Growth of Numerical Methods in Aerodynamics and Fluid Mechanics

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Abstract; In the 1970s, CFD in North America gained much practical value through the introduction of high-resolution finite-volume techniques developed both domestically and internationally. Since the Eu- ler and Navier-Stokes models were adopted as the norm in the 1980s, these techniques spread across aerodynamics; since then, aerospace engineering has been at the forefront of CFD advancements. The 1990s saw a change in research priorities away from underlying discretizations and toward more applied topics including high-performance computing and the generation and use of unstructured/adaptive grids. More sophisticated applications around the turn of the century are pushing researchers to seek for compact higher-order algorithms, which draw heavily on finite-element methods.

1 The Dawn of Modern CFD

1.1 The Starting Position, 40 Years Ago

Let's take a look at how the field of numerical fluid mechanics was developing in the United States in the late 1960s. The days of national labs doing pioneering research into first-order methods—research that was documented in great detail in the "Methods in Computational Physics" book series published by Academic Press [3]—are long gone.

Nevertheless, the accuracy gains that were expected from using second-order approaches such as the Lax and Wendroff method [79] for hyperbolic conservation laws and its predictor-corrector variations [22] were not being realized. As soon as shock waves arrive, numerical oscillations and nonlinear instabilities begin to haunt the solutions.

To their credit, Bernie Alder, John Killeen, and Sydney Fernbach, editors at Academic Press and Livermore, showed exceptional foresight in

The new Journal of Computational Physics has replaced the previous book series. Computational fluid dynamics (CFD) was once known as numerical fluid mechanics (NFM), and its development was chronicled in this publication.

The MUSCL algorithm of Van Leer [141] and Woodward, the gold standard in compressible CFD, was based on an essay by IBM scientist Jacob Fromm [44] in the third issue of J. Comp. Phys. (1968); see Section 2. The proceedings of the First International Conference on Numerical Techniques in Fluid

Mechanics, held in Novosibirsk, USSR, July 1969, were also published in the journal (Volume 5, 1970). The work of V. V. Rusanov [124] on third-order Euler techniques in this issue was the impetus for the work of Burstein and Mirin [21]. These higher-order extensions were useless until the issues with second-order approaches were resolved.

Yet, both within and outside of J. Comp. Phys., efforts to deal with second-order approaches persisted. This continuous Euler solution of flow over a blunt body was achieved by Burstein [22] using a 2-dimensional predictor-corrector variant of the Lax-Wendroff scheme (a step). In [79], for the 1-dimensional Lagrangean equations, the Euler extension of terms is provided to combat nonlinear instabilities and shock-induced oscillations; these terms are notable since they are third-order smoothing terms based on solution gradients.

Nonlin-ear 1-D and 2-D variations of the Lax-Wendroff scheme devised by R. W. MacCormack [90] to reduce the operation count dominated computational aerodynamics for many years after its publication in a well cited AIAA study. A simplified third-order smoothing factor is included into this scheme, and its coefficient is made to be a function of the pressure gradient.

1.2 The Birth of High-Resolution Schemes

Modeling the linear advection of a step function may help one understand the challenges involved in developing a second-order approach for the compressible Euler equations that yields shock structures devoid of oscillations. Godunov's [46] famous 1959 article contains a "barrier" theorem that states that if an advection scheme maintains the solution's monotonicity, it can only be accurate to the first order. This finding may discourage those working to enhance advection systems, however there is a workaround. It is implicit in the proof of this theorem that a linear discretization is used to approximate the linear advection equation, and once nonlinear discretizations are allowed, the theorem no longer holds.

In the first year of the 1970s, three separate strategies were initiated for building oscillation-free higher-order advection schemes, proving that Godunov's theorem could be avoided. Jay P. Boris (USA) [14], Bram van Leer (Netherlands) [139], and Vladimir P. Kolgan (USSR) [76] are the astrophysicist, astronomer, and engineer, respectively. The only two authors whose work I will analyze in this chapter are Boris and

collaborators [15, 16, 17, 158]; Van Leer's 1970s work was mostly carried out in the Netherlands, and is cited here solely for comparison. Kolgan's [76] technique is identical to Van Leer's, although it has not received as much attention or development as Van Leer's, in no little part due to Kolgan's untimely death in 1978. The Russian contribution to Computational Fluid Mechanics glosses right over it.

During a seminar course in Trieste, Italy, in August 1971 [14], Boris (then and now at the Naval Research Laboratory) presented the first non-oscillatory second-order advection system called

SHASTA - Sharp and Smooth Transport Algorithm. His method was a predictor-corrector, in which a non-oscillatory first-order scheme is followed by a corrector step that eliminates the leading, dissipative term of the truncation error ("anti-diffusion"). Yet, the corrector fluxes are throttled down when appropriate to forestall the emergence of new extremes. Flux-Corrected Transport (FCT) is the family of techniques that this process yields.

Nevertheless, FCT techniques have not caught on in aeronautical engineering, which is more concerned with stable flows, since they are better suited to and more extensively employed for turbulent high-energy flows, such as those that emerge in weapons development. A further problem is that the limiter in FCT schemes might flip on and off unexpectedly since it is so tightly tied to the update step, which can provide solution contours that resemble a staircase.

In Van Leer's method of numerical advection, the solution is represented by polynomial sub-cell distributions, and the values of their derivatives are limited. This method is basically a Discontinuous Galerkin approach. This method's finite-volume counterpart obtains sub-cell distributions by interpolating cell-averaged values, making the issue of preventing numerical oscillations a question of non-oscillatory initial-value interpolation independent of the update equation. In the United States, this perspective spawned the creation of Es- sentially Non-Oscillatory (ENO) interpolation (see Section 3.1) and left its impact on picture restoration, in particular edge sharpening [80].

The aforementioned method is distinguished by the discontinuity in all flow variables that occurs at the interface between cells. Godunov [46] pointed out in the 1950s that one can obtain unique fluxes by interpreting the situation at an interface at the beginning of a time step as Riemann's initial-value prob- lem (a generalization of what is known in gas dynamics as the "shock-tube problem"), for which there is only one known solution. The finite volume technique that takes into account these interface fluxes is automatically biased toward the upwind direction. Calculational algorithms that generate fluxes from either accurate or approximate1 solutions of Riemann's problem were soon called exact or approximate "Riemann solver" see further Sub-Section 3.1.

The first 2-D Euler code based on Van Leer's [140] advection schemes with piecewise linear subcell distributions, written and tested in 1975-77 by Van Leer's collaborator, astrophysicist Paul Woodward, was named MUSCL, for "Monotone Upstream Scheme for Conservation Laws" this acronym became generic for codes of this type. Woodward took the code to the Lawrence Livermore National Laboratory, where he further advanced and popularized the MUSCL approach and its sequel PPM (Piecewise Parabolic Method) in collaboration with numerical analyst Phil Colella [33, 34]. A landmark pa- per is their 1984 JCP review [156], an elaborate comparative study in which Godunov-type schemes, FCT and more traditional methods are pitted against one another.

The MUSCL scheme was greatly simplified when a predictor-corrector for- mulation by Steve Hancock (a former student of Maurice Holt at UC Berkeley) came along [136, 144]; this is an extension to hyperbolic systems of Van Leer's finite-volume version ([140], Scheme I) of Fromm's [44] advection scheme.

2 Computational Aerodynamics in the 1970s

While high-resolution methods were developed by researchers dedicated to a fully compressible flow model, the aerodynamics community was still served by simpler flow models, in particular, forms of the potential flow equations for homentropic, irrotational flow. Incompressible potential flow was treated by panel methods such as found in Boeing's PanAir code; Mach-number ef- fects for subsonic and supersonic flows were included in the small-disturbance equations, still linear. For transonic flow, however, the equations are inherently nonlinear.

The first successful numerical technique for steady transonic flow was based on the transonic small-disturbance equation and due to applied mathemati- cian Julian Cole and his student Earll Murman [100, 99]; here the centered stencil used in the subsonic flow region automatically switches to an upwind stencil in the supersonic region, and to a special stencil at sonic points. An in- triguing flaw of this scheme was that the transonic switch did not distinguish between an admissible compression shock and an inadmissible expansion shock, and thus could lead to the appearance of the latter in smooth flow[2]. This problem was later removed by Antony Jameson (economist by educa- tion) [66] through upstream biasing of density values appearing in the scheme, creating the artificial diffusion needed to break down expansion shocks. He also introduced differencing in a frame normal to the shock ("rotated differ- ences"), for greater robustness and precision. Jameson's techniques became part of the FLO22 code (developed with David Caughey), and of Boeing's influential TranAir code [72], formulated on a non-conforming Cartesian grid, with embedded solid-body boundary conditions. This workhorse code is still used extensively for airplane analysis and design.

[2] A decade later, expansion shocks turned up in Euler solutions obtained with Roe's numerical flux (see Sub-Section 3.1). The issue of "entropy-satisfying" fluxes be- came a topic of interest to applied mathematicians (Harten, Lax, Osher, Tadmor, Goodman, LeVeque); the standard of industry is an "entropy fix" based on the work of Harten, Goodman and LeVeque [145].

Jameson's influence on aeronautical CFD can hardly be overestimated. Starting in the late 60s he contributed a sequence of aerodynamics codes for in- creasingly complete flow models, from small-disturbance to full Navier-Stokes. Most influential were his efficient 2-D Euler code FLO57 and its multi-grid version FLO87, which definitively sold the aerospace community on the full Euler flow model.

Another strong force in the development of CFD in the aeronautical com- munity was Flow Research Corp., a company that counted among its em- ployees such influential scientists as Joe Steger, Earll Murman, Mohammed Hafez, Woodrow Whitlow and Wen-huei Jou, who all eventually ended up at high positions in academia, national labs and industry. Hafez and Whitlow are known for co-authoring the first transonic-flow code based on the full potential equation [53]. Hafez remained dedicated to the full potential equation after it had been superseded by the Euler equations, developing a non-isentropic correction [154] to the transonic shock position.

Yet the broadest effort in developing CFD algorithms and codes for aero- dynamics in the 1970s was located at NASA's Ames Research Center. While Terry Holst and collaborators were refining POTFLOW [60], a full-potential flow code, Dick Beam and Bob Warming pioneered an implicit, compressible Navier-Stokes scheme, implemented with aid of a kind of dimensional split- ting, "approximate factorization," due to Briley and McDonald, also at ARC [93]. This scheme formed the basis of the ARC2D/3D codes developed by Tom Pulliam, Joe Steger and others [112].

In retrospect the development of this Navier-Stokes solver must be regarded as premature. At this time knowledge of limiting had not yet reached aero-nautics, so the Euler discretization embedded in the Beam-Warming scheme, based on central differencing, was oscillatory in the presence of shocks, and not a good basis for a Navier-Stokes scheme.

Subsequent work by Steger and Warming on forward/backward splitting of the Euler fluxes [128], a crude approximate Riemann solver[3], was a step in a more promising direction, although the splitting was mainly intended for approximate LU factorization of implicit operators. Furthermore, a new inter- action of Peter Goorjian (ARC) with Björn Engquist and Stan Osher (both at UCLA) in 1979 gave birth to the entropy-satisfying upwind Engquist-Osher flux [42] (also based on flux splitting) for the small-disturbance transonic potential equation; it eventually morphed into a much-used approximate Rie- mann solver for the full Euler equations. This leads us right into the 1980s.

3 The Heyday of CFD: 1980-1998

3.1 Impact of High-Resolution Schemes

The emergence of higher-order Godunov-type methods created several strong research trends in the 1980s; much of the research activity was concentrated at and emanated from the Institute for Computer Applications in Science and Engineering (ICASE) at NASA's Langley Research Center, established in 1972 by the Universities Space Research Administration (USRA). After a modest start in 1972, ICASE came to play a crucial role in the further development of CFD, for aeronautics or for general use, in the US as well as worldwide; its period of high impact stretched from 1980 through 1998[4].

ICASE was set up to bring together Langley engineers and scientists from all over the country and the world, and it handled this task extremely well. One of its earliest successes was the result of introducing to LaRC of multigrid analyst Achi Brandt (Weizmann Institute, Rehovot, Israel). His collaboration with Jerry South, Jr., chief of the Theoretical Aerodynamics Branch (ThAB), on solving the full potential equation marks the first application of multi- grid relaxation to an aeronautical flow problem [73]. Another mathematician from Israel, David Gottlieb (now at Brown University) introduced spectral methods [50] to ICASE and LaRC. Spectral methods became a prominent tool for research of turbulence and the transition to turbulence; at ICASE a sizable group dedicated to such studies included M. Y. Husseini, T. A. Zang,
C. Canuto and A. Quarteroni [24].

Even more significant was the arrival of Van Leer at ICASE in 1979; this marks the introduction of Godunov-type high-resolution schemes to LaRC and, subsequently, to the general aeronautics community. Soon ICASE be- came a center of knowledge exchange and collaboration among applied math- ematicians, physicists and aerospace engineers on the subjects of limiters and non-oscillatory interpolation, as well as upwind fluxes based on approximate Riemann solvers; research in these topics proliferated. An anthology of ICASE- based papers on these topics, with historical and technical notes, can be found in the book *"Upwind and High-Resolution Schemes"* [61].

The use of upwind fluxes, which promote diagonal dominance in implicit schemes, further created a revival of classical relaxation methods, and a new perspective on convergence acceleration; see below in this section.

Among the regular visitors of ICASE, one of the most productive and in- fluential was Ami Harten (Tel Aviv University), because he also was a regular at ARC and UCLA. At ICASE he collaborated with his former advisor Peter Lax (NYU) and Van Leer on a review of upwind differencing [56], which fea- tures an approximate Riemann solver that is in wide use for large, complex hyperbolic systems[5]. At ICASE he also developed local sufficient conditions to make a scheme Total-Variation-Diminishing (TVD) [54]. The total varia- tion of a discrete solution (sum of absolute differences) will increase with the birth of a new extremum; thus, a TVD scheme guarantees a non-oscillatory solution when applied to a single *nonlinear* conservation law.

Harten's motivation for this work was to put the theory of limiting on a mathematical footing broad enough to allow extension to multiple space dimensions. Unfortunately it was shown by mathematicians Jonathan Goodman and Randy LeVeque [49] that the total variation is too crude a functional to be of use in constraining multi-dimensional discrete functions: a multi-dimensional TVD advection scheme can be no better than first-order accurate. Around 1985 Harten re-examined non-oscillatory interpolation theory while at UCLA and, together with Osher, Engquist, Sukumar Chakravarthy (Rock- well), and Chi-Wang Shu, developed the concept of ENO [58, 57, 55, 127], which does generalize to multi-dimensional solutions [1]. ENO is a systematic procedure that selects the discrete stencil whose data will give the smoothest interpolant, i. e. the function with the lowest values of its derivatives. ENO schemes are only Total-Variation-Bounded (TVB). ENO was succeeded by Weighted ENO (WENO) [71], which includes a higher-order target scheme and switches stencil only when really needed to prevent oscillations.

Another researcher whose career in CFD took off at ICASE was Philip Roe (Royal Aircraft Establishment, UK). His approximate Riemann solver [119], presented first in 1980 at the 7th International Conference on Numerical Methods in Fluid Dynamics (Stanford/ARC), became the most popular one among all such solvers. Though not developed in the USA, it is useful to describe it here, if only for the sake of comparison. It is based on a local linearization of the conservation laws, valid in the vicinity of the interface between two cells; the linearization is with respect to a smart average of the neighboring states ("Roe average"). While new for the Euler equations, it turns out that a similar linearization of the Lagrangean equations goes back to an early paper by Godunov [47].

The Riemann solver of Osher [107] treats any acoustic wave as a simple wave, whether it actually is an expansion wave, or a shock. Both Osher and Roe solvers can be used to split flux differences across a mesh into parts attributable to either forward- or backward-moving waves; this technique is called “fluctuation splitting” after Roe, or “flux-difference splitting”. Less ac- curate are the solvers based on the Boltzmann approach [56], in which the distribution functions of adjacent cells are merged; this leads to formulas commonly known as “flux-vector splitting” or simply “flux splitting.” The best-known representatives are the Steger-Warming splitting discussed earlier, and Van Leer’s flux splitting [143], developed at ICASE.

Van Leer and Wim Mulder [97, 148] demonstrated that classical relaxation methods for elliptic equations (from point-Jacobi to line-Gauss/Seidel) are effective when applied to upwind second-order discretizations of the Euler equations in two dimensions [NB: this work was not done in the USA]. Independently, Osher and Chakravarthy [106] soon came to the same conclusions. Mulder also experimented with multigrid relaxation for the Euler equations and in 1989, while at UCLA, developed a semi-coarsening strategy [98] that overcomes the lack of convergence caused by alignment of the grid with the flow.

Meanwhile, vector computing was becoming a standard capability of com- puter architecture, and this significantly upset the order of preference held by relaxation methods on the basis of their performance on scalar computers. Sequential methods such as Gauss-Seidel, where one result follows from another, can not make use of vector processing in one dimension; in multidimensional calculations, though, it is possible to process a stack of 1-D or 2-D Gauss-Seidel relaxations with vector operations. The same holds for line relax- ation, which by itself does not vectorize well. In view of these complications, the “checkerboard” variant of Jacobi relaxation (update every other point) and the “zebra” variant of line relaxation (update every other line), which vectorize well, became popular for a while. Note that most of these relaxation methods are inspired on structured hexahedral grids; it is cumbersome to extend them to unstructured tetrahedral grids [52].

The collective knowledge of limiters, Riemann solvers and relaxation meth- ods was put to use in a collaboration between Van Leer and Jim Thomas and Kyle Anderson, both at NASA Langley’s Analytical Methods Branch, and Bob Walters of Virginia Tech, in the development of the CFL2D/3D code [122], which is still in use. During this development it became clear that non-differentiable components in the residual calculations, notably, nonsmooth limiters and flux functions, could slow down or even halt convergence to a steady state. When using an implicit time-marching scheme

it is now cus- tomary to use only differentiable limiters such as Van Leer's harmonic limiter [140], Van Albada's [136], Koren's [77], or the one developed especially by
V. Venkatakrishnan [152] with easy convergence in mind.

A different approach to discretization of the Euler equations was launched in 1981 by Jameson, Wolfgang Schmidt († 2008) and Eli Turkel (Tel Aviv

University) [69]. Their numerical flux is never upwind; it is the sum of an alge- braic flux average and a third-order stabilizing artificial-diffusion term with a scalar coefficient; limiting is accomplished by trading this term for a first-order term with a coefficient proportional to the second difference of the pressure. While this approach is not automatically non-oscillatory when applied to a linear advection equation, it does give non-oscillatory shock profiles in the class of steady-flow problems for which it was intended. The time-marching method combined with this spatial discretization was a four-stage Runge- Kutta method, after Rizzi [118], who had pioneered the use of Runge-Kutta methods for Euler schemes. In addition the scheme included several explicit convergence-acceleration devices, in particular, residual smoothing (averaging of the local residual with neighboring values) and enthalpy damping. Later, Jameson added multigrid relaxation [67] and used up to five stages, with or without residual smoothing, in order to get strong high-frequency damping, as required in a multigrid strategy.

Jameson's design of multistage methods suited for multigrid relaxation was done by trial and error. The procedure was made automatic and in some sense optimized by Van Leer and students [150, 89].

Multigrid relaxation is only one of many convergence-acceleration tech-niques used in aerodynamics. Any type of vector-sequence acceleration, suchas GMRES [125], Bi-Conjugate-Gradients [137] or other Krylov methods [23], can be used to solve the large systems of nonlinear equations arising in CFD,or as a preconditioner for a final solver. Preconditioning can be a powerful toolfor clustering eigenvalues of a system to be solved; in Sub-Section 3.2 local preconditioning of the Euler and Navier-Stokes equations figures prominently.The Euler era in aeronautical CFD lasted only 5 years; by 1986, when a Euler solution of flow over a full fighter aircraft[6] adorned the cover of Avia-tion Week [9], Navier-Stokes solvers based on high-resolution Euler schemes had already been presented at the 7th AIAA CFD Conference in 1985, [134].Inclusion in a Navier-Stokes discretization does put a constraint on the ap-proximate Riemann solver used for computing the inviscid fluxes: its impliedartificial dissipation should not interfere with the structure of attached bound-ary layers [151]. This rules out the use of flux-vector splitting, which causesartificial diffusion of tangential momentum across the boundary layer [30],thus visually thickening the layer except on excessively fine grids. For thesame reason Jameson's Euler flux, which contains a scalar dissipation coef-ficient, is not tenable in a Navier-Stokes code, as demonstrated by Allmaras[4]. Turkel and Swanson [133] avoided the unwanted diffusion by replacing thescalar coefficient by a matrix; this makes Jameson's flux mimic an upwind flux, with the effect of limiting included; see Van Leer [142].

Liou and Steffen [85] succeeded in modifying Van Leer's Eulerian flux split- ting by taking out the advection terms and treating these by flux-difference splitting; only terms containing the pressure remain traditionally flux-split. The resulting numerical flux function, named Advection-Upwind/Splitting Method (AUSM), is still very simple and compatible with the Navier-Stokes equations; a number of variations exist [84].

Meanwhile, at the national laboratories (LANL, Sandia, LLNL), where CFD was intensively used in weapons and energy research (including radiative hydrodynamics), the impact of high-resolution schemes was felt in phases. The labs were quick to embrace the concept of limiting second-order terms, includ- ing it in the re-map step of their Eulerian-Lagrangean codes, which until then had been first-order accurate by necessity. This gave such an improvement in overall accuracy that no immediate need was felt to also include the other obvious component of Godunov-type schemes, the Riemann solver. It was ow- ing to the considerable efforts of Woodward, Phil Colella [156, 34] and others, that the full numerical technology of higher-order Godunov methods slowly became accepted at the national laboratories. In this regard it is interesting to note that the concept of Discontinuous Galerkin (DG) methods for fluid dynamics, which can be regarded as the ultimate way of generating Godunov- type methods, was actually invented at LANL by Reed and Hill [117], and has now become the focus of CFD method development in aeronautics; see Section 4.

Toward the end of the 1980s most developers and users of high-resolution codes for gas dynamics and aerodynamics were rather satisfied with the per- formance of their codes in a wide range of flow problems. Yet I must conclude this subsection with a discussion of one notable exception: the hypersonic flow regime. By 1988 it was clear that highly successful finite-volume codes like CFL2D produced bizarre solutions of steady flow around a blunt body on perfectly smooth grids, if the Mach number rose above 5. Typically, the bow- shock would exhibit a tumor-like growth or "carbuncle;" the correct steady solution, obtainable for symmetric flow problems by only solving for half of the flow field, no longer was an attractor.

Since then, insight into the carbuncle instability has greatly improved. There is a complete analysis of 1-D shock-position instability by Barth [11]; the instabilities become more complex when a 1-D normal shock, grid-aligned, is studied with a 2-D code [114] – this is called the 1.5-D case. Still greater complexity arises in genuinely 2-D and 3-D flow problems. Phil Roe and stu- dents have studied the carbuncle in great detail and come up with a variety of flux modifications combating the carbuncle [65], but to date no numerical flux function has been found that is carbuncle-proof in all dimensions [74].[7]

The carbuncle problem is exacerbated on unstructured grids. To this date it is recommended that hypersonics calculations be carried on multiblock struc- tured grids composed of hexahedrals [105].

This greatest unresolved problem of classical finite-volume schemes has been deemed worthy of the only illustration of this chapter, Figure 1 (from Kitamura et al. [74]).

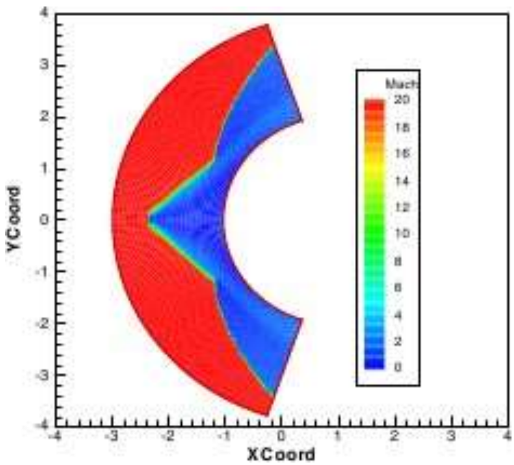

Fig. 1. The dreaded Carbuncle. Bow shock for Mach 6 flow about a cylinder. First- order Roe scheme. Contours of Pressure Coefficient.

3.2 Emphasis on Grids, Parallel Computing, and More

In spite of the carbuncle, toward 1990 research gradually shifted away from de- veloping basic Euler and Navier-Stokes discretizations, with one exception: the study of genuinely multi-dimensional Euler methods, to be discussed further below. Otherwise, CFD research turned to adaptive and unstructured grids, and formulating schemes for such grids. Convergence acceleration remained a research focus; furthermore, there was a growing research activity in more complex fluid problems, such as multi-fluid dynamics and multi-scale flow. Funding agencies were shifting moneys from focused fundamental research to high-performance (= massively parallel) computing and communication (HPCC) and grand-challenge applications; support for basic research never fully recovered.

Cartesian grids with cut cells at solid boundaries and tree-structured adap- tive refinement (quadtree, octree) were developed for pure Euler calculations and scored great successes in practical applications. A landmark is the study of Berger and Aftosmis [2] of the flow around a C-150 transport plane, in particular, the current in which exiting paratroopers would be immersed. The authors arrive at a recommendation of increasing the plane’s angle of attack when unloading troopers. Worth mentioning is also the space-weather predic- tion software BATS-R-US, which tracks a solar coronal emission all the way till it arrives at the earth, using adaptive meshes to represent a range of scales from tens of kilometers near the earth to the 1 AU distance from Sun to Earth (see the contribution by K. G. Powell in Part IV).

Fully unstructured grids for aeronautical problems, first with triangular, later with tetrahedral cells, were developed at the same time as the cut- Cartesian grids. Tim Baker (2006) and Jameson [68] were the first to produce 3-D inviscid flow solutions for a simplified airplane on a tetrahedral grid. When formulating the Euler conservation laws on such a grid, one has the choice be- tween a cell-based approach, where the cells are the volumes over which con- servation is guaranteed, and a node-based approached, where conservation is guaranteed on the cells of a dual grid centered around the nodal points. Ei- ther approach has produced efficient computational codes. Node-based codes include Jameson-Baker [68], LaRC's FUN3D [5], Mavriplis's NSU3D [92], and OVERFLOW [70]. AVUS [59] is and example of a cell-based code. In addi- tion, the so-called residual-distribution schemes, to be discussed below, are all node-based.

Pure cut-Cartesian grids proved to be unsuited for viscous flows [32]; they have to be blended with prismatic boundary-layer grid. The same is true if the main space-filling grid is tetrahedral. In some approaches developed later, e.g., those by M. S. Liou (DRAGON) [159] and Z.-J. Wang [155], the tetrahedral and prismatic grids are merged into in one framework without any distinction. The opposite is true in the CHIMERA [13] approach of Steger(1992) and Peter Buning, which is particularly effective in multi-body flow calculations. Here, each body gets its own grid wrapped around it, resulting in overset grids betweeen which interpolation routines are defined for data transfer. The approach is useful for fixed bodies as well as bodies moving with respect to each other, as with store separation or the launching of an escape vehicle. A landmark result was the flow around the Space Shuttle with booster rockets attached, computed as early as 1989 [20].

A key result on moving grids was the calculation in 1987 by Man Mohan Rai [116] of flow over a 2-D stationary blade row followed by a moving blade row, discretized on two grids sliding along one another.

In the area of convergence acceleration, some researchers concentrated on the key problem of reducing the complexity of computing steady solutions to the theoretical minimum. Specifically, solving a discrete problem with N unknowns should not require more than KN operations (the "complexity"), where K is a bounded number independent of N . It was clear that multi- grid relaxation should be part of the solution strategy. Multigrid expert Achi Brandt [18] used a slightly different terminology: to him "textbook multigrid convergence" means bringing down the residual to the level of the truncation error within a few (say, 5) multigrid cycles. This goal includes not just achiev- ing $O(N)$ complexity, but also bringing down the coefficient K to the lowest achievable value.

$O(N)$ complexity of steady Euler solutions was first achieved at the end of a long line of research started by Van Leer and collaborators [150, 89, 88] and finished by David Darmofal and K. Siu [37] in 1998. Key ingredients in this approach are optimal local preconditioning (to make the Euler equations behave as a scalar equation insofar as this is possible), optimally smoothing time-marching schemes (to efficiently damp high-frequency modes at each grid level), and multigrid relaxation with semi-coarsening (to overcome the flow- alignment problem; see Sub-Section 3.1). Darmofal and Siu showed that with regular full coarsening the complexity for an Euler calculation of lifting flow increases to about $O(N^{1.5})$, and without local preconditioning convergence stalls.

In contrast, $O(N)$ complexity of steady Navier-Stokes solutions has not been achieved; the computational work typically scales with N^2 or worse. One reason is that no optimal multi-D local preconditioner has been developed todate[8].

Local preconditioning itself has a long lineage; it descends from A. Chorin's [27] artificial compressibility technique, which allows to compute incompress- ible flow by marching in time with a hyperbolic system. This in turn was generalized by Turkel and optimized for subsonic flow [135], to speed up steady-flow calculations in the nearly incompressible regime. Many applica- tions of this basic preconditioning are due to C. Merkle and collaborators [153, 26, 43]. In 1991 Van Leer et al. [146] proved that the lowest condition number achievable among the characteristic speeds by local preconditioning of the Euler equations is $|1 - M^2|^{-\frac{1}{2}}$, where M is the Mach number. This preconditioning separates the residual component due to acoustic waves from the residual components due to advection; this allows separate scaling of the different processes, which in turn can be used to reduce the spread in wave speeds (equivalent to reducing the system's condition number), thus speeding up explicit marching toward a steady state at any Mach number. Another benefit of the residual splitting is its use in residual-distribution schemes, discussed toward the end of this section.

A general theory of optimal local preconditioning for 2-D hyperbolic sys- tems was developed by Roe [121]. It was applied successfully to the 2-D MHD equations [104], but obtaining the optimal preconditioner for MHD is suffi- ciently expensive to make its widespread application doubtful.

Two-fluid dynamics became greatly simplified with the appearance of the "level-set method" of Mulder, Osher and Sethian [96], related to older Volume- of-Fluid methods [45], but particularly easy to implement. In this method a scalar function measures the distance to the fluid interface; the zero level (contour) of the function indicates the interface itself. An advection equation or conservation law for this function is added to and integrated along with the Euler equations. Under the rule of this equation, the scalar function loses its property of distance function, so renormalization is needed at regular time intervals. The method can be used for compressible [113] as well as incom- pressible flow [130].

This chapter would not be complete without touching on the subject of genuinely multidimensional methods for the Euler equations. These started out as techniques of switching automatically to a shock-attached coordinate frame [38, 82, 35] in order to achieve a grid-insensitive shock representation, in particular, to avoid smearing of oblique steady shocks. A more fundamen- tal technique, proposed independently by Roe [123] and Ijaz Parpia [109], sought to enrich the rotated Riemann solver with a shear wave running nor- mal to the other waves. This model is suited for steady-flow calculations; it efficiently removes pressure oscillations across a detached boundary layer and, unexpectedly, leading-edge entropy errors.

In 1986, though, Roe [120] already published an even more ambitious con- cept based on an unstructured nodal-point scheme, in which the Riemann solver, previously used to decompose the flux imbalance at a cell interface, was interpreted in multiple dimensions as a multidimensional wave model that would explain the flux integral along the entire cell boundary, i.e., the residual [95]. Contributions due to the waves would be distributed in some suitable fashion over downwind nodes; the sum of all contributions at one node would serve to update the state at the node. This scatter-gather ap- proach had an Achilles heel: the wave model. The model was not unique and there were always more plane waves than state quantities, making the steady state a matter of cancelling rather than vanishing waves - not a road to high accuracy.

It took until 1994 before it was realized that the discrete acoustic waves had to be taken out of the model and treated collectively as the acoustic part of the residual. The tool by which this was achieved was a splitting of the Euler residual into a hyperbolic (advection) and an elliptic (acoustic) part, previously derived for the sake of locally preconditioning the Euler equations(see above).

This class of multi-D schemes, nowadays called “residual-distribution schemes,” matured during the 1990s owing chiefly to the efforts of Roe et al. at the University of Michigan in Ann Arbor and Herman Deconinck et al. at the Von Kármán Institute near Brussels. Milestones were the doctoral theses of Lisa Mesaros (1995, UMich [94]) and Henri Paillère (1995, VKI [108]).

The approach has become popular only in Europe, where it is actually used for solving industrial flow problems. A comprehensive report describing the European effort up to 1996 is the BRITE/EURAM project book edited by Deconinck and Koren (1997 [39]).

The state of the art is still represented reliably by the theses of Dutchman Erwin van der Weide (1998, TU Delft, Netherlands [138]) and Roumanian

Doru Caraeni (2000, TI Lund, Sweden [25]). Van der Weide solves complex steady viscous rocket-base-flow problems. His findings are that the method does fulfil its promise of uniform resolution regardless of direction, but that convergence to a steady solution suffers, probably because of the compact, highly nonlinear limiters. Caraeni develops a third-order-accurate scheme for Large-Eddy Simulation (LES). Temporal accuracy is achieved by using the scheme only in an inner iterative (pseudo-time) loop, which solves an outer, implicit update scheme.

It remains a challenge to include Navier-Stokes terms in a residual- distribution strategy, although theoretically this should be feasible. Some progress in this direction has recently been made by Nishikawa [102].

4 Latest Developments

During the past decade, CFD in the USA has become more powerful than ever, owing to the circumstance that massively parallel computing has come within reach of every research group. There is a great diversity in challenging applications; the trend seems to be toward handling increasingly complex physics in the presence of an increasingly complex geometry. It is not my intention to present an inventory of such applications; I will restrict myself to illuminating some accompanying developments in CFD methodology.

The first building block to be recast when describing a more complex phys- ical system is the inviscid part of the numerical flux function or, equiva- lently, the approximate Riemann solver. When the equation systems get larger and their eigenvector/value structure more intricate, detailed Riemann solvers with separate contributions from all waves are increasingly difficult and costly to obtain. For the 8 equations of magnetohydrodynamics[9] (MHD) a Roe-type solver is known [111], but in computational practice, specifically, in space- weather prediction (see Part IV of this book), one routinely resorts to a three-
wave solver of the Harten-Lax-Van Leer type, due to Linde (HLLL) [83]. And the even larger systems of equations ($\geq$ 10) obtainable for low-density flow by taking multiple moments of the Boltzmann equation [51, 81, 19] are now exclusively treated with the HLLL solver [132].

A completely different way of simplifying the inviscid numerical fluxes is to avoid the need for a Riemann solver by discretizing the equations on a staggered grid, in the spirit of the Lax-Friedrichs scheme [78]. Schemes of this type have the property that the solution changes even for a zero time-step, due to its projection onto the staggered grid; this projection gives an averaging or diffusion error. In consequence, the truncation error of such a scheme always has a term inversely proportional to Δt in its truncation error, and the time-step must not be made arbitrarily small on a fixed grid. These schemes therefore are not suited for defining the spatial operator in a Method- of-Lines (Runge-Kutta, multistage) time-marching approach. In spite of their inherent crudeness, a staggered scheme is a practical choice when the equation system is large or unexplored and a Riemann solver may be costly or not evenavailable.

While the Lax-Friedrichs scheme is only first-order accurate, the Tadmor- Nessyahu [101] scheme, formed on a more elaborate stencil, has second-order accuracy and is adequate for fluid dynamics. Particularly advanced are the formulations and applications of this method by the Canadian mathematician Paul Arminjon and students [6], who has used it as the basis of an efficient MHD code [7].

Much flow complexity in today's challenging applications derives from ge- ometrical complexity. The use of unstructured, adaptively refined grids can solve the problems of discretizing space in the presence of complex bound- aries, and making sure that the solution has the detail where needed. But on such grids conventional finite-volume methods lose or compromise at least one desirable property out of the following three: accuracy (one order is easily lost), monotonicity (oscillations arise in advection, or the maximum principle is violated in elliptic steady solutions), conservation (sometimes sacrificed for the sake of accuracy or monotonicity [31]). The higher the targeted accuracy of the method, the closer to impossible becomes the preservation of desirable properties. Thus, the use of the highest-order finite-volume schemes available, viz., WENO schemes, is restricted to fundamental flow research on uniform rectangular grids such as the study of turbulence (Direct Navier-Stokes or DNS simulations) or transition to turbulence [157].

The direction in which CFD methodology is currently evolving in the USA borrows generously from finite-element methods. Specifically, when expanding the subcell solution in terms of a set of basis functions, it is becoming com- monplace to treat the coefficients of the expansion as independent quantities, each with its own update equation, rather than to compute these by inter- polating the solution in the cell's neighborhood. This potentially allows one to maintain an arbitrarily high order of accuracy, which in turn may be used to counter the effects of poor grid quality. By trading the mesh size (h) for the order of accuracy (p) where the solution is smooth, and vice versa where intricate spatial detail asks to be resolved, one arrives at a so-called h p refinement strategy, also regarded as essential to modern CFD.

Examples of methods in this class are the vintage Discontinuous Galerkin (DG) method [117] and Spectral Element (SE) method [91], and the much more recent Spectral

Volume (SV) and Spectral Difference (SD) methods, both developed by Zhi-Jian Wang [129, 87]. DG typically uses a polynomial basis per cell, whereas SE obviously uses harmonic basis functions. SV and SD define the subcell solution by discrete solution values, but there is a polynomial basis in the background. There is increasing evidence that DG, SV and SD may be implementations of the same method by different quadrature- related formulas [63]; we may expect blending of the boundaries between these methods in the future.

DG is the oldest, most researched and most applied of the above methods, so it is worth being discussed here in more detail. Originally developed at LANL for neutron transport by Reed and Hill [117], it is a finite-element interpretation and implementation of the class of upwind advection schemes. It was developed independently in Europe by Van Leer ([140], Schemes III and VI), who extended it to a coupled space-time method, but at the time was unable to generalize this idea for a nonlinear hyperbolic system [141]. After that, the decelopment of DG for hyperbolic systems stalled for more than a decade.

Later applications to hyperbolic systems by Shu and Bernardo Cockburn [28], understandably, used the spatial DG operator in a semi-discretization, combined with multi-stage marching in time. It was not until 2004 that Hung Huynh [62] succeeded in formulating an explicit space-time scheme for the Eu- ler equations that reduces to Van Leer's 1977 Scheme III for linear advection; it is more efficient than DG/Runge-Kutta [131].

DG schemes for hyperbolic systems, just as finite-volume schemes, include Riemann solvers to compute inviscid fluxes, and limiters to make the solution non-oscillatory. A bottle-neck in the development of high-order DG methods is the absence of limiters suited for DG; current limiters are borrowed from finite-volume methods [29] and are too crude to preserve the subtleties of the DG discretization, resulting in loss of accuracy. For piecewise linear 1- D solutions Huynh [62] has developed a satisfactory DG limiter, but it is not clear how to extend it to multiple dimensions. In fact, one of the great unsolved problems remaining in CFD, whether one regards traditional finite- volume methods or DG methods, is to develop a multidimensional limiter for piecewise linear solutions, usable on unstructured grids.

Fortunately it is *not* necessary to develop such limiters for piecewise poly- nomial solutions of a higher degree, owing to the development of *hierarchical reconstruction* by Yingjie Liu [86] and others. Here one takes derivatives of the solution to the point that the distribution becomes piecewise linear; after limiting this derivative the linear part of the next lower derivative is limited, and so on, all the way back to the original solution.

While DG for advection was inspired by upwind finite-volume schemes and benefited from the available Riemann solvers and limiters, applying the DG concept to diffusion terms — as needed when solving advection-diffusion or Navier-Stokes problems — is not natural and had to be developed without a leading example. As a result the methodology got mired in finite-element tricks. To define a unique diffusive flux at a point where neither the solution nor its derivative are defined, penalty terms were evoked, with little physi- cal motivation. Going back as far as 1978, the first DG schemes for diffusion were inconsistent or marginally stable, until G.A. Baker [10] and Arnold [8] introduced a stabilizing interface penalty term. It took until 1998 before Shu and Cockburn came up with the now popular Local DG (LDG) method [29], inspired by rewriting the diffusion equation as a first-order system of two equations. This procedure, though, squares the condition number of the operator's eigenvalues, and therefore causes an overly restrictive stability condition on the time step.

Not suffering from this drawback are the methods of Bassi and Rebay [12]; Darmofal and his DG group at MIT [36] combined LDG with the compactness of Bassi-Rebay, and named the resulting scheme Central DG (CDG). Finally, the DG-for-diffusion scene was swept clean by Van Leer and coworkers [149, 147, 115] through the development of the Recovery-based DG method (RDG). In this technique one recovers from the piecewise polynomial solution on a pair of neighboring cells a single higher-order polynomial that is indistinguishable from the former in the weak sense. Great economy results from applying this recovery procedure to the piecewise continuous basis functions on the pair of cells; in this way a smooth *recovery basis* is obtained that can be used throughout any fixed-grid calculation. The solution is expanded in terms of the recovery basis when computing the diffusive fluxes, and in terms of the discontinuous basis when computing the advective fluxes; the sets of expansion coefficients are *identical*. Huynh [64] has shown that CDG and Bassi-Rebay can be interpreted as lower-order approximations to RDG.

In recent years it has been recognized that multistage time-marching, though convenient and versatile, does not bring out the best of the DG discretization. Space-time DG appears to be the way to go, but so far has been used only for linearized equation systems, such as encountered in aeroelasticity [75]. Relevant is that Suzuki [131] has shown an order-of-magnitude increase in efficiency when combining the spatial DG operator with Hancock's time-marching method as formulated by Huynh [62]. The latter becomes a true space-time DG method when applied to a linear hyperbolic system, and may be regarded as a first iteration step toward space-time DG for a nonlinear system.

At the start of the 21st century there clearly is no lack of challenging research topics in CFD-method development.

5 CFD in Canada

All of the aforementioned advances in CFD took occurred in the United States, and many of them would not have been possible without the contributions of immigrants drawn to the country by the expansion of the CFD industry. Nonetheless, it is important to note that Canada also has a thriving CFD community, with organizations like the CFD Society of Canada, which has an annual conference. The International Journal of Computational Fluid Dynam- ics, one of the most prestigious publications in CFD, is edited by Fred Habashi of McGill University in Montreal. Other other Canadians have made significant contributions to the field of computational fluid dynamics, including Paul Arminjon of the University of Montreal, David Zingg and Clinton Groth of the University of Toronto, Carl Ollivier-Gooch of the Jean-Yves Trepanier from Lécole Polytechnique de Montréal, Konstantin Kabin from the University of Alberta, and David Hewson from the University of British Columbia.

6 Concluding Remarks

Instead of evaluating several hundred individual research articles, I have attempted to tell the tale of four decades of CFD in the United States and Canada by focusing on technique development and following the longer arches of research. Participating in CFD research across the time period outlined has given me a unique understanding of these frequently overlapping and diverging areas of study.

I regret in advance to the many people whose names and contributions were left out, and to the readers who may not find their preferred sources among those named. Because of space and time constraints, I have had to leave off several of the topics that were originally on my ambitious list.

The goal of this chapter is twofold: to increase interest in CFD among individuals with just a passing knowledge with the field, and to provide fresh historical insights to those engaged in CFD research and/or applications.

Acknowledgments

This section of the book was written when I was going through a rough patch in my own life. Ken Powell's assistance in finalizing it via fact checking and referencing has been invaluable.

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