pi) = 0 \quad (190)$$

The parameter λ in (189) is free to assume any real value whatever, and part of our task is to discover the λ 's for which the problem can be solved. In our previous problems we have considered only *initial value problems*, in which the solution of a second-order equation is sought that satisfies two conditions at a single value of the independent variable. Here we have an entirely different situation, for we wish to satisfy one condition at each of two distinct values of x . Problems of this kind are called *boundary value problems (BVPs)*, and in general they are more difficult and far reaching — in both theory and practice — than initial value problems. Although we will not pursue the theory behind BVPs like equation (189) here, its non-trivial solutions are

$$y(x) = c_1 \sin \sqrt{\lambda} x, \quad (191)$$

with $\lambda = n^2$, $n = 1, 2, 3, \dots$ [39]

C.4.2 Systems of Ordinary Differential Equations

Sometimes we shall be concerned with a *first-order system of ordinary differential equations* of the form

$$\left. \begin{aligned} {}^1y' &= {}^1f(x, {}^1y, {}^2y, \dots, {}^my) \\ {}^2y' &= {}^2f(x, {}^1y, {}^2y, \dots, {}^my) \\ &\vdots \\ {}^my' &= {}^mf(x, {}^1y, {}^2y, \dots, {}^my) \end{aligned} \right\}, \quad (192)$$

where

$${}^jy' = \frac{d}{dx} {}^jy(x) \quad (193)$$

We immediately abbreviate the phrase italicized above to ‘first-order system’, or just ‘system’. The system (192) can be written in vector form as

$$\vec{y}' = \hat{f}(x, \vec{y}), \quad (194)$$

where $\vec{y} = ({}^1y, {}^2y, \dots, {}^my)^T$ and $\hat{f} = ({}^1f, {}^2f, \dots, {}^mf)^T$, so that $\hat{f}: \mathcal{R} \times \mathcal{R}^m \rightarrow \mathcal{R}^m$.

We note that each jf depends on ${}^1y, {}^2y, \dots, {}^my$, i.e., the system is *coupled*. Were it the case that each jf depended on jy alone, the system would be *uncoupled*, and each equation in it could be handled independently of the rest. It is this coupling that is the essence of a system; an uncoupled system is not essentially different from a scalar DE.

The general solution of a first-order system of dimension m contains, in general, m arbitrary constants; thus, e.g., it is easily checked by substitution that the 2-D system

$$\left. \begin{aligned} {}^1y' &= {}^1y/x + {}^2yx \\ {}^2y' &= x[({}^2y)^2 - 1]/{}^1y \end{aligned} \right\} \quad (195)$$

is satisfied by

$$\left. \begin{aligned} {}^1y(x) &= x[\cos(C_1x + C_2)]/C_1 \\ {}^2y(x) &= -\sin(C_1x + C_2) \end{aligned} \right\} \quad (196)$$

for any values (with the exception of $C_1 = 0$) of the arbitrary constants C_1, C_2 . For the general m -dimensional system, the m arbitrary constants can be fixed by imposing m initial conditions. If these m conditions take the form of demanding that the $^j y, j = 1, 2, \dots, m$ all take given values *at the same initial point*, then the system together with the conditions constitute an IVP. Writing the system in the vector form (194), the general IVP thus takes the form

$$\dot{y}' = \hat{f}(x, \hat{y}), \quad \hat{y}(a) = \hat{\eta}, \quad \hat{f}: \mathcal{R} \times \mathcal{R}^m \rightarrow \mathcal{R}^m, \quad (197)$$

where

$$\hat{\eta} = ({}^1\eta, {}^2\eta, \dots, {}^m\eta)^T \quad (198)$$

Once again, we abbreviate the nomenclature, and henceforth refer to (197) as a ‘problem’.

If in (197) $\hat{f}$ is independent of x , the problem (and the system it involves) is said to be *autonomous*, and to be *non-autonomous* otherwise. It is always possible, at the cost of raising the dimension by 1, to write a non-autonomous problem in autonomous form. All one need do is add an extra scalar equation ${}^{m+1}y' = 1$ with IC ${}^{m+1}y(a) = a$, which implies that ${}^{m+1}y \equiv x$, so that the new $(m+1)$ -dimensional system is clearly autonomous. E.g., if we add to (195) the ICs ${}^1y(1) = 1, {}^2y(1) = 0$, the resulting 2-D non-autonomous problem can be rewritten as

$$\begin{aligned} {}^1y' &= {}^1y/{}^3y + {}^2y^3y & {}^1y(1) &= 1 \\ {}^2y' &= {}^3y[({}^2y)^2 - 1]/{}^1y & {}^2y(1) &= 0 \\ {}^3y' &= 1 & {}^3y(1) &= 1, \end{aligned} \quad (199)$$

a 3-D autonomous problem, with solution

$$\begin{aligned} {}^1y(x) &= x \cos(x-1) \\ {}^2y(x) &= -\sin(x-1) \\ {}^3y(x) &= x \end{aligned} \quad (200)$$

Since we regard the dimension of the problem as being arbitrary, there is clearly no loss of generality in assuming that the general m -dimensional problem is autonomous [14].

C 4 3 Partial Differential Equations

Physical systems in many fields of applied science and engineering can be described in terms of mathematical systems composed of equations containing partial derivatives. A *partial differential equation (PDE)* is an equation involving several independent variables $x, y, z, \dots$, a function u of these variables, and the partial derivatives of the dependent function u with respect to the independent variables. These variables may be time and one or several coordinates in space. Symbolically, the general PDE is

$$F(x, y, z, \dots, u, u_x, u_y, u_z, \dots, u_{xx}, u_{yy}, \dots, u_{xy}, u_{xz}, \dots) = 0 \quad (201)$$

The order of the highest derivative is called the *order* of the equation. Just as in the case of ODEs, we say that a PDE is *linear* if it is of the first degree in the dependent variable and its partial derivatives [19].

Some important linear PDEs of the second-order are

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad (202)$$

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} \quad (203)$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad (204)$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \quad (205)$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0 \quad (206)$$

Equations (202–206) are called the 1-D *wave equation*, 1-D *heat equation*, 2-D *Laplace equation*, 2-D *Poisson equation*, and 3-D *Laplace equation*, respectively. Here c is a constant, t is time, and x, y, z are orthogonal space coordinates [29]. Each of the above equations is profoundly significant in theoretical physics, and their study has stimulated the development of many important mathematical ideas. In general, PDEs arise in the physics of continuous media — in problems involving electric fields, fluid dynamics, diffusion, and wave motion. Their theory is very different from that of ODEs, and is much more difficult in almost every respect [39].

A *solution* of a PDE in some region R of the space of the independent variables is a function which has all the partial derivatives appearing in the equation in some domain containing R , and satisfies the equation everywhere in R . (One often merely requires that the function is continuous at the boundary of R , has those derivatives in the interior of R , and satisfies the equation in the interior of R . [29]) E.g. if

$$u_{xx} - u_{tt} = 0, \quad (207)$$

which is equation (202) with $c = 1$, then

$$\begin{aligned} u_1(x, t) &= \sin \pi x \cos \pi t \\ u_2(x, t) &= \sin 2\pi x \cos 2\pi t \end{aligned} \quad (208)$$

$$u_n(x, t) = \sin n\pi x \cos n\pi t$$

are all solutions, as is easily seen by direct substitution. The result (208) reveals an important characteristic of PDEs that is common to ODEs, too: a single equation, like (207), for one function u may possess many *particular* solutions. Thus one concern in any problem is to develop certain *auxiliary conditions* that serve to isolate or characterize an *individual* solution for a given problem [19].

In general, the totality of solutions of a PDE is very large. E.g., the functions

$$u = x^2 - y^2, \quad u = e^x \cos y, \quad u = \ln(x^2 + y^2), \quad (209)$$

which are entirely different from each other, are solutions of (204), as one may easily verify. The unique solution of a PDE corresponding to a given physical problem will be obtained by the use of additional information arising from the physical situation. E.g., in some cases the values of the required solution of the problem on the boundary of some domain, *boundary conditions* (BCs) will be given, in other cases when the time t is one of the variables, the values of the solution at $t = 0$, *initial conditions* (ICs) will be prescribed [29].

Certain types of boundary conditions appear and are appropriate in the mathematical models of *initial-boundary-value-problems* (IBVPs). These common conditions are classified as boundary conditions of

- 1 the first type, or the *Dirichlet* condition: the dependent variable is prescribed along the boundary
- 2 the second type, or the *Neumann* condition: the normal derivative of the dependent variable is prescribed along the boundary
- 3 the third type: a relation between the dependent variable and its normal derivative is prescribed along the boundary [19]

Special cases of the 2-D second-order equation

$$a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2} + d \frac{\partial u}{\partial x} + e \frac{\partial u}{\partial y} + fu + g = 0, \quad (210)$$

where a, b, c, d, e, f , and g may be functions of the independent variables x and y and of the dependent variable u , occur more frequently than any other because they are often the mathematical form of one of the conservation principles of physics. Equation (210) is said to be *elliptic* when $b^2 - 4ac < 0$, *parabolic* when $b^2 - 4ac = 0$, and *hyperbolic* when $b^2 - 4ac > 0$. These are called *canonical forms* of (210) [40].

As an important application, let us consider the temperature in a long thin bar or wire of constant cross section and homogeneous material which is oriented along the x -axis and is perfectly insulated laterally, so that heat flows in the x -direction only. Then u depends only on x and time t , and the heat equation (96) becomes the 1-D heat equation (203), with $c^2 = k$. Let us examine the case when the ends $x = 0$ and $x = L$ of the bar are kept at temperature zero. Then the Dirichlet BCs are

$$u(0, t) = u(L, t) = 0 \quad \forall t \quad (211)$$

Let the initial temperature distribution in the bar be

$$u(x, 0) = \sin\left(\frac{\pi x}{L}\right) \quad (212)$$

The individual solution $u(x, t)$ of this linear, second-order, 1-D, parabolic IBVP (203, 211, 212) is [29]

$$u(x, t) = \sin\left(\frac{\pi x}{L}\right) e^{-(c\pi/L)^2 t} \quad (213)$$

D Numerical Methods

D.1 Introduction

The ultimate aim of the field of numerical analysis is to provide convenient methods for obtaining useful solutions to mathematical problems and for extracting useful information from available solutions which are not expressed in tractable forms. Such problems may each be formulated, e.g., in terms of an algebraic or transcendental equation, an ODE or PDE, or an integral equation, or in terms of a set of such equations [41]. As a simple algebraic example, the problem of finding the zeroes of an n th-degree real polynomial with $n \geq 5$ may have no analytical solution. As a more complex PDE example, the Navier-Stokes equations (85), for which there is no known analytical solution.

This formulation may correspond exactly to the situation which it is intended to describe, more often, it will not. Analytical solutions, when available, may be precise in themselves, but may be of unacceptable form because of the fact that they are not amenable to direct interpretation in numerical terms, in which case the numerical analyst may attempt to devise a method for effecting that interpretation in a satisfactory way, or he may prefer to base his analysis instead upon the original formulation [41]. As a simple algebraic example, the problem of finding the zeroes of $p(x) = x^2 - 2$, whose exact analytical solution is clearly $x_1 = -\sqrt{2}$, $x_2 = +\sqrt{2}$, which are expressible in closed symbolic form but are not in a usable numerical form. As a more complex example, the integral formula for the solution of a first-order linear ODE (178).

More frequently, there is no known method of obtaining the solution in a precise form, convenient or otherwise. In such a case, it is necessary either to attempt to approximate the problem satisfactorily by one which is amenable to precise analysis, to obtain an approximate solution to the original problem by methods of numerical analysis, or to combine the two approaches.

On the other hand, the problem itself may not be clearly defined, and the analyst may be provided only with its partial solution, perhaps in the form of a table of approximate data, together with a certain amount of information with regard to its reliability, or perhaps in terms of an integral defining a function which cannot be expressed in terms of a finite number of tabulated functions. His purpose then is to obtain additional useful information concerning the function so described.

Generally the numerical analyst does not strive for exactness. Instead, he attempts to devise a method which will yield an approximation differing from exactness by less than a specified tolerance, or by an amount which has less than a specified probability of exceeding that tolerance. When the information supplied to him is inexact, he attempts both to obtain a dependable measure of the uncertainty which results from that inexactness and also to obtain an approximation which possesses a specified reliability compatible with that uncertainty.

He tries to devise a procedure which would be capable of affording an arbitrarily high degree of accuracy, in a wide class of situations, if the reliability of given information and of available calculating devices were correspondingly high. Even when successful in this attempt, he still seeks alternative procedures which may possess certain advantages in convenience or efficiency in certain situations, but which may be of less general applicability, or which may have the property that the degree of accuracy obtainable, even under ideal circumstances, cannot exceed a certain limit which depends upon the function to be analyzed. In this last case, which is of frequent occurrence, he attempts to ascertain that limit and to classify the situations in which it is not sufficiently high.

Needless to say, there are relatively few situations in which all these objectives have been or can be, perfectly attained. However, research with these aims in view continues to provide new procedures, as well as additional information with regard to the basic advantages and disadvantages of the older ones. Additional impetus has been afforded by the development

of automatic desk calculators and, more recently, of large-scale computers. For example, certain methods had long been known to possess important theoretical advantages, but had not been *convenient*, from the point of view of the labor and time involved, for use in hand calculation or in calculation based on the use of the slide rule or of tables of logarithms, and hence had been considered as little more than mathematical curiosities. However, technological developments have promoted several of them into a much more active status and have also created additional need for detailed reexamination and modification of other existing methods and for a search for new ones.

One of the most rapidly expanding phases of numerical analysis is that which deals with the approximate solution of PDEs. But a basic understanding of the more involved problems which arise in that phase of the analysis depends strongly upon familiarity with similar problems which arise, in a somewhat simpler way, in connection with the solution of algebraic and transcendental equations, the processes of interpolation and approximation, numerical differentiation and integration, and the approximate solution of ODEs, in which only one independent variable is involved [41].

In the process of problem solving, it is possible to distinguish several more or less distinct phases. The first phase is *formulation*. In formulating a mathematical model of a physical system, scientists should take into account beforehand the fact that they expect to solve a problem on a computer. They will therefore provide for specific objectives, proper input data, adequate checks, and for the type and amount of output.

Once a problem has been formulated, numerical methods, together with a preliminary error analysis, must be devised for solving the problem. A numerical method which can be used to solve a problem will be called an *algorithm*. An algorithm is a complete and unambiguous set of procedures leading to the solution of a mathematical problem. The selection or construction of appropriate algorithms properly falls within the scope of *numerical analysis*. Having decided on a specific algorithm or set of algorithms for solving the problem, numerical analysts should consider all the sources of error that may affect the results. They must consider how much accuracy is required, estimate the magnitude of the round-off and discretization errors, determine an appropriate step size or the number of iterations required, provide for adequate checks on the accuracy, and make allowance for corrective action in cases of nonconvergence.

The third phase of problem solving is *programming*. The programmer must transform the suggested algorithm into a set of unambiguous step-by-step instructions to the computer [42].

D.2 Euler's Method

Although Euler's method is seldom used in practice, the simplicity of its derivation can be used to illustrate the techniques involved in the construction of some of the more advanced techniques, without the cumbersome algebra that accompanies these constructions.

The object of the method is to obtain an approximation to the solution to the well-posed IVP

$$\frac{dy}{dt} = f(y, t), \quad a \leq t \leq b, \quad y(a) = \alpha \quad (214)$$

In actuality, a continuous approximation to the solution $y(t)$ will not be obtained, instead, approximations to y will be generated at various values, called *mesh points*, in the interval $[a, b]$. Once the approximate solution is obtained at these points, the approximate solution at other points in the interval can be obtained by interpolation. The process of producing the approximate solution to (214) at mesh points is often called *integration* of the IVP, since integration and differentiation are inverse processes. A particular solution to an IVP is often called a *particular integral*.

In this section, we make the stipulation that the mesh points are equally distributed throughout the interval $[a, b]$. This condition is ensured by choosing a positive integer N

and selecting the mesh points $\{t_0, t_1, t_2, \dots, t_N\}$ where

$$t_i = a + ih, \quad i = 0, 1, 2, \dots, N \quad (215)$$

The common distance, $h = (b - a)/N$, between successive points, is called the *stepsize*, or *steplength*. A step between points of time is called a *timestep*. (Mesh points are not always equally distributed however.)

Suppose that $y(t)$, the unique solution to (214), has two continuous derivatives on $[a, b]$. Then we can represent $y(t)$ with a Taylor series and for each $i = 0, 1, 2, \dots, N - 1$,

$$y(t_{i+1}) = y(t_i) + (t_{i+1} - t_i)y'(t_i) + \frac{(t_{i+1} - t_i)^2}{2}y''(\xi_i) \quad (216)$$

for some number ξ_i in (t_i, t_{i+1}) . If $h = t_{i+1} - t_i$, then

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\xi_i) \quad (217)$$

and, since $y(t)$ satisfies the ODE (214),

$$y(t_{i+1}) = y(t_i) + h f(y(t_i), t_i) + \frac{h^2}{2}y''(\xi_i) \quad (218)$$

Euler's method constructs $y^i \approx y(t_i)$ for each $i = 1, 2, \dots, N$, by deleting the remainder term. Thus [37]

$$\begin{aligned} y^0 &= \alpha, \\ y^{i+1} &= y^i + hf(y^i, t_i), \quad i = 0, 1, \dots, N - 1 \end{aligned} \quad (219)$$

Equation (219) is called the *Forward Euler (FE)* method because the derivative $f(y^i, t_i)$ “looks forward” to generate y^{i+1} . In vector form, (219) becomes

$$\begin{aligned} \hat{y}^0 &= \hat{\alpha}, \\ \hat{y}^{i+1} &= \hat{y}^i + h\hat{f}(\hat{y}^i, t_i), \quad i = 0, 1, \dots, N - 1 \end{aligned} \quad (220)$$

A similar Taylor approximation, the *Backward Euler (BE)* method is defined by

$$\begin{aligned} \hat{y}^0 &= \hat{\alpha}, \\ \hat{y}^{i+1} &= \hat{y}^i + h\hat{f}(\hat{y}^{i+1}, t_{i+1}), \quad i = 0, 1, \dots, N - 1 \end{aligned} \quad (221)$$

Equation (221) is called the Backward Euler method because the derivative $\hat{f}(\hat{y}^{i+1}, t_{i+1})$ “looks backward” to generate $\hat{y}^{i+1}$.

D.3 Explicit Methods

If the current mesh point $\hat{y}^{n+k}$ is defined in terms of only the previous mesh points $\hat{y}^{n+k-1}, \hat{y}^{n+k-2}, \dots$, then the method is *explicit*. FE is explicit [37].

Advantages

- simple to implement
- often very efficient on parallel and vector computers

Disadvantages

- typically unstable for reasonably large stepsize
- frequently require prohibitively small stepsizes and therefore require long execution times

D.4 Implicit Methods

If the method is not explicit, then the method is *implicit*. BE is implicit [37]

Advantages

- typically has good stability characteristics
- often not constrained by stability to a small stepsize

Disadvantages

- much computational overhead is usually necessary to solve the (potentially nonlinear) simultaneous algebraic system at each timestep

D.5 One-Step Method

A method which can be written

$$\tilde{y}^{n+1} = \tilde{y}^n + h\psi(\tilde{y}^n, t_n, h), \quad (222)$$

where h is given and the *increment function* ψ is determined by $\hat{f}$ and is a function of $\tilde{y}^n$, t_n and h only, is called a *one-step method* [14]. FE is a one-step method. BE is implicitly one-step, i.e. although we may not be able to write the increment function $\hat{\psi}$, ψ exists.

D.6 Local Truncation Error

Since the object of numerical techniques is to determine sufficiently accurate approximations with minimal effort, we need a means for comparing the efficiency of various approximation methods. The first device we consider is called the *Local Truncation Error (LTE, $\tilde{d}^{i+1}$)*, or *local discretization error* of the method. The LTE at a specified step measures the locally produced amount by which the exact solution to the problem fails to satisfy the method being used for the approximation [37].

If the approximation is calculated by

$$\tilde{y}^{i+1} = \phi(\tilde{y}^i, h), \quad (223)$$

then the LTE at t_{i+1} is given by

$$\tilde{d}^{i+1} = \hat{\phi}(\tilde{y}(t_i), h) - \tilde{y}(t_{i+1}) \quad (224)$$

The term $\hat{\phi}(\tilde{y}(t_i), h)$ in equation (224) is the value which the method would yield as an *approximation* to $\tilde{y}(t)$ at t_{i+1} by taking one step h from the actual value of $\tilde{y}(t)$ at t_i . The term $\tilde{y}(t_{i+1})$ is the *actual* value of $\tilde{y}(t)$ at t_{i+1} . Hence the LTE is in essence a measure of the amount by which the method deviates from the actual solution locally, due to discretization [14].

Let us consider as a test problem, the 1-D IVP

$$\begin{aligned} y &= -5y, \\ y(0) &= 1, \end{aligned} \quad (225)$$

whose actual solution is

$$y(t) = e^{-5t} \quad (226)$$

Using FE with $h = 0.1$, we have

$$\begin{aligned} \phi(y^i, h) &= y^i + hf(y^i, t_i) \\ &= y^i + (0.1)(-5y^i) \\ &= (0.5)y^i, \end{aligned} \quad (227)$$

and

$$\begin{aligned} d^{i+1} &= \phi(y(t_i), h) - y(t_{i+1}) \\ &= (0.5)y(t_i) - y(t_{i+1}) \\ &= (0.5)e^{-5t_i} - e^{-5t_{i+1}} \end{aligned} \quad (228)$$

At $t_{10} = 1.0$,

$$\begin{aligned} d^{10} &= (0.5)e^{(-5)(0.9)} - e^{(-5)(1.0)} \\ &\approx -0.0011834 \end{aligned} \quad (229)$$

D.7 Total Accumulated Error

The next device we consider is called the *Total Accumulated Error (TAE)*, or *global truncation error*. The TAE at a specified step measures the total amount by which the exact solution to the problem fails to satisfy the method being used for the approximation. The TAE at t_i is given by [14]

$$e^i = y^i - y(t_i) \quad (230)$$

In the test problem, (225), using FE with $h = 0.1$, at $t_{10} = 1.0$, we have

$$\begin{aligned} e^i &= y^i - y(t_i) \\ &= (0.5)^i y^0 - e^{(-5)t_i} \\ &= (0.5)^{10}(1) - e^{(-5)(1.0)} \\ &\approx -0.0057614 \end{aligned} \quad (231)$$

D.8 Order of Accuracy

We frequently use the notation

$$F(h) = O(h^p) \text{ as } h \rightarrow 0, \quad (232)$$

where h is a scalar and F may be either a scalar or a vector. Notation (232) means that there exists a positive constant K such that $\|F(h)\| \leq Kh^p$ for h sufficiently close to zero. Normally, we do not bother to add the phrase ‘as $h \rightarrow 0$ ’ and merely write $F(h) = O(h^p)$, but ‘as $h \rightarrow 0$ ’ is still implied. This is of some importance, since $F(h) = O(h^p)$ is an *asymptotic* statement concerning what happens for sufficiently small h , its interpretation must not be debased into implying that $F(h)$ is roughly the same size as h^p , regardless of the size of h [14].

If the LTE of a numerical method is $O(h^{p+1})$, then we say that the method is *order p* . We commonly say, ‘ F of h is big O of h to the p ’, or ‘ F of h equals O of h to the p ’, or ‘ F of h is order h to the p ’, etc., or that ‘a method is p -order accurate’. E.g. FE and BE are first-order accurate, since the terms omitted from the Taylor series to derive these methods are

$$F(h) = \frac{h^2}{2}y''(t_i) + \frac{h^3}{3!}y'''(t_i) + \quad (233)$$

and $F(h)$ is $O(h^2)$.

A distinction should be made here between the use of $O(h^p)$ for *small* stepsizes h in the analysis of numerical methods, and the use of $O(h^p)$ for *large* data set size in the analysis of computer algorithms. If the LTE of a numerical method is

$$F(h) = ah^3 + bh^2 + ch, \quad (234)$$

e.g., then the LTE is $O(h)$, since the other terms of (234) are insignificant when $h \rightarrow 0$ and the method is zeroth-order accurate. However, if a computer algorithm takes $F(h)$ time to run, then the algorithm is $O(h^3)$, since the other terms of (234) are insignificant when $h \rightarrow \infty$.

D.9 Stability

We are interested in using methods that will produce dependably accurate results for a wide range of problems. One criterion we like to impose upon an algorithm whenever possible is that small changes in the initial data produce correspondingly small changes in the final results. An algorithm that satisfies this property is called *stable*, it is *unstable* when this criterion is not fulfilled. Some algorithms will be stable for certain choices of initial data but not for all choices [37]. Small changes in the initial data are called *perturbations*.

Although definitions of many different kinds of stability are in use, we will use the following definition: a method is said to be *absolutely stable* for a given step size h , if a perturbation $\hat{\epsilon}_0$ in the IC, results in a change no greater than $\hat{\epsilon}_0$ in the computed solution at all subsequent steps.

E.g. we will show that FE is stable for the *test equation*,

$$\dot{y}' = \lambda \hat{y}, \quad \lambda \in \mathcal{C}, \quad (235)$$

which is a very specific ODE, used here in place of an arbitrary problem. We define the perturbations

$$\begin{aligned} \hat{z}^0 &= \hat{y}^0 + \hat{\epsilon}^0 & \text{IC}, \\ \hat{z}^k &= \hat{y}^k + \hat{\epsilon}^k & \text{for any step } k \end{aligned} \quad (236)$$

We apply FE to (235)

$$\begin{aligned} \hat{z}^{k+1} &= \hat{z}^k + h\lambda \hat{z}^k & \text{perturbed,} \\ \hat{y}^{k+1} &= \hat{y}^k + h\lambda \hat{y}^k & \text{non-perturbed} \end{aligned} \quad (237)$$

Subtracting

$$\hat{\epsilon}^{k+1} = \hat{\epsilon}^k + h\lambda \hat{\epsilon}^k = (1 + h\lambda)\hat{\epsilon}^k \quad (238)$$

Thus $|\hat{\epsilon}^k| \leq |\hat{\epsilon}^0|$, $\forall k \geq 0 \Rightarrow |1 + h\lambda| \leq 1$, i.e. FE applied to (235) with stepsize h is stable $\forall \lambda \ni$

$$|1 + h\lambda| \leq 1 \quad (239)$$

The inequality (239) defines the *stability region* in the complex h plane in which the method is stable.

Similarly we can show that BE applied to (235) with stepsize h is stable $\forall \lambda \ni$

$$|1 - h\lambda| \geq 1 \quad (240)$$

D.10 Stiffness

When integrating a DE, one would expect the requisite stepsize to be relatively small in a region where the solution curve displays much variation, and to be relatively large where the solution curve straightens out to approach a line with slope nearly zero. For some problems this is not the case. Sometimes the stepsize is forced down to an unacceptably small level in a region where the solution curve is very smooth. The phenomenon being exhibited here is known as *stiffness*. In some cases we may have two different problems with the same solution, yet problem 1 is *not* stiff and problem 2 *is* stiff. Clearly the phenomenon cannot be a function of the exact solution, since this is the same for both problems, and must be a property of the differential system itself. It is thus more appropriate to talk of *stiff systems* rather than of *stiff problems*.

In this section we consider various aspects of the phenomenon of stiffness. ‘Phenomenon’ is probably a more appropriate word than ‘property’, since the latter rather implies that stiffness can be defined in precise mathematical terms, it turns out not to be possible to do this in a satisfactory manner, even for the restricted class of linear constant coefficient systems. We shall also see several qualitative statements that can be (and mostly have been)

made in an attempt to encapsulate the notion of stiffness, and state what is probably the most satisfactory of these as a ‘definition’ of stiffness

Before we address this issue, we will need to define some concepts. Consider the linear constant coefficient inhomogeneous system

$$\hat{y}' = A\hat{y} + \phi(x), \quad (241)$$

where $\hat{y}, \hat{\phi} \in \mathcal{R}^n$ and A is a constant $n \times n$ matrix with eigenvalues $\lambda_t \in \mathcal{C}, t = 1, 2, \dots, n$ (assumed distinct) and corresponding eigenvectors $\hat{c}_t \in \mathcal{C}^n, t = 1, 2, \dots, n$. The general solution of (241) takes the form

$$\hat{y}(x) = \sum_{t=1}^n \kappa_t \exp(\lambda_t x) \hat{c}_t + \hat{\psi}(x), \quad (242)$$

where the κ_t are arbitrary constants and $\hat{\psi}(x)$ is a particular integral. Now let us suppose that

$$\text{Re}(\lambda_t) < 0, \quad t = 1, 2, \dots, n, \quad (243)$$

which implies that each of the terms $\exp(\lambda_t x) \hat{c}_t \rightarrow 0$ as $x \rightarrow \infty$, so that the solution $\hat{y}(x)$ approaches $\hat{\psi}(x)$ asymptotically as $x \rightarrow \infty$, the term $\exp(\lambda_t x) \hat{c}_t$ will decay monotonically if λ_t is real and sinusoidally if λ_t is complex. Interpreting x to be time (as it often is in physical problems) it is appropriate to call $\sum_{t=1}^n \kappa_t \exp(\lambda_t x) \hat{c}_t$ the *transient solution* and $\hat{\psi}(x)$ the *steady-state solution*. If $|\text{Re}(\lambda_t)|$ is large, then the corresponding term $\kappa_t \exp(\lambda_t x) \hat{c}_t$ will decay quickly as x increases and is thus called a *fast transient*, if $|\text{Re}(\lambda_t)|$ is small, the corresponding term $\kappa_t \exp(\lambda_t x) \hat{c}_t$ decays slowly and is called a *slow transient*. Let $\bar{\lambda}, \underline{\lambda} \in \{\lambda_t, t = 1, 2, \dots, n\}$ be defined by

$$|\text{Re}(\bar{\lambda})| \geq |\text{Re}(\lambda_t)| \geq |\text{Re}(\underline{\lambda})|, \quad t = 1, 2, \dots, n, \quad (244)$$

so that $\kappa_t \exp(\bar{\lambda} x) \hat{c}_t$ is the fastest transient and $\kappa_t \exp(\underline{\lambda} x) \hat{c}_t$ the slowest. We now define the *stiffness ratio* as

$$\frac{|\text{Re}(\bar{\lambda})|}{|\text{Re}(\underline{\lambda})|} \quad (245)$$

J. D. Lambert defines *stiffness* as follows

If a numerical method with a finite region of absolute stability, applied to a system with any ICs, is forced to use in a certain interval of integration a steplength which is excessively small in relation to the smoothness of the exact solution in that interval, then the system is said to be *stiff* in that interval.

There are other characteristics which are exhibited by many examples of stiff problems, but for each there are counterexamples, so these characteristics do not make good definitions of stiffness. Nonetheless, definitions based upon these characteristics are in common use by some authors and are good clues as to the presence of stiffness. Lambert refers to these as ‘statements’ rather than definitions, for the reasons stated above. A few of these are

Statement 1. A linear constant coefficient system is stiff if all of its eigenvalues have negative real part and the stiffness ratio is large.

Statement 2. Stiffness occurs when stability requirements, rather than those of accuracy, constrain the steplength.

Statement 3. Stiffness occurs when some components of the solution decay much more rapidly than others [14].

The origin of the term ‘stiffness’ seems to be somewhat of a mystery. According to J. O. Hirschfelder, the term ‘stiff’ is used because such systems correspond to tight coupling between the driver and driven in servo-mechanisms [43]. According to Richard L. Burden and J. Douglas Faires, systems of DEs are called ‘stiff’ (mathematical stiffness) due to their

application in analyzing the motion of spring, damping and mass systems having large spring constants (physical stiffness) [37] E.g. the IVP

$$m\ddot{x} + c\dot{x} + kx = 0, \quad x(0) = x_0, \quad \dot{x}(0) = 0, \quad (246)$$

with $m = 1, c = 1001, k = 1000$, can be written in the form (241) with $n = 2$ and

$$A = \begin{pmatrix} 0 & 1 \\ -1000 & -1001 \end{pmatrix}, \quad (247)$$

$$\phi(t) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (248)$$

$$\dot{x}(0) = \begin{pmatrix} x_0 \\ 0 \end{pmatrix}, \quad (249)$$

and has eigenvalues $\bar{\lambda} = -1000, \underline{\lambda} = -1$. Both eigenvalues have negative real part and the stiffness ratio is

$$\frac{|-1000|}{|-1|} = 1000, \quad (250)$$

which is fairly large. System (246) then certainly satisfies statements 1 & 3. Here the spring constant k is large and the damping constant c is even larger [29]. The exact solution to (246) is

$$x(t) = x_0 \left(-\frac{1}{999} e^{-1000t} + \frac{1000}{999} e^{-t} \right) \approx x_0 e^{-t} \quad (251)$$

Note that (251) behaves quite nearly as a simple exponential $x_0 \exp(-t)$, but the presence of the $\exp(-1000t)$ term, even with a small coefficient is enough to make the numerical computation very sensitive to stepsize. Stable integration of (246) requires a very small stepsize until well into the smooth part of the solution curve, resulting in an error much smaller than required for accuracy. Thus the system also satisfies statement 2 and Lambert's definition.

D.11 Functional Iteration

A *fixed point* for a given function $\hat{g}$ is a value $\hat{p}$ for which

$$\hat{g}(\hat{p}) = \hat{p} \quad (252)$$

Functional iteration or *fixed point iteration* consists of constructing a sequence

$$\hat{p}^{n+1} = \hat{g}(\hat{p}^n) \quad (253)$$

Problem (252) possesses a unique solution to which the iteration (253) will converge if $\hat{g}$ satisfies a Lipschitz condition in a neighborhood of $\hat{p}$. [14]

Certain problems, e.g. a *root-finding* problem $f(p) = 0$ can be transformed into a *fixed point* problem such that repeated applications of (253) converge to the solution of the problem. Root-finding problems and fixed-point problems are equivalent classes in the following sense. Given a root-finding problem $f(p) = 0$ we can define a function g with a fixed point at p in a number of ways, e.g., as $g(x) = x - f(x)$ or as $g(x) = x + 3f(x)$. Conversely, if the function g has a fixed point at p , then the function defined by $f(x) = x - g(x)$ has a zero at p . The fixed-point form of a problem is easier to analyze than the root-finding form and certain fixed-point choices lead to very powerful root-finding techniques [37].

E.g. to find a root of

$$f(x) = \sin x, \quad (254)$$

in the interval $[1, 6]$, we could iterate

$$g_1(x) = x + \frac{1}{2} \sin x, \quad (255)$$

beginning at

$$x^0 = 4.000, \quad (256)$$

until a fixed point is approximated within a tolerance of $\epsilon = 0.01$

$$\begin{aligned} x^0 &= 4.000, \\ x^1 &= 3.622, \\ x^2 &= 3.391, \\ x^3 &= 3.267, \\ x^4 &= 3.205, \\ x^5 &= 3.173, \\ x^6 &= 3.157, \\ x^7 &= 3.149 \end{aligned} \quad (257)$$

x^7 then is within the specified tolerance of a root of (254)

Certain choices for g converge faster than (255), e.g.

$$g_2(x) = x + \sin x \quad (258)$$

produces

$$\begin{aligned} x^0 &= 4.000, \\ x^1 &= 3.243, \\ x^2 &= 3.142 \end{aligned} \quad (259)$$

The linear systems arising from special cases of implicit numerical methods for ODEs and PDEs are generally solved by iterative methods

D.12 Newton-Raphson Method

Another iterative method for root-finding is the *Newton-Raphson method* (NR), or simply *Newton's method*. Suppose that f is twice continuously differentiable on $[a, b]$. Let $\bar{x} \in [a, b]$ be an approximation to a root p such that $f'(\bar{x}) \neq 0$ and $\|\bar{x} - p\|$ is “small”. Consider the first Taylor polynomial for $f(x)$ expanded about $\bar{x}$,

$$f(x) = f(\bar{x}) + f'(\bar{x})(x - \bar{x}) + \frac{f''(\xi(x))}{2}(x - \bar{x})^2, \quad (260)$$

where $\xi(x)$ lies between x and $\bar{x}$. Since $f(p) = 0$, this equation, with $x = p$, gives

$$0 = f(\bar{x}) + f'(\bar{x})(p - \bar{x}) + \frac{f''(\xi(p))}{2}(p - \bar{x})^2 \quad (261)$$

Newton's method is derived by assuming that, since $\|p - \bar{x}\|$ is small, the term involving $(p - \bar{x})^2$ is negligible and that

$$0 \approx f(\bar{x}) + f'(\bar{x})(p - \bar{x}) \quad (262)$$

Solving for p in equation (262) gives

$$p \approx \bar{x} - \frac{f(\bar{x})}{f'(\bar{x})} \quad (263)$$

This sets the stage for the Newton-Raphson method, which starts with an initial approximation p_0 and generates the sequence p_n , defined by

$$p_n \approx p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}, \quad n \geq 1 \quad (264)$$

Newton's method is not guaranteed to converge, but when it does converge, it converges very quickly [37]

D.13 The Trapezoidal Rule

Suppose that $f(x)$ is continuous for $a \leq x \leq b$, and let $a = x_0 < x_1 < x_2 < \dots < x_n = b$ be a subdivision of $[a, b]$ into n equal intervals of length $h = (b - a)/n$. Then

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(x_0) + 2f(x_1) + 2f(x_2) + \dots + 2f(x_{n-1}) + f(x_n)] \quad (265)$$

D.14 Linear Multistep Methods

Using the shortened notation

$$\hat{f}^{n+j} = \hat{f}(\hat{y}^{n+j}, t_{n+j}), \quad j = 0, 1, \dots, k \quad (266)$$

we define a *Linear Multistep Method (LMM)* or *linear k -step method* in standard form by

$$\sum_{j=0}^k \alpha_j \hat{y}^{n+j} = h \sum_{j=0}^k \beta_j \hat{f}^{n+j}, \quad (267)$$

where α_j and β_j are constants subject to the conditions

$$\alpha_k = 1, \quad |\alpha_0| + |\beta_0| \neq 0 \quad (268)$$

The first of these conditions removes, in a convenient manner, the arbitrariness that arises from the fact that we could multiply both sides of (267) by the same constant without altering the method. The second condition prevents both α_0 and β_0 being zero, and thus precludes methods such as

$$\hat{y}^{n+2} - \hat{y}^{n+1} = h \hat{f}^{n+1}, \quad (269)$$

which is essentially a 1-step and not a 2-step method, and is in practice indistinguishable from the 1-step method

$$\hat{y}^{n+1} - \hat{y}^n = h \hat{f}^n \quad (270)$$

Method (270) is FE, the simplest of all numerical methods for DEs [14]. BE is then

$$\hat{y}^{n+1} - \hat{y}^n = h \hat{f}^{n+1} \quad (271)$$

Note that in (270), $\alpha_k = \alpha_1 = 1$, $\alpha_0 = -1$, $\beta_k = \beta_1 = 0$, and $\beta_0 = 1$, and that in (271), $\alpha_k = \alpha_1 = 1$, $\alpha_0 = -1$, $\beta_k = \beta_1 = 1$, and $\beta_0 = 0$. In general, if $\beta_k = 0$, the method is explicit, otherwise the method is implicit.

D.15 Predictor-Corrector Methods

Suppose that we wish to solve the standard IVP by an implicit LMM. Then at each step we have to solve for $\hat{y}^{n+k}$ the implicit system

$$\hat{y}^{n+k} + \sum_{j=0}^{k-1} \alpha_j \hat{y}^{n+j} = h \beta_k \hat{f}(\hat{y}^{n+k}, t_{n+k}) + h \sum_{j=0}^{k-1} \beta_j \hat{f}^{n+j} \quad (272)$$

We normally do this by the fixed point iteration

$$\begin{aligned} \hat{y}^{n+k,s+1} + \sum_{j=0}^{k-1} \alpha_j \hat{y}^{n+j} &= h \beta_k \hat{f}(\hat{y}^{n+k,s}, t_{n+k}) + h \sum_{j=0}^{k-1} \beta_j \hat{f}^{n+j}, \\ \hat{y}^{n+k,0} &\text{arbitrary,} \quad s = 0, 1, \end{aligned} \quad (273)$$

which will converge to the unique solution of (272) provided that

$$h < \frac{1}{|\beta_k|L}, \quad (274)$$

where L is the Lipschitz constant of f with respect to y . For non-stiff problems, this restriction on h is not significant, in practice, considerations of accuracy put a much more restrictive constraint on h . Although (273) will converge for arbitrary $\hat{y}^{n+k,0}$, each iteration calls for one evaluation of the function f , and computation can obviously be saved if we can provide as good a guess as possible for $\hat{y}^{n+k,0}$. This is conveniently done by using a separate *explicit* LMM to provide the initial guess $\hat{y}^{n+k,0}$. We call this explicit method the *predictor* and the implicit method (272) the *corrector*, the two together comprise a *Predictor-Corrector (PC) pair* [14].

D.16 Adaptive Stepsize

During the course of the integration of an IVP it is periodically necessary to change the stepsize to minimize computational work while maintaining prescribed accuracy [44] (and stability). Any worthwhile numerical ODE package varies the stepsize dynamically as it integrates, and its methods are called *adaptive stepsize* methods. In parts of the interval (t_0, t_N) where the solution $\hat{y}(t)$ varies rapidly, we typically want smaller steps, whereas in parts where the solution is nearly constant, we usually want larger steps. In practice, we have a parameter ϵ and we want $\|d^n\| \leq \epsilon$, for each step we take. Of course we would like to take as big a step as we can. One adaptive stepsize method estimates the LTE $\hat{d}^n(h)$ as

$$\hat{d}^n(h) = \frac{\hat{y}^{n+2,2h} - \hat{y}^{n+2,h}}{2^r - 1}, \quad (275)$$

where r is the order of the numerical method, h is the current stepsize, and $\hat{y}^{n+2,2h}$ and $\hat{y}^{n+2,h}$ are approximations of $\hat{y}(t_{n+2})$ using stepsizes of $2h$ and h , respectively, and estimates the desired stepsize h^* as

$$h^* = h \left(\frac{\epsilon}{\|\hat{d}^n(h)\|} \right)^{1/(r+1)}, \quad (276)$$

where ϵ is the tolerance, and then does the following

- 1 if $h \leq h^*$, then set $\hat{y}^{n+2} = \hat{y}^{n+2,h}$ and proceed with h^* as the current stepsize,
- 2 otherwise, set $h = h^*$ and retry the combination

D.17 Runge-Kutta Methods

The simplest of all numerical methods is FE,

$$\hat{y}^{n+1} = \hat{y}^n + h \hat{f}^n \quad (277)$$

FE is linear in $\hat{y}^n$ and $\hat{f}^n$ and, being a one-step method, presents no difficulty when we want to change the steplength, but of course it has very low accuracy. Linear multistep methods achieve higher accuracy by retaining linearity with respect to $\hat{y}^{n+j}$ and $\hat{f}^{n+j}$, $j = 0, 1, \dots, k$, but sacrificing the one-step format. The result of retaining the linearity is that the local error has a relatively simple structure, which is why we are able to estimate it so easily, the cost of moving to a multistep format is the considerable difficulties encountered when we want to change steplength.

Runge-Kutta (RK) methods develop from Euler's Rule in exactly the opposite direction, higher order is achieved by retaining the one-step form but sacrificing the linearity. The

result is that there is no difficulty in changing the steplength, but the structure of the local error is much more complicated, and there exists no easy and cheap error estimate. We are rather in a Catch-22 situation, with linear multistep methods it is easy to tell when we ought to change steplength but hard to change it, while with Runge-Kutta Methods it is hard to tell when to change steplength but easy to change it!

The general s -stage Runge-Kutta method for the IVP

$$\dot{y} = \hat{f}(x, y), \quad y(a) = \hat{\eta}, \quad \hat{f}: \mathcal{R} \times \mathcal{R}^m \rightarrow \mathcal{R}^m \quad (278)$$

is defined by

$$\left. \begin{aligned} \hat{y}^{n+1} &= \hat{y}^n + h \sum_{i=1}^s b_i \hat{k}_i, \\ \hat{k}_i &= \hat{f}(\hat{x}^n + c_i h, \hat{y}^n + h \sum_{j=1}^s a_{ij} \hat{k}_j), \quad i = 1, 2, \dots, s \end{aligned} \right\} \quad (279)$$

We shall always assume that the following (the *row-sum condition*) holds [14]

$$c_i = \sum_{j=1}^s a_{ij}, \quad i = 1, 2, \dots, s \quad (280)$$

E.g. the classical 4th-order RK method is

$$\left\{ \begin{aligned} \hat{k}_1 &= h \hat{f}(\hat{y}^n, t_n), \\ \hat{k}_2 &= h \hat{f}(\hat{y}^n + \tfrac{1}{2} \hat{k}_1, t_n + \tfrac{1}{2} h), \\ \hat{k}_3 &= h \hat{f}(\hat{y}^n + \tfrac{1}{2} \hat{k}_2, t_n + \tfrac{1}{2} h), \\ \hat{k}_4 &= h \hat{f}(\hat{y}^n + \hat{k}_3, t_n + h), \\ \hat{y}^{n+1} &= \hat{y}^n + \tfrac{1}{6} (\hat{k}_1 + 2\hat{k}_2 + 2\hat{k}_3 + \hat{k}_4) \end{aligned} \right. \quad (281)$$

D.18 Iterative Techniques for Linear Systems

Numerical methods which yield solutions after an amount of computation that can be specified in advance are called *direct methods*. An example of a direct method for approximating the solution of a system of linear equations is *Gauss elimination*. We will not pursue direct methods here. In contrast, an *indirect method* or *iterative method* is one in which we start from an approximation to the true solution and, if successful, obtain better and better approximations from a computational cycle repeated as often as may be necessary for achieving a required accuracy, so that the amount of arithmetic depends upon the accuracy required.

Iterative methods are used mainly in those problems for which convergence is known to be rapid, so that the solution is obtained with much less work than that of a direct method, and for systems of large order but with many zero coefficients, the so-called “*sparse*” systems, for which elimination methods would be relatively laborious and need much storage. Such systems occur in connection with vibrational problems, BVPs, PDEs, circuit analysis, and other applications and have given rise to a rapidly growing literature [29].

An iterative technique to solve the linear system $A\hat{x} = \hat{b}$ begins with an initial approximation $\hat{x}^0$ to the solution $\hat{x}$, and generates a sequence of vectors $\{\hat{x}^k\}_{k=0}^{\infty}$ which converges to $\hat{x}$. Iterative techniques involve a process that converts the system $A\hat{x} = \hat{b}$ into an equivalent system of the form $\hat{x} = T\hat{x} + \hat{c}$ for some matrix T and vector $\hat{c}$. After the initial vector $\hat{x}^0$ is selected, the sequence of approximate solution vectors is generated by computing

$$\hat{x}^k = T\hat{x}^{k-1} + \hat{c}, \quad k = 1, 2, \quad (282)$$

This is a form of fixed-point iteration [37].

converges, to 3 decimal places, to the solution

$$\hat{x} = (5\,000, 3\,000, 1\,000)^T \quad (291)$$

in 59 iterations. Jacobi iteration applied to the system

$$\begin{array}{rclcl} E_1 & -14x_1 & + & -91x_2 & + & 52x_3 & = & 4617 \\ E_2 & -68x_1 & + & 79x_2 & + & 76x_3 & = & -649 \\ E_3 & 64x_1 & + & 16x_2 & + & 83x_3 & = & -4872 \end{array} \quad (292)$$

does not converge at all. Also, in practice, the linear system is often much larger than the 3×3 systems illustrated here.

The Jacobi iterative method is called a method of *simultaneous corrections* because no element x_i^k of an approximation $\hat{x}^k$ is used until all the elements of $\hat{x}^k$ have been calculated [29]. Jacobi iteration is not very fast in itself, but simple and completely parallel, and thus very fast when implemented on a parallel computer architecture.

D.18.2 Gauss-Seidel Iteration

An improvement over Jacobi iteration is suggested by an analysis of (284). To compute x_i^k , the components of $\hat{x}^{k-1}$ are used. Since, for $i > 1$, $x_1^k, \dots, x_{i-1}^k$ have already been computed and are likely to be better approximations to the actual solutions $x_1, \dots, x_{i-1}$ than $x_1^{k-1}, \dots, x_{i-1}^{k-1}$, it seems reasonable to compute x_i^k using these most recently calculated values. This is called the *Gauss-Seidel iterative technique (GS)* [37]. The system (283) is then iterated as

$$\begin{array}{rclcl} x_1^k & = & & -\frac{1}{2}x_2^{k-1} & - & \frac{1}{2} \\ x_2^k & = & -\frac{1}{15}x_1^k & & + & \frac{2}{15}x_3^{k-1} & + & \frac{4}{5} \\ x_3^k & = & & -\frac{3}{20}x_2^k & & & + & \frac{23}{20} \end{array} \quad (293)$$

Letting $\hat{x}^0 = (0\,000, 0\,000, 0\,000)^T$, the iterates generated to 3 decimal places are

$$\begin{array}{rcl} \hat{x}^0 & = & (0\,000, 0\,000, 0\,000)^T, \\ \hat{x}^1 & = & (-0\,500, 0\,833, 1\,025)^T, \\ \hat{x}^2 & = & (-0\,917, 0\,998, 1\,000)^T, \\ \hat{x}^3 & = & (-0\,999, 1\,000, 1\,000)^T, \\ \hat{x}^4 & = & (-1\,000, 1\,000, 1\,000)^T \end{array} \quad (294)$$

Note that this method converges to the solution

$$\hat{x} = (-1\,000, 1\,000, 1\,000)^T \quad (295)$$

of (283) to an accuracy of 3 decimal places in 4 iterations—a 20% saving over Jacobi iteration. Gauss-Seidel iteration applied to (290) converges, to 3 decimal places, to the solution

$$\hat{x} = (5\,000, 3\,000, 1\,000)^T \quad (296)$$

in 28 iterations—a 53% saving over Jacobi iteration.

Gauss-Seidel is a method of *successive corrections* because each element x_i^k of an approximation $\hat{x}^k$ is used as soon as it is calculated [29]. Gauss-Seidel iteration is not obviously parallel, but when used to solve PDEs, there is much parallelism hidden in it.

D.18.3 Relaxation Method

In Jacobi iteration, rather than correct $\hat{x}^k$ using the Jacobi correction $\hat{x}^{k+1,J}$, defined by

$$\hat{x}^{k+1,J} = T\hat{x}^k + \hat{c}, \quad (297)$$

which can over-correct, resulting in oscillatory behavior which may retard convergence, we can use a weighted average of this computed value and the previous iterate,

$$\hat{x}^{k+1} = \omega \hat{x}^{k+1,J} + (1 - \omega) \hat{x}^k, \quad (298)$$

in hopes of damping out the oscillations and accelerating convergence. This technique can be applied similarly to Gauss-Seidel iteration. Methods employing this weighted average are called *relaxation methods*. For choices of the weighting factor $0 < \omega < 1$, the procedures are called *under-relaxation methods*. For choices $1 < \omega$, the procedures are called *over-relaxation methods*. These methods are abbreviated *SOR* for *Successive Over-Relaxation* and are particularly useful for solving the linear systems that occur in the numerical solution of certain PDEs [37].

Over-relaxation can increase the effects of iteration and make a stable method converge faster. E.g. relaxed Gauss-Seidel with $\omega = 1.34$ applied to (290) converges, to 3 decimal places, to the solution

$$\hat{x} = (5.000, 3.000, 1.000)^T \quad (299)$$

in 9 iterations—a 68% saving over Gauss-Seidel iteration, an 85% saving over Jacobi iteration.

Under-relaxation can decrease the effects of iteration and make an otherwise unstable method stable. E.g. relaxed Gauss-Seidel with $\omega = 0.5$ applied to (292) converges, to 3 decimal places, to the solution

$$\hat{x} = (-54.000, -47.000, -8.000)^T \quad (300)$$

in 38 iterations—a problem for which Jacobi and Gauss-Seidel do not converge at all.

D.18.4 Matrix-Splitting

A decomposition of a matrix A into a sum of matrices, which simplifies manipulation of $A\hat{x} = \hat{b}$ is called a *matrix splitting*. E.g. let

$$\begin{aligned} -U &= \text{strictly upper triangular part of } A, \\ D &= \text{diagonal part of } A, \\ -L &= \text{strictly lower triangular part of } A, \end{aligned} \quad (301)$$

then the matrix A is split into simpler matrices as

$$A = D - U - L \quad (302)$$

The Jacobi method can then be represented in matrix form as a splitting

$$\hat{x}^{k+1} = D^{-1}(U + L)\hat{x}^k + D^{-1}\hat{b}, \quad (303)$$

the Gauss-Seidel splitting is

$$\hat{x}^{k+1} = (D - L)^{-1}U\hat{x}^k + (D - L)^{-1}\hat{b}, \quad (304)$$

and the relaxed Gauss-Seidel splitting is [37]

$$\hat{x}^{k+1} = (D - \omega L)^{-1}[(1 - \omega)D + \omega U]\hat{x}^k + \omega(D - \omega L)^{-1}\hat{b} \quad (305)$$

D.19 Subroutine Packages

Collections of subroutines for solving systems of ODEs, called *subroutine packages*, or *solvers*, etc., are available. The *Livermore Solver for Ordinary Differential Equations (LSODE)* is designed to produce numerical solutions to IVPs, especially for stiff chemical kinetics problems. This FORTRAN-callable package, written by Alan C. Hindmarsh at *Lawrence Livermore National Laboratory (LLNL)*, uses the *backward-difference formula (BDF)* method, and implicit Adams methods [44].

Another FORTRAN collection is *CHEMSODE* a *stiff ODE solver for the equations of chemical kinetics*, developed by Colin J. Aio at LLNL. This package implements three different types of preconditioned time differencing techniques, along with a choice of steplength control, which eliminate the need for the matrix algebra typically associated with implicit numerical methods, while retaining the numerical stability [10].

E Parallel Processing

Some terminology from Parallel Processing is defined here

- 1 *CPU* — Central Processing Unit, a single computer
- 2 *OS* — Operating System
- 3 *bandwidth* — the bandwidth of a memory system is the maximum number of bytes that can be transferred in one second between the processing component and the memory. This concept can be extended to describe the rate at which other system components involved in the transport of data can operate [45]
- 4 *pipelining* — the process of putting portions of a problem into an *assembly line*. E.g. consider adding two floating point numbers $a = 1.0123e-3$, $b = 1.0000e-1$. We can perform this addition in stages

(a) Shift so radix points align

$$\begin{array}{r} 0.010123e-1 \\ 1.000000e-1 \end{array} \quad (306)$$

(b) Add

$$\begin{array}{r} 0.010123e-1 \\ + 1.000000e-1 \\ \hline 1.010123e-1 \end{array} \quad (307)$$

(c) Shift

$$0.1010123 \quad (308)$$

(d) Round

$$0.10101 \quad (309)$$

We can now use the 4-stage scheme above to add two floating point vectors $\hat{a} = ({}_1a, \dots, {}_Na)^T$ and $\hat{b} = ({}_1b, \dots, {}_Nb)^T$ component-wise. I.e. while ${}_ia$ and ${}_ib$ are being shifted, ${}_{i-1}a$ and ${}_{i-1}b$ are being added, ${}_{i-2}a + {}_{i-2}b$ is being shifted, ${}_{i-3}a + {}_{i-3}b$ is being rounded, ${}_{i-4}a + {}_{i-4}b$ is being output. The total time t required to add two vectors of length N is

$$t = t_s + t_l(N - 1), \quad (310)$$

where t_s is the *setup time* required to get the first result (i.e. for the first component sum, ${}_1a + {}_1b$ to pass completely through the pipeline), and t_l is the time required for the longest (slowest) operation in the pipeline. Pipelining is also called *vector processing*.

- 5 *vector machine* — a computer implementing the pipelining paradigm
- 6 *parallelism* — the process of performing tasks concurrently, the degree to which portions of a problem can be processed concurrently
- 7 *problem size* — the number of pieces of data that we want to update
- 8 *parallel machine* — a computer consisting of two or more CPUs connected via some interconnection network, a collection of multiple processors that work on a single problem. Such a computer system is capable of achieving tremendous cost/performance benefits. Parallel processors are classified as either *shared memory* or *distributed memory* machines. Machines consisting of 1,000,000 or more CPUs are called *massively parallel computers*.

- 9 *parallel wall clock time, t_p* — the maximum time for a CPU in a parallel machine to complete its portion of the problem. If t_i is the time required for CPU i to complete, and there are m CPUs, then $t_p = \max_{i=1}^m t_i$. t_p is essentially the time required for a parallel machine to complete the problem.
- 10 *serial wall clock time, t_s* — the total time for all CPUs in a parallel machine to complete their portions of the problem. $t_s = \sum_{i=1}^m t_i$. t_s is essentially the time that would be required for a single machine to complete all portions of the problem sequentially.
- 11 A *node* in a network consists of a processor and its local memory. The *size n* of a network is the number of nodes it contains. A *partition* is a particular scheme for dividing a problem into portions, or a corresponding configuration of nodes in a parallel processor.
- 12 *speedup* — t_s/t_p .
- 13 *RP* — Relative Performance. $RP = (t_s/t_p)/n$. RP is essentially the efficiency of the parallelization of the problem. If the problem is divided evenly between CPUs, then $RP = 1$. If $RP = 1$, then we have a perfectly *scalable* problem. A value of $RP > 1$ is said to be *superlinear*. If dividing the problem into small portions results in the problem fitting completely into the CPUs' local cache memories, then we have eliminated the time spent in communication with slow memory, and not replaced it with time spent in message-passing. Thus we have $t_p < t_s/n$, and therefore $RP > 1$. For performance vs. processors, any value of RP better than 1 is a good return.
- 14 *load balancing* — sharing the processing burden equally across all CPUs in a parallel machine, to minimize t_p . The goal of load balancing is to keep processor nodes busy and have them finish roughly at the same time. Valuable processor cycles are wasted if some nodes have to wait on others to finish. The greatest speedup is possible only when all processors are busy all of the time.
- 15 *SIMD* — Single-Instruction Multi-Data. All CPUs execute the same instruction simultaneously. In the SIMD paradigm, all CPUs do the same thing at the same time or else they remain idle. E.g. a vector processor.
- 16 *MIMD* — Multi-Instruction Multi-Data. Many CPUs can be simultaneously executing different instructions on different data. Furthermore, these CPUs operate in a largely autonomous manner as though they were separate computers.
- 17 *interconnection network (IN) topology* — a mapping function from the set of processors and memories onto the same set of processors and memories.
- 18 A *shared memory* architecture is one which accomplishes interprocessor coordination through a global memory shared by all CPUs (cf. distributed memory).
- 19 *cache memory* — a special-purpose random access memory designed to reduce a number of contention problems which arise from a bus-structured shared-memory IN topology.
- 20 In a shared memory architecture, each CPU has its own *local cache*. A typical bus-structured parallel computer attempts to reduce contention for the bus by fetching instructions and data directly from each individual cache, as much as possible.
- 21 *MPI* — Message-Passing Interface. A distributed-memory IN consists of processors and their local memories connected by communication links. There is no global memory so it is necessary to move data from one local memory to another by means of *message-passing*. This is typically done by a SEND/RECEIVE pair of commands.

which must be written into the application software by a programmer. Thus, programmers must learn the message-passing paradigm, and cope with the details of data copying and the attendant consistency issues.

- 22 A *distributed memory* architecture typically combines a local memory and a processor at each node of the IN. Message-passing is used to communicate between any two CPUs, and there is no global, shared memory (cf. shared memory).
- 23 *Meiko CS-2* -- a distributed memory system. Communication must be requested; no shared memory [46, 27].

F Related Methods

F.1 Introduction

Several numerical methods are in use which although not germane to our discussion, are often used alternately on similar problems. These related methods are presented here for comparison.

F.2 Finite Difference Approximations to Derivatives.

When a function F and its derivatives are single-valued, finite and continuous functions of x , then by Taylor's theorem,

$$F(x+h) = F(x) + hF'(x) + \frac{1}{2}h^2F''(x) + \frac{1}{6}h^3F'''(x) + \quad (311)$$

and

$$F(x-h) = F(x) - hF'(x) + \frac{1}{2}h^2F''(x) - \frac{1}{6}h^3F'''(x) + \quad (312)$$

Addition of these expansions gives

$$F(x+h) + F(x-h) = 2F(x) + h^2F''(x) + O(h^4), \quad (313)$$

where $O(h^4)$ denotes terms containing fourth and higher powers of h . Assuming these are negligible in comparison with lower powers of h it follows that,

$$F''(x) = \left(\frac{d^2F}{dx^2} \right)_{x=x} \approx \frac{1}{h^2} \{ F(x+h) - 2F(x) + F(x-h) \}, \quad (314)$$

with a leading error on the right-hand side of order h^2 .

Subtraction of equation (312) from equation (311) and neglect of terms of order h^3 leads to

$$F'(x) = \left(\frac{dF}{dx} \right)_{x=x} \approx \frac{1}{2h} \{ F(x+h) - F(x-h) \}, \quad (315)$$

with an error of order h^2 .

Let $A = (x-h, u(x-h))$, $P = (x, u(x))$, $B = (x+h, u(x+h))$. Then (315) clearly approximates the slope of the tangent at P by the slope of the chord AB , and is called a *central-difference* approximation. We can also approximate the slope of the tangent at P by either the slope of the chord PB , giving the *forward-difference* formula,

$$F'(x) \approx \frac{1}{h} \{ F(x+h) - F(x) \}, \quad (316)$$

or the slope of the chord AP giving the *backward-difference formula* (BDF)

$$F'(x) \approx \frac{1}{h} \{ F(x) - F(x-h) \}, \quad (317)$$

Both (316) and (317) can be derived immediately from (311) and (312) respectively, assuming second and higher powers of h are negligible. This shows that the leading errors in these forward and backward-difference formulae are both $O(h)$. [40]

F.3 Finite Difference Method

In the *Finite Difference Method* (FDM), derivatives at a point are approximated by difference quotients over a small interval. E.g. for the 1-D diffusion equation,

$$u_t = Du_{xx}, \quad (318)$$

we set up a grid in the x - t plane with grid spacings Δx and Δt . The basis of the simplest finite difference method is to replace the second derivative on the right-hand side of (318) by a *central difference* quotient in x and replace u_t by a *forward difference* in time. Then, one advances the approximate solution forward in time, one time level after another. More precisely, if we let u_j^n denote the approximate solution at $x_j = j\Delta x$ and $t_n = n\Delta t$, then the finite difference analog of (318) is

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{D}{(\Delta x)^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) \quad (319)$$

or

$$u_j^{n+1} = u_j^n + \mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n), \quad j = 1, \dots, q \quad (320)$$

where

$$\mu = \frac{D\Delta t}{(\Delta x)^2} \quad (321)$$

Generalization to more than one spatial dimension is a natural extension of (320)

The classical *stability condition* for FDM is

$$\Delta t \leq \frac{(\Delta x)^2}{2D}, \quad (322)$$

and is slightly stronger than the actual stability restriction which can be derived for (320) [20]

Note that once the right-hand side of (318) is approximated by a central difference quotient, u_t can be approximated by, e.g. a forward difference (explicit method), a backward difference (implicit method), the Numerical Method of Lines, a Preconditioned Time Difference, etc. wherein different numerical methods arise.

F.4 Finite Element Method

The *Finite Element Method (FEM)* was originally developed for use in civil engineering but is now used for approximating the solutions to partial differential equations that arise in all areas of applied mathematics. One advantage of the finite element method over finite difference methods is the relative ease with which the boundary conditions of the problem are handled. Many physical problems have boundary conditions involving derivatives and irregularly shaped boundaries. Boundary conditions of this type are difficult to handle using finite difference techniques since each boundary condition involving a derivative must be approximated by a difference quotient at the gridpoints, and irregular shaping of the boundary makes placing the gridpoints difficult. The finite element method includes the boundary conditions as integrals in a functional that is being minimized, so the construction procedure is independent of the particular boundary conditions of the problem.

Consider, e.g. the partial differential equation

$$\frac{\partial}{\partial x} \left(p(x, y) \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(q(x, y) \frac{\partial u}{\partial y} \right) + r(x, y)u(x, y) = f(x, y), \quad (323)$$

with $(x, y) \in \mathcal{D}$, where $\mathcal{D}$ is a plane region with boundary $\mathcal{S}$.

Boundary conditions of the form

$$u(x, y) = g(x, y) \quad (324)$$

are imposed on a portion $\mathcal{S}_1$ of the boundary. On the remainder of the boundary $\mathcal{S}_2$, $u(x, y)$ is required to satisfy

$$p(x, y) \frac{\partial u}{\partial x}(x, y) \cos \theta_1 + q(x, y) \frac{\partial u}{\partial y}(x, y) \cos \theta_2 + g_1(x, y)u(x, y) = g_2(x, y), \quad (325)$$

where θ_1 and θ_2 are the direction angles of the outward normal to the boundary at the point (x, y)

Physical problems in the areas of solid mechanics and elasticity have associated partial differential equations similar to (323). The solution to a problem of this type is typically the minimization of a certain functional, involving integrals, over a class of functions determined by the problem.

Suppose p , q , r , and f are all continuous in $\mathcal{D} \cup \mathcal{S}$, p and q have continuous first partial derivatives, and g_1 and g_2 are continuous on $\mathcal{S}_2$. Suppose, in addition, that $p(x, y) > 0$, $q(x, y) > 0$, $r(x, y) \leq 0$, and $g_1(x, y) > 0$. Then a solution to (323) uniquely minimizes the functional

$$\begin{aligned} I[w] = & \int_{\mathcal{D}} \int \left\{ \frac{1}{2} \left[p(x, y) \left(\frac{\partial w}{\partial x} \right)^2 + q(x, y) \left(\frac{\partial w}{\partial y} \right)^2 - r(x, y) w^2 \right] + f(x, y) w \right\} dx \, dy \\ & + \int_{\mathcal{S}_2} \left\{ -g_2(x, y) w + \frac{1}{2} g_1(x, y) w^2 \right\} dS \end{aligned} \quad (326)$$

over all functions w satisfying (324) on $\mathcal{S}_1$ which are twice continuously differentiable. The finite element method approximates this solution by minimizing the functional I over a smaller class of functions.

The first step is to divide the region into a finite number of sections, or elements, of a regular shape, either rectangles or triangles.

The set of functions used for approximation is generally a set of piecewise polynomials of fixed degree in x and y , and the approximation requires that the polynomials be pieced together in such a manner that the resulting function is continuous with an integrable or continuous first or second derivative on the entire region. Polynomials of linear type in x and y ,

$$\phi(x, y) = a + bx + cy, \quad (327)$$

are commonly used with triangular elements, while polynomials of bilinear type in x and y ,

$$\phi(x, y) = a + bx + cy + dxy, \quad (328)$$

are used with rectangular elements [37].

F.5 Numerical Method of Lines

To solve the 1-D pure diffusion equation

$$u_t = Du_{xx}, \quad (329)$$

with *Initial Conditions (IC)*

$$u(x, 0) = \sin(\pi x/L), \quad (330)$$

and *Boundary Conditions (BC)*

$$u(0, t) = u(L, t) = 0, \quad (331)$$

we could replace the partial derivatives with *algebraic approximations* evaluated at a general point with indices (j, n) , this would lead to a set of algebraic equations that approximate equation (329). Once the approximation algebraic equations have been defined, they could be solved using any standard linear equation solver to obtain an *approximate numerical solution* to equation (329), of course, the auxiliary conditions, equations (330–331), would also have to be included in the algebraic equations. This procedure is the basis for well-known classical finite difference and finite element methods for PDEs. The *Numerical Method of Lines (NUMOL)* is really just a small departure from this basic approach. In the NUMOL,

we retain the index j to account for variations of u with x , but we treat t as a continuous variable (rather than t evaluated at discrete points corresponding to the index n). Thus, we will replace the partial derivative u_{xx} in equation (329) with an algebraic approximation evaluated at point j , but keep the derivative u_t , this will lead to a system of differential equations in t , and since we now have only one independent variable t , the differential equations will be ODEs. This is the essence of the NUMOL [16]

F.6 Method of Characteristics

Consider the equation

$$a \frac{\partial u}{\partial x} + b \frac{\partial u}{\partial y} = c, \quad (332)$$

where a , b , and c are, in general, functions of x , y , and u but not of $\partial u / \partial x$ and $\partial u / \partial y$, i.e. the first-order derivatives occur only to the first degree although the equation need not be linear in u . Such an equation is said to be quasi-linear. It is customary to put $\partial u / \partial x = p$ and $\partial u / \partial y = q$ and to write the equation as

$$ap + bq = c \quad (333)$$

At each point of the solution domain of such an equation there is a direction along which the integration of equation (333) transforms to the integration of an ordinary differential equation. In other words, *in this direction* the expression to be integrated will be independent of partial derivatives in other directions, such as p and q .

Assume we know the solution values u of equation (333) at every point on a curve C in the x - y plane, where C does *not* coincide with the curve Γ on which initial values of u are specified. The question to be asked at this stage is this: "Can we determine values for p and q on C from the values of u on C so that they satisfy equation (333)?"

If we can, then in directions tangential to C from points on C we shall automatically satisfy the differential relationship

$$du = \frac{\partial u}{\partial x} dx + \frac{\partial u}{\partial y} dy = p dx + q dy, \quad (334)$$

where dy/dx is the slope of the tangent to C at $P(x, y)$ on C .

Equations (333–334) are two equations for p and q . Elimination of p between them gives

$$du = \frac{c - bq}{a} dx + q dy, \quad (335)$$

which can be written as

$$q(a dy - b dx) + (c dx - a du) = 0 \quad (336)$$

This equation is explicitly independent of p because the coefficients a , b and c are functions of x , y and u only. It can also be made independent of q by choosing the curve C so that its slope dy/dx satisfies the equation

$$a dy - b dx = 0 \quad (337)$$

By equations (336–337) it then follows that

$$c dx - a du = 0 \quad (338)$$

Equation (337) is a differential equation for the curve C and (338) is a differential equation for the solution values of u along C . The curve C is called a *characteristic curve* or *characteristic*. These equations are easy to remember because they can be written as

$$\frac{dx}{a} = \frac{dy}{b} = \frac{du}{c} \quad (339)$$

This also shows that u may be found from either the equation $du = (c/a)dx$ or the equation $du = (c/b)dy$ [40]

F.7 Particle Methods

Smoothed Particle Hydrodynamics (SPH) was invented to deal with problems in astrophysics involving fluid masses moving arbitrarily in 3-D in the absence of boundaries. A typical example is the numerical simulation of the fission of a rapidly rotating star. The wide variety of applications of SPH which range from post-Newtonian fluid dynamics to highly supersonic metal and rock collisions show that SPH is a versatile tool. There are arguments to suggest that SPH is most effective in 3-D calculations and least efficient in 1-D, but the full effectiveness of SPH is yet to be determined. SPH involves the motion of a set of points. At any time the velocity and thermal energy are known at these points. A mass is also assigned to each point and, for this reason, the points are referred to as particles. In order to move the particles correctly during a time step it is necessary to construct the forces which an element of fluid would experience. These forces must be constructed from the information carried by the particles [47].

The *Particle In Cell (PIC)* method, a combined Eulerian-Lagrangian scheme, has been applied successfully to solve a wide variety of multifluid problems where the fluid distortions are large. It utilizes Lagrangian fluid particles to transport mass, momentum, and energy through an Eulerian mesh of cells. While the use of these particles facilitates the calculation of multifluid problems, it also results in nonphysical fluctuations of the fluid quantities. Furthermore, the dual mesh system of the PIC method makes great demands on computer memory capacity and calculation time.

In the *Fluid In Cell (FLIC)* method, the difference equations are very similar to those used in the PIC method. However, it employs a different transport calculation which does not require the use of particles. This reduces the memory storage requirements for a given problem and reduces the computing time, since it is not necessary to compute the motion of the particles. Furthermore, the elimination of particles allows solutions which are free of the fluctuations which are characteristic of PIC [48].

F.8 Monte Carlo Method

Many problems in physics involve averaging over many variables. For example, suppose we know the position and velocity dependence of the total energy of ten interacting particles. Since in 3-D each particle has three velocity components and three components of position, the total energy is a function of 60 variables. Hence a calculation of the average energy per particle involves computing an $N = 60$ dimensional integral. If we divide each coordinate into p intervals, there will be p^{60} points to sum in this example. Clearly we cannot apply the usual numerical techniques for large N , however for N in the range 2-5, the standard methods are still useful. The *Monte Carlo* method of integration is most suitable for the evaluation of multiple integrals for which conventional numerical methods are not generally useful.

How can we use a pile of stones to measure the area of a pond? Suppose the pond is in the middle of a field of known area A . Throw the stones at random such that they land at random within the boundary of the field and count the splashes when a stone lands in the pond. The area of the pond is approximately the area of the field times the fraction of stones which make a splash. This simple procedure is an example of a *Monte Carlo* method.

More explicitly, imagine a rectangle of height H and width $(b - a)$ such that $f(x)$ is within its boundaries. Compute n pairs of random numbers x_i and y_i such that $a \leq x_i \leq b$ and $0 \leq y_i \leq H$. The fraction of points x_i, y_i which satisfy the condition $y_i \leq f(x_i)$ is an estimate of the ratio of the integral of $f(x)$ to the area of the rectangle. Hence the estimate F_n in the "hit or miss" method is given by

$$F_n = A \frac{n_s}{n} \quad (340)$$

where n_s is the number of "splashes" or points below the curve, n is the total of points, and

A is the area of the rectangle. Note that n in (340) should not be confused with the number of intervals used in classical numerical methods.

Another Monte Carlo procedure is based on a theorem of calculus which states that the integral is determined by the average value of the integrand $f(x)$ in the range $a \leq x \leq b$. In order to determine this average, we choose the x_i at random instead of at regular intervals and *sample* the value of $f(x)$. For the 1-D integral, the estimate F_n of the integral in the “sample mean” method is given by

$$F_n = (b - a)\langle f \rangle = (b - a) \frac{1}{n} \sum_{i=1}^n f(x_i) \quad (341)$$

where the x_i are random numbers distributed uniformly in the interval $a \leq x_i \leq b$, and n is the number of *trials*. Note that the n points are chosen with random spacing in (341). For low dimensional integrals, classical methods are more accurate, but for higher dimensional integrals (341) does better [49].

G Related Problems

Certain physical problems have been under examination recently which are similar to our reaction-transport problem. Two of these related problems are presented here for comparison.

G.1 The Non-linear Burgers' Equation

Burgers' equation is a 1-D version (without pressure gradient) of the Navier-Stokes equations (85). It governs the time evolution of a 1-D velocity field $v(x, t)$

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} = \frac{1}{R} \frac{\partial^2 v}{\partial x^2} \quad (342)$$

where R denotes the Reynolds number (in dimensionless units the Reynolds number R is defined as $R = \nu^{-1}$ where ν denotes the kinematic viscosity) [50]

G.2 The Fisher Equation

The Fisher equation

$$\frac{\partial u}{\partial t} = u(1 - u) + \frac{\partial^2 u}{\partial x^2} \quad (343)$$

where $u(x, t)$ refers to the population density at a point x at time t , was proposed by R. A. Fisher in 1937 as a model of mutant gene propagation [51]

H Notation

Various symbols are in use in this text. Most of them are defined when they first occur in use. An effort was made to tabulate them here as well, so they will all be in one place for reference. Some of the most frequently used familiar symbols, e.g. e , π and ∞ , are intentionally omitted for brevity. Emphasized text appears in *italic* style type, especially when a term is defined. Variable names are in *italics*. Units are in **typewriter** style.

a	1. advection parameter, 2. acceleration
(aq)	aqueous
A	1. matrix, 2. area, 3. chemical species absorbing solar radiation, 4. point
A^*	chemical species A in an excited state
A^T	transpose of matrix A
A^{-1}	inverse of matrix A
$\det A, A $	determinant of matrix A
$\text{diag } A$	diagonal part of matrix A
AB	line segment from point A to point B
$\hat{a}, \hat{b}, \hat{c}$	vector constants
B	point
c	1. scalar constant, 2. velocity of light in a vacuum, $\approx 2.9979 \times 10^8 \text{ m s}^{-1}$
C	1. concentration of an arbitrary gaseous species, 2. a curve in the x - y plane, 3. heat capacity
$\mathcal{C}$	field of complex numbers
$\mathcal{C}^n$	n -dimensional complex vector space, $= \{(z_1, z_2, \dots, z_n) z_1, z_2, \dots, z_n \in \mathcal{C}\}$
$^{\circ}\text{C}$	centigrade, $= \text{K} - 273.15$
δ^{i+1}	Local Truncation Error (LTE)
D	1. matrix, 2. diffusion parameter
D_i	chemical product of dissociation
$\mathcal{D}$	two-dimensional plane region
d	day
$\hat{e}^i$	Total Accumulated Error (TAE)
e	electronic charge
E_i	i th equation in linear system
f, F	1. functions, 2. force
$\mathbf{F}$	field of scalars
$\langle f \rangle$	average value of f
f_c	fluid flux due to convection
f_D	fluid flux due to diffusion
$\hat{f}(\vec{y}, t)$	vector function of vector variable $\vec{y}$ and time variable t
g	acceleration due to gravity, $\approx 9.81 \text{ m s}^{-2}$ at the earth's surface
(g)	gas
$g(p)$	scalar function of scalar variable p
h	1. time increment (stepsize), 2. Planck's constant, $\approx 4.135669 \times 10^{-15} \text{ eVs}$
H	heat flow
h	hour
i, j, k	indices
$\hat{i}, \hat{j}, \hat{k}$	orthonormal unit coordinate vectors
I, I_n	n -dimensional identity matrix
$I[w]$	functional

$Im(\lambda)$	imaginary component of complex λ
k	1 reaction rate constant, 2 thermal diffusivity, 3 wave number, $= 2\pi/\lambda$
k_a	photon absorption rate
$k_j(x, t)$	reaction rate coefficient functions
K	1 thermal conductivity, 2 eddy diffusion coefficient
km	kilometer, $= 10^3$ m
K	kelvin
(l)	liquid
L	1 matrix, 2 Lipschitz constant
${}_i\ddot{L}, {}_i\bar{L}$	chemical loss rates
L	liter
m	1 fixed number of iterations, 2 mass, 3 system size
m	meter
M	1 matrix, 2 catalyst
M	mole/liter
min	minute
mol	mole, $\approx 6.0221 \times 10^{23}$
n	1 number of iterations, 2 system size
nm	nanometer, $= 10^{-9}$ m
N	1 matrix, 2 total number of chemical species involved in the simulation
$[NO_2]$	concentration of NO_2 , e.g.
$O()$	order of accuracy (big O)
O	atomic oxygen
O_2	molecular oxygen
O_3	ozone
p	1 power of h , 2 fixed point of an independent variable, 3 pressure, 4 polynomial function
ppm	parts per million
P	point
${}_iP$	chemical production rates
q	total number of discrete space points in x , i.e. number of gridpoints
Q	heat
R	1 chemical reaction rate, 2 Reynolds number
R_0	initial chemical reaction rate
${}_iR(u, t)$	reactive term for i th chemical species
R	1 field of real numbers, 2 space region
R^n	n -dimensional real vector space, $= \{(x_1, x_2, \dots, x_n) x_1, x_2, \dots, x_n \in \mathcal{R}\}$
$Re(\lambda)$	real component of complex λ
rev	revolution
s	number of iterations
(s)	solid
s	second
$\mathcal{S}$	one-dimensional plane boundary
t	independent time variable, usually in seconds
t_0	initial value of t
t_n	n th iteration of t . If Δt is constant, $t_n = t_0 + n\Delta t$
T	1 matrix, 2 period of traveling wave, 3 temperature
u	dependent scalar variable
u^n	n th time iteration of u
u_j^n	j th spatial iteration and n th temporal iteration of u
$\bar{u}^{n+1, s+1}$	$s+1$ corrector iteration of $n+1$ predictor iteration of u

$u = (u_1, \dots, u_q)^T$	column vector of q components, usually of q spatial points
u_x	partial derivative of u with respect to x
u_{xy}	second partial derivative of u
$i u$	concentration of i th chemical species
$i u_j^n$	j th spatial iteration and n th temporal iteration of concentration of i th chemical species
$\mathbf{u} = ({}_1u, \dots, {}_Nu)^T$	column vector of N components, usually of concentrations of N chemical constituents
U	matrix
v	phase velocity of traveling wave, $= \lambda/T = \omega/k$
V	volume
$\mathbf{v}$	velocity of a fluid
$\mathbf{V}$	vector space
V	volt
x, y, z	independent space variables
$\hat{x}, \hat{y}$	dependent vector variables
$\hat{x}^0$	initial value of $\hat{x}$
$\hat{x}^j$	i th component of j th iteration of vector $\hat{x}$
$\hat{x}^{k+1, l}$	Jacobi correction, computed as iteration $k+1$ of Jacobi method
$\{\hat{x}^k\}_{k=0}^\infty$	infinite sequence of vectors $\hat{x}^k$
$\dot{x}, \ddot{x},$	first, second, etc. derivative of $x(t)$ with respect to t
$y', y'',$	first, second, etc. derivative of y
${}_j y$	j th dependent variable y in a system of ODEs
y_m	amplitude of traveling wave
$y^{(n)}$	n th derivative of y
$\hat{y}(t_i)$	actual value of $\hat{y}(t)$ evaluated at t_i
$\hat{y}^i$	numerical approximation to $\hat{y}(t_i)$
α	diffusion coefficient
Γ	a curve in the x - y plane
δ_{ij}	Kronecker delta, $= 1$ if $i = j$, 0 if $i \neq j$
Δt	time increment (may be constant, may be variable) $\Delta t = t_{n+1} - t_n$
Δx	space increment
$\Delta[NO_2]$	change in concentration of NO_2 , e.g.
∇	differential vector operator, in 3-D $= \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}$
ϵ	tolerance
$\hat{\eta}$	initial condition vector
θ_1, θ_2	direction angles of outward normal to plane region boundary
κ_t	arbitrary constants in ODE solution
λ	1 wavelength of solar radiation photon, 2 wavelength of traveling wave, 3 eigenvalue
μ	combined iteration constant
ν	1 frequency of solar radiation photon, 2 kinematic viscosity
ξ	point in interval of interest where Taylor remainder is a single term
ρ	1 advection coefficient, 2 density
$\rho(4)$	spectral radius of matrix A
σ	specific heat
ϕ	1 quantum yield, 2 atmospheric eddy flux
$\hat{\phi}$	approximating function
$\phi(\hat{y}, t)$	vector function of vector variable $\hat{y}$ and time variable t
ψ	increment function
$\psi(x)$	particular integral in ODE solution
ω	1 relaxation weighting factor, 2 angular frequency, $= 2\pi/T$

Ω

region in $\mathcal{R}^n$

I Abbreviations

Various abbreviations are in use in this text. As was noted previously for the notation, most of the abbreviations are defined when they first occur in use, but are tabulated here as well.

BC	Boundary Condition
BDF	Backward-Difference Formula
BE	Backward Euler
BVP	Boundary Value Problem
CHEMSODE	a stiff ODE solver for the equations of chemical kinetics
CPU	Central Processing Unit
DE	Differential Equation
DEC	Digital Equipment Corporation
DHM	Damped Harmonic Motion
FDM	Finite Difference Method
FE	Forward Euler
FEM	Finite Element Method
FLIC	Fluid In Cell
FTCS	Finite Time Central Space
GS	Gauss-Seidel
IBVP	Initial Boundary Value Problem
IC	Initial Condition
IN	Interconnection Network
IVP	Initial Value Problem
LLNL	Lawrence Livermore National Laboratory
LMM	Linear Multistep Method
LSODE	Livermore Solver for Ordinary Differential Equations
LTE	Local Truncation Error
LW	Lax-Wendroff
MIMD	Multi-Instruction Multi-Data
MPI	Message-Passing Interface
NR	Newton-Raphson
NUMOL	Numerical Method of Lines
ODE	Ordinary Differential Equation
OS	Operating System
PC	Predictor-Corrector
PD	Positive Definite
PDE	Partial Differential Equation
PIC	Particle In Cell
PTD	Preconditioned Time Differencing
RISC	Reduced Instruction Set Computer
RK	Runge-Kutta
RP	Relative Performance
SDD	Strictly Diagonally Dominant
SHM	Simple Harmonic Motion
SIMD	Single-Instruction Multi-Data
SOR	Successive Over-Relaxation
SPH	Smoothed Particle Hydrodynamics
TAE	Total Accumulated Error
UW	Upwind Differencing

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