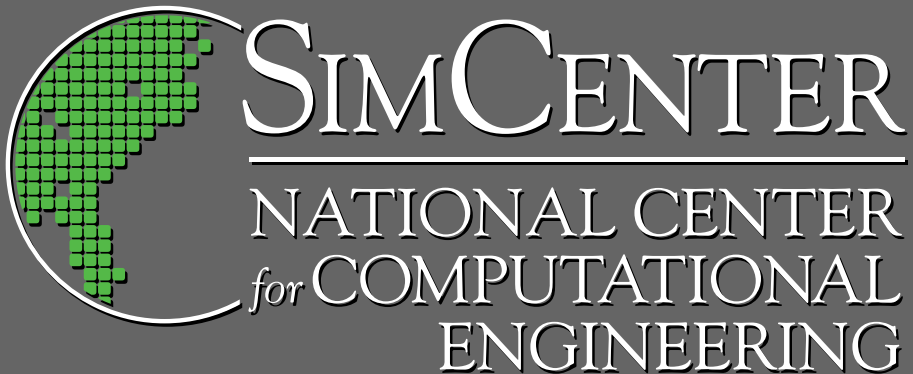


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Reflections on the Evolution of Implicit Navier-Stokes Algorithms

A Technical Report by

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UTC-CECS-SimCenter-2008-04

September 2008

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- Pre-Publication Manuscript -

This article was prepared by invitation to discuss the history and progress of joint work related to the authors' 1973 implicit method for solution of the compressible Navier-Stokes equations. It will appear (with possible revision) in a future special issue of Computers and Fluids.

Reflections on the Evolution of Implicit Navier-Stokes Algorithms

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We are very grateful for the editor's invitation to reflect on the history and progress of our joint work on implicit solution of the Navier-Stokes equations. It has prompted us to better appreciate how far our field has come since the early days of limited computer resources and of incomplete understanding of the important and necessary advances that would emerge to solve really complicated problems. We will briefly comment here on the development of our own noniterative time-linearized, block-coupled, alternating-direction implicit (ADI) scheme reported during 1973-1977, and then give some personal reflections on the subsequent evolution of these ideas and some of the progress achieved through related ideas and innovations introduced by others. References for much of the work mentioned here are given in our 2001 article in volume 30 of this journal, which commemorates the retirements of R.M. Beam and R.W. Warming. The literature on even this subset of CFD includes many more contributions than we could possibly mention here, however, and so we ask forbearance for the unavoidable omission of important work by our colleagues and even our own coworkers at the UTC SimCenter.

The impetus for implicit viscous flow solvers has been the need to solve complex flows requiring highly nonuniform grids and with multiple time and length scales. Such problems can present severe algorithmic challenges when resolving disparate local length scales introduced by geometry, very thin shear layers, and other localized flow structures. In addition, the differing time scales of convection, diffusion, sound propagation, and chemical reaction can result in equation stiffness, a term used for ordinary differential equations whose system matrices have a wide range of eigenvalues. In both instances, the enhanced stability properties available from implicit schemes can help by allowing larger time steps, within an objective of either time accuracy or convergence to a steady solution.

The challenge facing our community at that time is exemplified by considering a three-dimensional flow of Reynolds number 10^8 past a moderately complex geometry. Allowing for possible length-scale variations of 10^{-3} for small geometric features, 10^{-3} for shear layers and another 10^{-3} for viscous sublayer resolution, it was easy to foresee grids with 10 million points and with minimum to maximum cell-volume ratios of 10^{-12} and perhaps much worse. Such variations in mesh length scale and cell-volume ratios required for resolution of geometry and thin shear layers greatly affect the stability and convergence behavior of Navier-Stokes algorithms. Such algorithmic challenges appeared very formidable or even intractable in the early days of CFD.

Our work in this area began in 1968 with McDonald's work on implicit compressible boundary-layer methods and Briley's dissertation on a two-dimensional ADI scheme for the incompressible vorticity and stream-function equations. This use of ADI schemes for the vorticity and stream function equations was successful in producing validated, time-accurate incompressible solutions for axisymmetric flow in a cylindrical vessel for $Re < O(10^3)$, using time steps with Courant number over 20. However, some of the advantage of using large Courant number enabled by implicit methods was erased by the need for 4-5 iterations at each time step to couple the equations and vorticity boundary conditions. Given that computing resources were extremely limited by current standards, a more efficient implicit Navier-Stokes algorithm was needed. We initially explored extensions of the vorticity-based algorithm and developed a coupled ADI scheme requiring 2×2 block-tridiagonal solutions. This was used for prediction of laminar and transitional separation bubbles using both the Navier-Stokes and boundary-layer equations with a local viscous-inviscid interaction model. This block-tridiagonal ADI scheme was significant because it eliminated the need for iteration to couple equations and boundary conditions in this particular case. Looking ahead to three-dimensional and compressible flow applications, however, we soon abandoned vorticity-based algorithms.

The Noniterative Time-Linearized Block-Coupled ADI Scheme

With much appreciated support from Dr. Morton Cooper at the Office of Naval Research, we began work that led to our 1973 implicit algorithm for the three-dimensional compressible Navier-Stokes equations in primitive variables. This algorithm combined a) a noniterative implicit time or local linearization, b) a coupled block-tridiagonal adaptation of the 1963 Douglas-Gunn formalism for generating n -dimensional ADI schemes from any linear scalar implicit time-marching scheme, and c) the use of implicitly coupled, characteristic-compatible boundary conditions. Once we recognized the utility of the Douglas-Gunn formalism to generate a three-dimensional block-tridiagonal ADI scheme for coupled sets of linear parabolic/hyperbolic equations, we needed to develop a suitable linearization for the Navier-Stokes equations and stable boundary conditions. We did this by experimenting with different techniques using the trivial one-dimensional test problem of inviscid uniform flow at constant Mach number. This test problem was ideal because a) the exact solutions to the differential and difference equations are known and identical, b) solutions with central differences are independent of artificial dissipation, and c) it is parametric in Mach number. We became convinced that the noniterative time linearization was a key ingredient when it provided stability for large Courant numbers over a full range of Mach numbers without added dissipation, provided that implicit characteristic-compatible inflow/outflow boundary conditions were used. The time linearization fully coupled the equations, thus obviating *ad hoc* decoupling techniques, and it was also unambiguous in guiding the implicit treatment of nonlinear boundary conditions, for example the subsonic "wind tunnel" conditions of total pressure and temperature at inflow and static pressure at outflow. A somewhat related two-dimensional scheme for magnetohydrodynamics was developed independently in 1973 by I. Lindemuth and J. Killeen. They applied the Peaceman-Rachford ADI scheme without linearization, and then linearized progressively about the two successive solutions obtained for each of the half steps.

During the period 1973-1980, our group applied the time-linearized ADI scheme to numerous three-dimensional steady subsonic flows in straight and curved ducts and pipes, multiphase multispecies turbulent combusting flows, horseshoe vortex flows, and discrete-hole cooling jets. It was also used in 1975 as a spatial marching algorithm for three-dimensional supersonic flow.

It was significant that the noniterative linearization has second-order time accuracy and does not reduce the order of first or second-order time differencing. Thus Newton iteration to solve a nonlinear implicit equation was unnecessary in principle because halving the time step could reduce both linearization and time differencing errors at the same cost as a single Newton iteration. Furthermore, both of these errors vanish in steady solutions, and the use of a pseudo-time iteration avoided the need for an accurate initial guess for Newton iteration. In fact, the time step could control the linearization error during iteration toward a steady solution.

The cost of a single time step using the noniterative implicit scheme was only about twice that of explicit methods, and it generally had much faster convergence to steady solutions. This efficiency was needed for implicit solution at a time when computers were inadequate for many practical CFD problems, especially in three dimensions. However, many subsequent improvements in implicit algorithms and solution methodology would be needed to achieve modern high-fidelity simulations, as increasingly powerful computers enabled them.

In our view, the primary long-term contribution of our Navier-Stokes algorithm was to introduce the noniterative time or local linearization to systems of nonlinear partial differential equations and boundary conditions, and to recognize the value of the scalar Douglas Gunn formalization to generate implicit coupled ADI schemes for the time linearized equations. This stimulated considerable interest and further research in implicit algorithms for the Navier-Stokes equations.

Early Work at NASA Ames Research Center

Our 1974 seminar at NASA Ames helped to generate some of this interest, and many important contributions were made there. In 1976, Beam and Warming developed an implicit approximate factorization (AF) algorithm for the Euler equations using conservative equations that admit discontinuous solutions. They gave a very concise and elegant derivation of their algorithm by expressing the time linearization in terms of flux Jacobian matrices for conserved variables \mathbf{Q} , and then using approximate factorization in terms of the implicit solution variable \mathbf{Q}^{n+1} to generate the one-dimensional block-tridiagonal systems. Their 1978 Navier-Stokes algorithm was similar but introduced the “delta-form” factorization in terms of $\Delta \mathbf{Q} = (\mathbf{Q}^{n+1} - \mathbf{Q}^n)$. Although written in a different form, the approximate factorization in terms of $\Delta \mathbf{Q}$ and the Douglas-Gunn procedure for generating ADI methods give the same result for \mathbf{Q}^{n+1} ; however, approximate factorization is much more direct and quickly became the standard derivation. J. L. Steger and P. Kutler also gave an early adaptation of this time-linearized AF scheme for incompressible flows in 1977, using Chorin’s artificial compressibility formulation.

Warming and Beam did extensive work on stability of implicit schemes, and one important development was their local stability analysis indicating that the Douglas-Gunn ADI scheme for the first-order wave equation is unconditionally unstable in three dimensions. In the context of implicit algorithms, the von Neumann stability analysis assumes linear equations with constant coefficients, a uniform grid, and periodic boundary conditions. We later performed a matrix stability analysis for this inviscid equation showing that when the periodic conditions are replaced by characteristic-based inflow/outflow conditions, the algorithm is conditionally stable for inviscid Courant number less than about 1.2. This may explain why many researchers including ourselves were able to obtain numerous steady solutions in three dimensions. Although it is unlikely that any algorithm would be unconditionally stable for complex nonlinear systems, the lack of unconditional stability for this model problem properly motivated the subsequent development of much improved two-factor AF schemes for three dimensions, most

notably the lower-upper (LU) factorization.

Some Post-1980 Developments

Characteristic-Based Upwind Schemes - A major algorithmic advance came in the early 1980s when Steger and Warming, B. van Leer, A. Harten, P. L. Roe, and others developed high-resolution characteristic-based (upwind) numerical fluxes. These flux formulas are used with conservative finite-volume or integral formulations that are capable of preserving discontinuities, with consequent higher resolution properties than finite-difference schemes for flows with discontinuities and/or thin viscous layers. Upwind flux formulations are also widely used for artificial compressibility formulations. While perhaps originally motivated by their discontinuity-preserving properties, their local upwind properties later were a key to developing more effective two-factor three-dimensional implicit methods.

Reducing Factorization Error in Time-Linearized Schemes - The efficiency of the noniterative implicit algorithms was procured at expense of both time-linearization and factorization errors. Both of these errors are absent in converged steady solutions, which was their primary use at the time, especially in three dimensions. However, it became evident that stability and convergence were degraded by factorization error, especially by the three-factor stability limitation and by increased stiffness at very low Mach numbers. Two additional algorithmic advances were significant in reducing these factorization errors.

Steger and Warming's 1981 noniterative implicit lower-upper factorization (LU/AF) algorithm based on flux-vector splitting was a very important development. The well-posed and stable steps of this and other LU/AF schemes are enabled by characteristic-based numerical flux formulas and a suitable technique for obtaining exact or approximate implicit flux Jacobian matrices. They provide a stable two-factor framework for three dimensions and were eventually a key ingredient in developing effective implicit schemes for unstructured grids. Riemann-based numerical fluxes such as Roe's 1981 flux-difference scheme are now widely used in conjunction with LU/AF schemes.

Another means for reducing factorization error is the use of low Mach number preconditioning techniques, and in 1983 we first developed a constant global preconditioning matrix that reduced factorization error at low Mach number and greatly improved convergence to steady solutions. This basic idea has evolved into other well known preconditioning techniques that alter system eigenvalues locally, as introduced by E. Turkel (1984) and D. Choi and C. L. Merkle (1985).

Iterative Time-Linearized Schemes for Structured and Unstructured Grids - More progress came with the use of iteration at each time step to completely eliminate the factorization error. S. R. Chakravarthy (1984) and R. W. MacCormack (1985) began using iterative relaxation methods that eliminated factorization errors in the time-linearized scheme. Iterative schemes later became the basis for successful implicit algorithms that are applicable to unstructured grids.

Although line-oriented factorizations are not applicable for unstructured grids, the time-linearized equations can be solved by point or line iterative methods and by LU relaxation or factorization. Iterative time-linearized implicit schemes for unstructured meshes were introduced in the early 1990s by J. T. Batina using point-implicit, two-sweep Gauss-Seidel, and two-sweep point-Jacobi relaxation, by V. Venkatakrishnan and D. J. Mavriplis using preconditioned generalized minimal residual (GMRES) iteration, and by W. K. Anderson using multicolor vectorizable Gauss-Seidel relaxation.

Iterative Newton-Linearized Unsteady Schemes – Another significant advance came when Chakravarthy and M. M. Rai (1986) introduced an (approximate) Newton linearization with iterative relaxation that, upon convergence, gives a solution of the nonlinear unsteady discrete approximation. This introduction of Newton-iterative schemes became feasible with improvements in computer processing speed and memory, which allowed both larger problem sizes and algorithm improvements. Although the Newton iterations themselves were solved approximately using relaxation or factorization techniques, the converged Newton iteration eliminates both time-linearization and factorization errors at each time step. Newton-linearized iterative schemes were also developed for the incompressible artificial compressibility equations by D. Pan and Chakravarthy (1989), and S. E. Rogers and D. Kwak (1990). The Newton-linearized methods are distinct from time-linearized methods, which approach Newton linearization of the steady equations as the time step becomes infinite.

In 1991, we began our current long-term collaboration with Dave Whitfield and his group, then at the National Science Foundation Engineering Research Center at Mississippi State University. Whitfield and L. K. Taylor had developed an iterative Newton-linearized unsteady upwind artificial-compressibility scheme that incorporated symmetric Gauss-Seidel (LU/SGS) relaxation to solve the Newton linearization. This method also used numerical differentiation to compute accurate Roe-flux Jacobian matrices instead of using approximate Jacobians. Their implementation exploited CPU/memory trade-offs enabled by large memory resources that had become available, at that time Cray SSD. By organizing the computation into sequential blocks and storing the residuals and large numerical Jacobian matrices, the linear LU/SGS iteration sweeps became extremely inexpensive, and the factorization error could be eliminated at very little cost. They subsequently modified this algorithm to perform multiple Newton iteration cycles, using LU/SGS sub-iteration to solve each linear Newton iterate. Another significant advance came in 1998, when J.C. Newman III, Anderson and Whitfield began using complex-variable numerical differentiation to compute highly accurate flux Jacobians and sensitivity derivatives.

There is some algorithmic unity in the fact that symmetric Gauss-Seidel relaxation and two-factor AF are equivalent linear iteration schemes, although they are generally written in different forms. The Newton-linearized schemes work well for steady solutions and can be used without the added cost of Newton iterations, but they are especially beneficial for time-accurate simulations, since they permit fully implicit nonlinear time-integration schemes. Accordingly, the Newton linearization of the unsteady equations is commonly used instead of the noniterative time linearization.

Scalable Parallel Algorithms for Structured and Unstructured Grids - In the early 1990s, we began exploring methods for transitioning implicit algorithms to parallel computers. In 1995, R. Pankajakshan and Briley modified Taylor and Whitfield's iterative Newton-linearized Navier-Stokes algorithm to enable parallel solution with minimal effect on its algorithmic performance. The parallel algorithm used a modified block-Jacobi symmetric Gauss-Seidel (BJ-SGS) sub-iteration scheme with coarse-grained domain decomposition for mapping to distributed-memory processors. In his 1997 dissertation, Pankajakshan developed a parallel iteration hierarchy for time-accurate solutions that encompassed multigrid, Newton and BJ-SGS iterations, and evaluated both algorithmic and software performance. A semi-empirical parallel performance model for his MPICH software implementation indicated constrained-memory scalability to at least 400 processors using contemporaneous distributed-memory computers such as the IBM-

SP2 and Cray-T3E. In 1997, C. Sheng and Whitfield began working with Kyle Anderson's implicit unstructured time-linearized flow solver and developed a multi-block implementation to reduce memory requirements on single-processor machines. Building on this work, D. G. Hyams's 2000 dissertation developed a scalable parallel implicit viscous flow solver for highly nonuniform multi-element unstructured grids. His work addressed issues of parallel iteration hierarchy for the Newton-linearized method and of the treatment of connectivity and coupling of the sub-domain interfaces. Finally, after our current group was formed in 2002, K. Sreenivas, Hyams, D. S. Nichols III, Pankajakshan, and Taylor developed a new code (now called Tenasi) based on this same algorithm but with many refinements, extensions and new capabilities for complex computational engineering analysis and design applications.

Implicit methods that have evolved from our early work continue to be applied to a wide range of problems. Many of these methods appear sufficiently attractive that a significant number of researchers are exploring algorithmic development to improve or extend these methods to an even broader range of practical problems. Our own work in recent years has focused on various application problems and related algorithm developments. These interests have included multiphase and chemically reacting flows, the shallow-water and Maxwell's equations, preconditioning, treatment of source terms and discontinuities other than shocks, and complex-variable differentiation.

Historical Examples of Runtime and Problem Size

We conclude by giving in Table I some historical examples of flow cases our group has run on different computers over the years. The first six cases (A-F) illustrate the evolution over time in problem size and runtime. The last case (G) is a hypothetical case having 10^6 grid points and 10^3 time steps. Runtime and cost are estimated for case G by assuming it would run on each computer at the same rate of runtime per point per step as in the corresponding cases A-F.

It is remarkable that the hardware cost for running the standardized case G has decreased from an estimated \$328,000 for the 1968 CDC-6600 to just \$0.23 on the current University of Tennessee at Chattanooga SimCenter Linux cluster of in-house design. Although the runtime varies with the number of processors used (constrained by available memory), the cost is more or less independent of the number of processors used, within the range of linear scalability for a given problem size. Our current benchmarks show a near-linear scalability up to 1200 processors on a problem size of 96 M points.

Although not evident from Table I, the Navier-Stokes algorithms have also improved greatly in regard to geometric and problem complexity, solution accuracy, and general robustness. Although these algorithms continue to evolve, CFD as a specialty is now having a tremendous impact on practical engineering analysis and design problems, and it appears that this impact will continue and accelerate for the foreseeable future.

Table I – Historical examples of actual Navier-Stokes flow cases

Historical Cases						Case G (Hypothetical)	
Year	Computer	Case [@]	Grid Size	Time Steps	Actual Runtime Hrs (Proc)	Runtime Hrs (Proc)	Cost [†] (in 2007 \$)
1968	CDC-6600	A	26x101	100	0.38 (1)	1447 (1) [*]	\$328,000
1973	Univac 1108	B	11x11x11	60	0.22 (1)	2713 (1) [*]	\$124,000
1985	Cray X-MP	C	29x29x29	60	0.13 (1)	89 (1) [*]	\$5,000
1998	Cray T-3E	D	4.5 M	14000	320 (50)	5 (50)	\$68
2004	SimCenter Cluster 1	E	18 M	5400	44 (100)	0.45 (100)	\$0.80
2007	SimCenter Cluster 2	F	21.5 M	2000	8.2 (160)	0.19 (160)	\$0.23

^{*} Hypothetical: if memory were available to run Case G

[†] Typical published hardware-only cost without discount, operating continuously without down time, depreciated over three years, in 2007 dollars

[@] Explanation of Cases:

- A. **University of Texas Austin 1968** - Time-accurate, incompressible, axisymmetric rotating flow: ADI scheme, vorticity/stream-function method (2D)
- B. **United Technologies Research Center 1973** - Steady flow in a straight square duct: Noniterative Time-linearized ADI/AF scheme (3D)
- C. **Scientific Research Associates, Inc. 1985** - Steady horseshoe vortex flow: Noniterative time-linearized ADI/AF scheme (3D)
- D. **NSF ERC Mississippi State University 1998** - Time-accurate 6-DOF maneuver of submarine with rotating propulsor and moving control surfaces, 2 hull lengths, 40 propeller revolutions: Parallel, structured Newton-iterative LU/BJ-SGS scheme (3D)
- E. **University of Tennessee SimCenter 2004** - Time-accurate release of contaminant in urban environment: Parallel unstructured Newton-iterative LU/BJ-SGS scheme (3D)
- F. **University of Tennessee SimCenter 2007** - Steady 360-deg compressor rotor with 36 blades: Parallel unstructured Newton-iterative LU/BJ-SGS scheme (3D)
- G. A hypothetical standardized case having 10^6 grid points and 10^3 time steps

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