Appendix A
Vector Formulae

A.1 Identities

For any vectors $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ and any scalar ψ:

$$\mathbf{A}\cdot(\mathbf{B}\times\mathbf{C}) = \mathbf{B}\cdot(\mathbf{C}\times\mathbf{A}) = \mathbf{C}\cdot(\mathbf{A}\times\mathbf{B}) \tag{A.1}$$

$$\mathbf{A}\times(\mathbf{B}\times\mathbf{C}) = (\mathbf{A}\cdot\mathbf{C})\mathbf{B} - (\mathbf{A}\cdot\mathbf{B})\mathbf{C} \tag{A.2}$$

$$(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{B}\times\mathbf{D}) = (\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D}) - (\mathbf{A}\cdot\mathbf{D})(\mathbf{B}\cdot\mathbf{C}) \tag{A.3}$$

$$\nabla\times\nabla\psi = 0 \tag{A.4}$$

$$\nabla\cdot(\nabla\times\mathbf{A}) = 0 \tag{A.5}$$

$$\nabla\times(\nabla\times\mathbf{A}) = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A} \tag{A.6}$$

$$\nabla\cdot(\psi\mathbf{A}) = \mathbf{A}\cdot\nabla\psi + \psi\nabla\cdot\mathbf{A} \tag{A.7}$$

$$\nabla\times(\psi\mathbf{A}) = \nabla\psi\times\mathbf{A} + \psi\nabla\times\mathbf{A} \tag{A.8}$$

$$\nabla(\mathbf{A}\cdot\mathbf{B}) = (\mathbf{A}\cdot\nabla)\mathbf{B} + (\mathbf{B}\cdot\nabla)\mathbf{A} + \mathbf{A}\times(\nabla\times\mathbf{B}) + \mathbf{B}\times(\nabla\times\mathbf{A}) \tag{A.9}$$

$$\nabla\cdot(\mathbf{A}\times\mathbf{B}) = \mathbf{B}\cdot(\nabla\times\mathbf{A}) - \mathbf{A}\cdot(\nabla\times\mathbf{B}) \tag{A.10}$$

$$\nabla\times(\mathbf{A}\times\mathbf{B}) = \mathbf{A}(\nabla\cdot\mathbf{B}) - \mathbf{B}(\nabla\cdot\mathbf{A}) + (\mathbf{B}\cdot\nabla)\mathbf{A} - (\mathbf{A}\cdot\nabla)\mathbf{B} \tag{A.11}$$

If $\mathbf{x}$ is the coordinate of an arbitrary point, P, say, with respect to some origin, O, say, and we denote the radial distance of this point from the origin by $r \equiv |\mathbf{x}|$, then $\mathbf{n} \equiv \hat{\mathbf{x}}$ is a unit radial vector pointing along the direction $\overline{OP}$. Assume that $f(r)$ is a sufficiently well-behaved function. The following identities hold:

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$$\nabla \cdot \mathbf{x} = 3 \tag{A.12}$$

$$\nabla \times \mathbf{x} = 0 \tag{A.13}$$

$$\nabla \cdot [\mathbf{n} f(r)] = \frac{2}{r} f + \frac{df}{dr} \tag{A.14}$$

$$\nabla \times [\mathbf{n} f(r)] = 0 \tag{A.15}$$

$$(\mathbf{A} \cdot \nabla)\, \mathbf{n} f(r) = \frac{f(r)}{r} [\mathbf{A} - \mathbf{n}(\mathbf{A} \cdot \mathbf{n})] + \mathbf{n}\, (\mathbf{A} \cdot \mathbf{n}) + \frac{df}{dr} \tag{A.16}$$

A.2 Integral Theorems from Calculus

In the following $\mathbf{A}(\mathbf{x})$ and $\phi(\mathbf{x}), \psi(\mathbf{x})$ are sufficiently well-behaved functions (vector or scalar) of the coordinates. We denote here by $\mathscr{V}$ a three-dimensional volume bounded by the surface $\partial\mathscr{V}$. The differential element of the volume is written as d^3x and that of the surface as dS; however, the latter has a direction (outward), and it is thus considered as a vector quantity, viz., $\mathbf{n}dS$, where n is the unit normal perpendicular to the element in the *outward* of the closed surface direction. Sometimes we also denote $\mathbf{n}\,dS = \mathbf{dS}$. The following theorems are important in vector calculus:

$$\int_{\mathscr{V}} \nabla \cdot \mathbf{A}\; d^3x = \oint_{\partial\mathscr{V}} \mathbf{A} \cdot \mathbf{n}\, dS \quad (\text{Divergence, or the Gauss theorem}) \tag{A.17}$$

$$\int_{\mathscr{V}} \nabla \psi\; d^3x = \oint_{\partial\mathscr{V}} \psi\, \mathbf{n}\, dS \tag{A.18}$$

$$\int_{\mathscr{V}} \nabla \times \mathbf{A}\; d^3x = \oint_{\partial\mathscr{V}} \mathbf{n} \times \mathbf{A}\, dS \tag{A.19}$$

$$\int_{\mathscr{V}} \left(\phi \nabla^2 \psi - \nabla\phi \cdot \nabla\psi\right)\; d^3x = \oint_{\partial\mathscr{V}} \phi\, \mathbf{n} \cdot \nabla\psi\, dS \quad (\text{Green}'\text{s first identity}) \tag{A.20}$$

Let now S be an open surface and C the contour binding it having a line element $\mathbf{dl}$ along it. The normal $\mathbf{n}$ to S defines by the right-hand screw "law," the positive direction along the contour C. The following theorems hold:

$$\int_S (\nabla \times \mathbf{A}) \cdot \mathbf{n}\, dS = \oint_C \mathbf{A} \cdot \mathbf{dl} \quad (\text{Stokes}' \text{ theorem}) \tag{A.21}$$

$$\int_S (\mathbf{n} \times \nabla)\; \psi\, dS = \oint_C \psi\, \mathbf{dl} \tag{A.22}$$

Appendix B
A Primer of Numerical Methods for Computational Fluid Dynamics

B.1 Introduction

Computational fluid dynamics (CFD) has been advancing rapidly together with the development of increasingly powerful high-performance computing infrastructure and more sophisticated numerical methods. In the beginning, this field of study was mainly applied to high-tech engineering areas of aeronautics and astronautics. Gradually, however, CFD found its way to the study of *bona fide* theoretical and experimental fluid dynamical problems. The most general equations, governing the latter, are *nonlinear* PDE, and thus analytical approaches to the full problems were bound to fail.

The field of fluid dynamics is much older than computers. In this book we tried to describe and understand fluid dynamical problems, which usually included a significant number of simplifying assumptions, so as to lend themselves to be treatable without recourse to CFD calculations. We exhibited analytical or perturbative methods of solutions, with only few instances where numerical calculations were exploited, but it remained clear, we hope, that more general problems, e.g., certain complex flows, require numerical simulation. Numerical simulations serve as a proxy for difficult or dangerous experiments, as well as to prod our intuition. Indeed, recently numerical calculations acquired sometimes the name of *numerical experiments*, but obviously, the question of the CFD result's *reliability* has continued to loom. The fast development of computer hardware and numerical algorithms has also reduced the researcher's cost to conduct big computational flow simulations. On the other hand, the need to simulate more extreme physical conditions, higher Reynolds and/or Mach numbers, higher temperature, etc., has brought an increase in effort associated with experimental testing. Thus, it has become sometimes more economical to conduct big CFD calculation and treat them as "experiments."

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In this appendix, we shall try to give a short primer of available numerical methods, indicating their advantages and disadvantages together with some caveats. In an appendix to a book of this size, we are able to give only the basics. After all, this is not a book on CFD (on the contrary, if one may say so). There exists, today, an immense modern literature on computational methods in fluid dynamics. We shall mention in the text of this appendix some of the best (in our opinion) bibliographical sources. Clearly, a successful "attack" on a specific fluid dynamical problem should contain experiments, if possible, analytical and semi-analytical, methods (this book) to understand the basics of the problem, and numerical simulations, where it should be remembered that analytical, semi-analytical, and approximate methods may contribute to the *physical understanding* of the processes taking place in a given setting. Numerical simulation results in a solution to *one* case; however, if several such calculations are done so as to experiment with certain input parameters, it significantly increases the cost. Still the "sea" of numbers has to be visually analyzed, but the physics behind the results often remains obscure. A prominent professor of one of us (O.R.) insisted that *one should not learn physics from a computer*. Today, this may seem to some perhaps old-fashioned, but in the present state of affairs we find still much wisdom in this saying.

B.2 Short Summary and References for the Local Methods

We shall concentrate here on methods for the numerical solution of fluid dynamical equations. As we know, these equations are a nonlinear set of partial differential equations (PDEs) in space and time variables, valid in well-defined spatial domains, with appropriate *boundary* and *initial conditions*. Unfortunately, there are rigorous mathematical results on the existence and uniqueness of solutions in only special cases. This usually does not prevent the fluid numericists from applying their methods obtaining some result, which they call a solution. Again, how reliable is this result? Indeed a lot of analysis (mainly based on linear and quasilinear equations) is performed, in order to unravel what is being called a *well-posed problem*, one that hopefully will numerically yield a unique, well-defined solution. We shall end this short paragraph by saying that it is very often advantageous to write the equation in the form of conservation laws (cf. Randall J. LeVeque, *Numerical methods for conservation laws, 2nd ed.*, 1999, Bikhäuser). In this section we shall mention methods of expressing a PDE on a finite grid (or finite volumes) created in the domain of the calculation. Necessary derivatives (usually not of high order) are approximated using the (truncated) Taylor series expansion or by using other methods of calculus, e.g., integrating over the small, almost local volume and using the Gauss theorem.

B.2.1 Finite Difference Methods

The finite difference method is the oldest of the numerical methods for the solution of PDE. It is believed that already L. Euler had in 1768 "discretized" differential equation on a grid and sought their solution by hand calculations. The finite difference method, as it was already hinted above, consists of dividing the computational domain into a *grid*, that is, each coordinate domain is divided to a number of points. At each point of the grid, the Taylor series expansion is utilized to generate finite difference approximations. In this way at each grid point an *algebraic equation* arises. The method is most commonly applied to structured grids, even though the grid spacing need not be uniform (remembering that grid stretching and distortion may hurt accuracy). We shall give here some basic possibilities in two dimensions, where the function discretized is $\phi(x,y)$. We may write

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j}^{\mathrm{c}} = \frac{\phi_{i+1,j}-\phi_{i-1,j}}{2\Delta x} + \mathscr{O}\left(\Delta x^2\right)$$

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j}^{\mathrm{f}} = \frac{\phi_{i+1,j}-\phi_{i,j}}{\Delta x} + \mathscr{O}\left(\Delta x\right)$$

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j}^{\mathrm{b}} = \frac{\phi_{i,j}-\phi_{i-1,j}}{\Delta x} + \mathscr{O}\left(\Delta x\right), \tag{B.1}$$

where for the sake of simplicity we have chosen a fixed grid spacing $\Delta x = x_j - x_{j-1} = x_{j+1} - x_j$. The remainder in each case estimates the accuracy of the scheme.

Different ways of differencing (in particular when also the time variable is discretized) exist, and we will not be able to bring even most of the accepted schemes (they are usually named) here. See, e.g., C.A.J. Fletcher, *Computational Techniques for Fluid Dynamics, vol 1, ed, 2*, 1990, Springer. Fletcher's book contains in Chap. 3 and especially in Sect. 3.5 most of the known finite difference schemes and their estimated accuracy. In addition, he discusses also the conditions for numerical stability of explicit methods, using the celebrated Courant-Friedrichs-Lewy (CFL) condition, which in its simplest formulation reads $\mathrm{C} \equiv u\Delta t/\Delta x \leq C_m$. If the numerical calculation is stable (i.e., does not develop growing oscillations with a short, i.e., of very few grid points, "wavelength"), C the Courant number has to be less than C_m. In simplest explicit schemes $C_m = 1$. This effectively bounds from above the allowed timestep and makes calculations more expensive in computer time. Implicit methods also exist, which suffer from much less stringent conditions, but they require usually complex iterative calculations. Do you understand the *physical* basis for the CFL condition?

B.2.2 Finite Volume Methods

This method is not applied on PDE in their conservation form (as mentioned in the first paragraph of Sect. B.2) but rather on the integral form of the conservation equations in physical space. The computational domain is subdivided into a finite number of contiguous volumes, which go under the name of control volumes. The value of the relevant functions is formally evaluated at the centroid of the control volume. The surfaces bound the control volumes in the appropriate integral conservation relations. For example, we shall give here the appropriate approximation in two dimensions of the x and y derivative of the function $\phi(x,y)$. We shall apply the Gauss divergence theorem in the second equality of each formula below, with dS^x and dS^y denoting the *projected* areas, in the x and y directions, respectively, of the bounding surfaces of a volume element.

Thus,

$$\left(\frac{\partial\phi}{\partial x}\right) = \frac{1}{\Delta V}\int_{\Delta V}\frac{\partial\phi}{\partial x}d^3x = \frac{1}{\Delta V}\int_A \phi\, dS^x \approx \frac{1}{\Delta V}\sum_{j=1}^{N}\phi_j S_j^x, \tag{B.2}$$

where ϕ^j are the values of the function at the elemental surfaces, ΔV is the element volume, and N denotes the number of bounding surfaces of this volume. Similarly,

$$\left(\frac{\partial\phi}{\partial y}\right) = \frac{1}{\Delta V}\int_{\Delta V}\frac{\partial\phi}{\partial y}d^3x = \frac{1}{\Delta V}\int_A \phi\, dS^y \approx \frac{1}{\Delta V}\sum_{j=1}^{N}\phi_j S_j^y. \tag{B.3}$$

For a more detailed description of the finite volume method, including examples, see Sect. 5.2 of the book by C.A.J. Fletcher, *Computational Techniques for Fluid Dynamics, vol 1, ed, 2*, 1990, Springer.

B.3 Weighted Residual Methods

Weighted residual methods (WRM) are different in their basic concept from finite difference and volume methods. The approximations, necessary for numerical solutions to be extracted from, are defined by truncated series expansions, such that the *residual* (actually the error) is made as small as possible, at least in the mean. Consider the following approximation to the solution function $\phi(x)$ (all is done in one dimension, for simplicity, in some finite segment, (a,b), say):

$$\phi_N(x) = \sum_{j=0}^{N}\hat{\phi}_j\varphi_j(x), \tag{B.4}$$

where $\varphi_j(x)$ are a set of basis (a.k.a. "approximating") functions, assumed here orthogonal, for the sake of simplicity (however, see below).

The residual is thus $R_N(x) = \psi - \psi_N$ and we shall now show how it may be canceled, at least in the mean. One way of canceling the residual can be understood in the following sense: first form

$$(R_N, \Psi_j)_{w_*} = \int_a^b w_* R_N \overline{\Psi}_j \, dx, \qquad j = 0, 1, 2 \ldots, N \tag{B.5}$$

Note that the above is a kind of $w^*(x)$ weighted scalar product of the residual with a member of a set of *trial* functions: $\Psi_j(x)$. One of the possibilities ("traditional Galerkin approach") to proceed is to choose the trial functions to coincide with the basis functions, $\varphi_k(x) = \Psi_k(x)$. Orthogonality of the basis/trial functions now allows one to determine the coefficients $\hat{\phi}_j$; thus,

$$\hat{\phi}_j = \int_a^b \phi \overline{\Psi}_j \, w_* \, dx, \qquad j = 0, 1 \ldots, N. \tag{B.6}$$

Doesn't this remind one of the well-known "least squares method"? The above mentioned book by Fletcher devotes his Chap. 5 to WRM.

B.3.1 Spectral Methods

Spectral methods belong to the broad category of WRM. The first possibility of a *spectral* method uses a similar form as the Galerkin method, mentioned above. The approximating functions and the weight functions are nonzero throughout the computational domain. In this sense these are *global* methods. The important attribute of a *spectral* method that it uses *orthogonal*, under the constant weight w, functions for *both* the approximating functions and the weight functions, written here in one dimension, for simplicity. Note that we have chosen the basis function to be orthogonal for simplicity of presentation only, they need not be:

$$(\varphi_j, \varphi_k)_w = \int \varphi_j(x) \varphi_k(x) w \, dx = \delta_{jk} \tag{B.7}$$

Fourier series, Legendre polynomials, and Chebyshev polynomials are well-known examples of orthogonal functions.

Another possibility is to select the trial functions as

$$\overline{\Psi}_j = \delta(x - x_j), \qquad x \in (a, b), \tag{B.8}$$

where the points x_j are chosen in a nonarbitrary manner and the weight function is $w_* = w = 1$. This is called a *collocation* approach and the method is called *pseudo-spectral*. In general, a pseudo-spectral method is closely related to spectral methods, but it complements the basis by an additional pseudo-spectral basis, which

allows one to represent functions on a quadrature grid. This simplifies the evaluation of certain operators and can considerably speed up the calculation when using fast algorithms such as the fast Fourier transform.

Spectral methods gained prominence in the 1970s. Substantial work started to appear in the professional literature, culminating by the seminal treatise of D. Gottlieb and S.A. Orszag, *Numerical Analysis of Spectral Methods*, 1977, SIAM-CMBS. Today spectral and pseudo-spectral methods are considered the most accurate and reliable and are routinely used for the most difficult direct numerical simulations (DNS) of complex and, in particular, turbulent flows. Today, there exist a substantial number of books on spectral methods. Suffice it to say that the huge work of C. Canuto, M.Y. Hussaini, A. Quateroni, and T.A. Zang, *Spectal Methods, 2 vols*, 2006, Springer, contains over a thousand pages in its two volumes. This excellent book, written by experts in the field, is recommended for any student who wishes to learn and perhaps use these powerful methods.

B.4 Summary and Some Caveats

We hope that it is clear to the reader that this appendix is *not* the extension of our book to include numerical methods in CFD. Rather than that, it is a short primer, mentioning the methods and their principles and citing the extensive bibliography that on the subject. Successful and careful application of the right CFD method (finding the most appropriate one is not an easy task) in physics, astrophysics, and indeed all the physical sciences has become an important part of modern research. However, it should not be forgotten that theoretical physics and astrophysics are not just computation. There is the danger that inaccurate or just wrong results of numerical calculations may mislead a generation of researchers. CFD *by itself* cannot lead, in our opinion, to proper physical understanding and progress. It can, if it is carefully and correctly executed, *simulate* nature, but as it is attributed to F. Dyson "We have already one nature (Universe), we want to understand it." This is one of the main reasons that this book was written.

Finally, some caveats: we think that it would be fair to say that the knowledge of the solution can go a long way in deciding on the proper numerical scheme. More seriously, *accuracy, scheme stability, and convergence* strengthen the computation reliability. By *convergence* we mean here sufficient resolution, which can be tested by examining how the result changes with the amount of grid points or spectral functions. Obviously, it is a must to perform tests on problems to which analytical solutions are known. Feasibility (as far as computer resources allow) is also an important factor in the choice of a CFD method for a particular problem. Here it seems that progress is unlimited, having perhaps the power to change our science, one day. Right now, it would be still fair to say that choosing the right problem plus a CFD method that is the best for it and conducting a successful simulation contain an element of "art," similarly to knowing how to employ analytical methods.

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