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# Towards the Next Generation in CFD

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**The impact of computational fluid dynamics (CFD) on aerospace design is hindered by the lack of certainty inherent in CFD simulations as they are typically performed today. The next generation of CFD must be capable of producing simulations at engineering-required accuracy in a reasonable time and in an automated manner. The purpose of this paper is to highlight the research topics that are critical to the development of a reliable, timely, and automated CFD capability. In particular, we discuss the need for and potential impact of solution-based adaptation, higher-order discretizations and corresponding solvers, and direct integration of CFD with CAD geometry models.**

## I. Introduction

Computational fluid dynamics (CFD) has made a significant impact on the aerospace design process. While experimental testing will always remain an integral part of aerospace design, especially for vehicles with high safety requirements, CFD has decreased the reliance on experimental testing.[1] CFD is clearly capable of approximating flows even for extremely complex problems, whether those complexities are due to geometry, physics, or both. As a result, CFD is viewed by many as a mature technology.

The impact of CFD on aerospace design, however, is hindered by the lack of certainty inherent in CFD simulations as they are typically performed today. Currently, the risks involved in using CFD for design are managed by developing standard practices for the desired applications.[2] These practices involve prescriptions for grid topologies and densities, turbulence models, iterative methods, corrections to simulation results, etc. However, when applied to problems outside of the scope for which they were developed, these standards can prove unreliable. Thus, for off-design conditions or novel design concepts, the utilization of CFD requires significant expert involvement and time in an attempt to manage the associated risks.

In our view, CFD has not reached its full potential. To do so, the next generation of CFD must be capable of producing simulations at engineering-required accuracy in a reasonable time and in an automated manner. With these capabilities, CFD technology can make an even greater impact on aerospace design. Novel design concepts can be explored allowing engineers to ask 'what-if' questions and receive reliable answers in a timely manner. Databases for on-design and off-design conditions could be generated facilitating screening of evolutionary and revolutionary designs.

The purpose of this paper is to highlight the research topics that are likely to be critical to the development of a reliable, timely, and automated CFD capability. The chosen topics are admittedly biased towards the authors' opinions. While some new results are given, the primary focus is to motivate the importance of each topic, briefly describe previous research, and highlight existing challenges.

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## II. Error Estimation & Adaptation

Most applications of CFD rely on previous experience to define an adequate mesh. Then, if time permits, the simulation on this initial mesh can be interrogated and a new mesh could be generated if concerns exist about the quality of the initial results. For off-design conditions, novel design concepts, or applications with complex physics, this is a time-consuming process that severely limits the utility of CFD.[1] Grid convergence studies can also be performed, however if the solution is far from the asymptotic regime, this approach could also fail to reduce the uncertainty.

One approach to achieve engineering accuracy in an automated fashion is error estimation and adaptation.[1,3] Research in adaptive methods has often stressed the potential to attain desired accuracy in fewer degrees of freedom and less computational time than through global refinement. However, this emphasis tends to ignore the large time spent developing an initial mesh especially for complex problems as well as the labor-intensive aspect of mesh generation. For simple problems where efficient meshes of high-quality can be readily generated, adaptive methods are unlikely to be competitive. The critical feature which adaptive methods offer is automated reliability for all problems.

Solution–based, automatic grid adaptation has demonstrated the potential to iteratively improve the solution quality by modifying the local grid resolution.[4–12] For high Reynolds number flows, two factors that limit the application of solution–based adaptation are reliable error indicators and adaptive generation of anisotropic meshes especially around complex geometries.

### A. Error Estimation

Several types of error indicators have been investigated. Many methods use indicators based on large flow gradients or undivided differences.[5,7,9] These methods tend to increase the grid density near certain flow features such as shocks, wakes, and boundary layers. Unfortunately, indicators of this type may lead to incorrect results. For example, continuously refining the grid near a shock does not necessarily lead to an improvement in overall solution accuracy. Predicting the proper shock strength and location, as well as other derived quantities, may depend more on the quality of the grid well upstream of the shock rather than in its immediate vicinity.[5]

Adaptive indicators have also been derived from interpolation error estimates for linear finite elements.[4,5,8,10] These methods attempt to equidistribute the estimated interpolation error in one or more scalars throughout the computational domain. Essentially, this amounts to adapting on the local second–derivatives or Hessian of the solution and, therefore, shares some of the potential deficiencies associated with feature–based indicators. Traditional feature– and Hessian–based indicators are local in nature and do not provide a reliable indication of how the discretization error is distributed or transported throughout the domain.

An alternate approach to making error estimation more relevant for engineering applications is to assess the error made in predicting integral quantities representing basic engineering outputs. Examples include the lift and drag forces acting on an aircraft wing, the mass-averaged total–pressure drop across a high–pressure turbine stage, or the average noise levels generated by an aircraft at takeoff condition. There has been a significant volume of research into *a posteriori* error analysis and grid adaptation for functional outputs within the context of finite element methods for fluid dynamics.[13–22] To estimate the error in an output, local residual errors are related to the output error through the adjoint solution. This relationship allows local error contributions to be used as indicators in a grid adaptive method designed to produce specially-tuned grids for accurately estimating the chosen output. For general discretizations, Pierce and Giles[23–26] have developed an adjoint-based error correction technique for functional outputs that extends superconvergence properties, automatically inherent in many finite element methods, to cover numerical results from any numerical method, including finite difference, finite volume, or finite element without natural superconvergence.

The work of Pierce and Giles was the stimulus for our recent work in output-based adaptation for compressible Navier-Stokes. Our approach merges an output-based indicator for cell size[27,28] with a Hessian-based indicator for cell shape.[29,30] We have demonstrated the method on a large variety of aerodynamic applications including inviscid subsonic to supersonic ($0 < M < 6$) flows, transonic Reynolds-averaged Navier-Stokes (RANS), multi-element high-lift flows, and recently sonic boom.[31] Park has extended and applied the methods to three-dimensional flows.[32,33] A key result from this work has been the reliability of the output-based adaptation; specifically, in all test cases, the output-based method has converged to globally-refined solutions.

While the output-based adaptive method has been very reliable, unsteady flows represent a severe challenge to method, and in fact time-dependent adjoint-based adaptation has not yet been pursued. The major difficulty with time-dependent flows is that the adjoint problem requires backwards integration in time. Thus, the primal equations must first be solved and then stored in some fashion. Then, the adjoint equations are marched backward from the final time linearizing about the stored primal iterates. This represents an enormous computational cost and at present does not seem viable for three-dimensional problems.

Even for steady flows, adjoint-based adaptation can face another challenge. For many applications, CFD simulations do not converge to a steady state solution, but rather remain somewhat unsteady. This is frequently observed with wakes and separated flows in three-dimensions. When this effect is relatively small, the impact on the outputs of interest can be minor and the non-converged solution is still frequently used (though perhaps in some average sense). However, this unsteadiness is often a result of a weak linear instability which is damped by nonlinearities. Thus, when the adjoint problem is solved, this nonlinearity is no longer present and the adjoint solution method will diverge. This problem has already been observed in the application of adjoints to optimization.[34,35] One solution to this problem is to increase the strength of the iterative solver.[36] When the unsteadiness observed in the simulation is due to a weak numerical instability (e.g. a physically stable mode exists that is outside the stability region of the iterative algorithm), this approach makes sense. However, when the flow is truly unsteady, strengthening the solver could stabilize the flow leading to significant errors.

Given the difficulties with adjoint-based adaptation for unsteady flows, alternative approaches may prove attractive. Aftosmis and Berger have recently applied residual-based indicators.[12] Unfortunately, the specification of desired residual levels is not obvious (compared to specifying output error), and this problem is exacerbated by the need to account for residuals from multiple equations. Regardless, residual-based indicators are an improvement over interpolation-based indicators since the local residual is a direct measure of the error even for highly convective systems.

In addition to discretization errors, modeling errors must also be considered. This is a much more difficult task but one that will be important as discretization errors are better controlled.

### B. Anisotropic Adaptation

A major bottleneck in automating the generation and adaptation of grids is the ability to robustly generate stretched (anisotropic) cells near complex, three-dimensional geometries. While the generation of isotropic meshes is relatively in-hand, we are not aware of any existing tools (whether from CFD software suppliers, government laboratories, or academia) that can robustly generate stretched (anisotropic) meshes near complex, three-dimensional geometries. The existing tools (e.g. NASA Langleys Vgrid) that come closest to this ability require significant manual intervention to specify near-surface resolution requirements, lack robustness near complex surfaces, and have no capability to generate stretched meshes off-surface. In contrast, for two dimensional problems, we have found BAMG from INRIA to robustly perform anisotropic adaptation.[37]

## III. Higher-order Discretizations

The accuracy of many discretizations currently used in aerodynamics is at best second order. For problems with high accuracy demands, the use of higher order discretizations can lead to significant gains in computational efficiency. This is clearly the case for long timescale unsteady problems where discretization errors compound as the flow is evolved. These situations are increasingly important in aerospace applications as the use of Detached Eddy and Large Eddy Simulations continues to expand. Acoustic simulations are another example where the need for high accuracy drives discretizations to higher order.

Even for traditional, steady state CFD simulations, higher order accuracy could offer significant computational benefits. In particular, boundary layer flows could be resolved with substantially fewer degrees of freedom than the essentially linear-varying approximations that dominate current practice. A common criticism for the application of higher-order methods to RANS is that the inaccuracy of turbulent models does not warrant reduced discretization error. However, the results from the recent AIAA Drag Prediction Workshops[38, 39] indicate that the spread in CFD-based drag estimates may be equally shared by discretization and modeling errors.

Numerous reasons exist for why current discretizations are not practical at higher order and have remained second-order. The root cause lies in the extended stencils that these algorithms employ. For discretizations that explicitly add numerical dissipation, the extended stencils arise from higher-order stabilization terms. For algorithms that introduce stabilization through upwinding, the extended stencils arise through local interpolants used to increase accuracy. These extended stencils contribute to difficulties in:

- *Stable iterative algorithms.* A well-known fact is that the iterative solution of these discretizations requires multi-stage methods and/or implicitness beyond a locally implicit scheme. Another common iterative approach employs backward Euler in which the Jacobian of the higher-order discretization is replaced by a lower-order approximation. Unfortunately, Mavriplis[40] has shown that the use of lower-order approximations severely limits the convergence rate attainable for higher-order finite-volume simulations of complex problems even when the lower-order systems are solved exactly.

- *Memory requirements.* Extended stencils degrade the sparsity of the linearized systems of equations used in implicit solution methods. This increased fill results in very high memory requirements and is the reason that lower-order approximations are often utilized.

- *Boundary conditions.* At boundaries, the construction of higher-order operators or higher-order reconstructions is difficult due to a lack of neighbors.

By contrast, finite element formulations introduce higher-order effects compactly within the element. Thus, viewed from the element level, the stencils are the same for all orders. Recently, Venkatakrishnan *et al*[41] showed that higher-order finite element schemes have significant advantages for smooth inviscid and viscous flows; however, they also delineated several remaining challenges that must be addressed before higher-order methods will be robust and efficient for practical applications containing shocks or other under-resolved flow features.

An attractive approach for achieving high-order accuracy is the discontinuous Galerkin (DG) formulation, in which element-to-element coupling exists only through fluxes at the shared boundaries between elements. This limited coupling is an enabling feature which permits the development of an efficient high-order solver. Furthermore, the DG formulation is well-suited for general unstructured meshes, and, due to its elementwise discontinuous representation, it is a natural method for $h$ and $p$ adaptation.

DG methods have been developed extensively for hyperbolic conservation laws, and, to a lesser extent, for diffusive operators. Bassi and Rebay have performed numerous studies for the Euler and Navier-Stokes equations,[42–44] showing the potential benefits of high-order accuracy with DG in these applications. Further details on DG methods are given by Cockburn and Shu,[45] who outline the state-of-the-art in this field and provide implementation details. For viscous problems, Arnold et al.[46] have analyzed a majority of the DG discretizations for Poisson's equation.

As noted by Cockburn and Shu, an area which has received less attention is solution algorithms for high-order DG discretizations. Hemker et al.[47] analyzed block Jacobi smoothing strategies with $h$-multigrid for one-dimensional diffusion problems. In addition, $p$-multigrid, or multi-order, solution strategies have been studied for high-order DG,[48, 49] showing several advantages such as ease of implementation and order-independent convergence rates.

Recently, we have developed a multigrid method for a higher-order DG discretization of the Navier-Stokes equations.[50–54] The algorithm employs $p$-multigrid with an element line Jacobi smoother. We have chosen the DG discretization of the compressible Navier-Stokes equations developed by Bassi and Rebay,[44] commonly refered to as the BR2 discretization.[55] This discretization has several advantages including a compact nearest-neighbor stencil and provable optimal accuracy ($O(h^{p+1})$ for the $L_2$ error). The element lines are formed from the strongest element-to-element coupling as determined by a low-order ($p = 0$) discretization of the convection-diffusion equation. Fourier analysis of the two-level $p$-multigrid algorithm for convection-diffusion shows that element line Jacobi is significantly better than element Jacobi especially for high Reynolds number flows and stretched grids.

A representative viscous case is that of $M = 0.5$, $Re = 5000$, laminar flow over a NACA 0012 airfoil at $\alpha = 0^o$. A set of four structured grids was used to generate the data. The meshes were created by modifying a baseline grid provided by Swanson[56] and coarsening three times, resulting in four nested meshes containing 672, 2688, 10752, and 43008 elements. The coarsest mesh is shown in Figure 1. On the airfoil

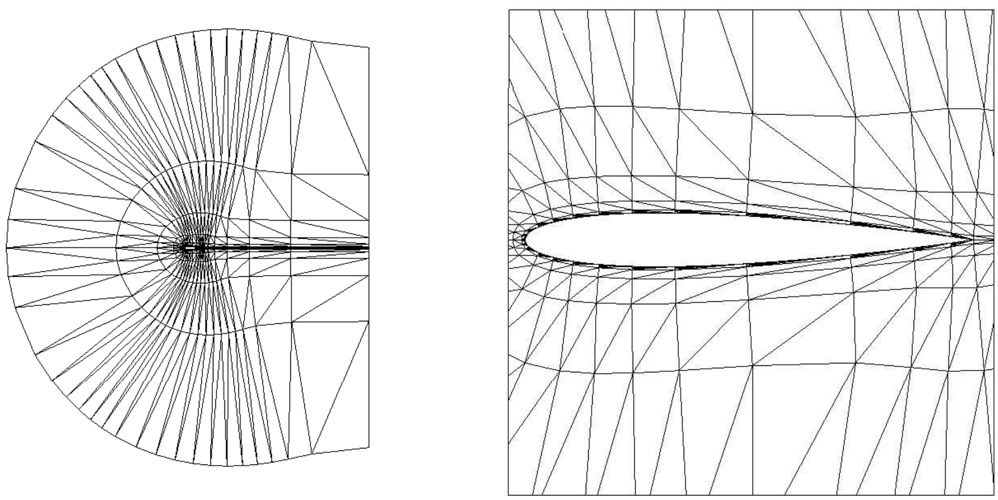
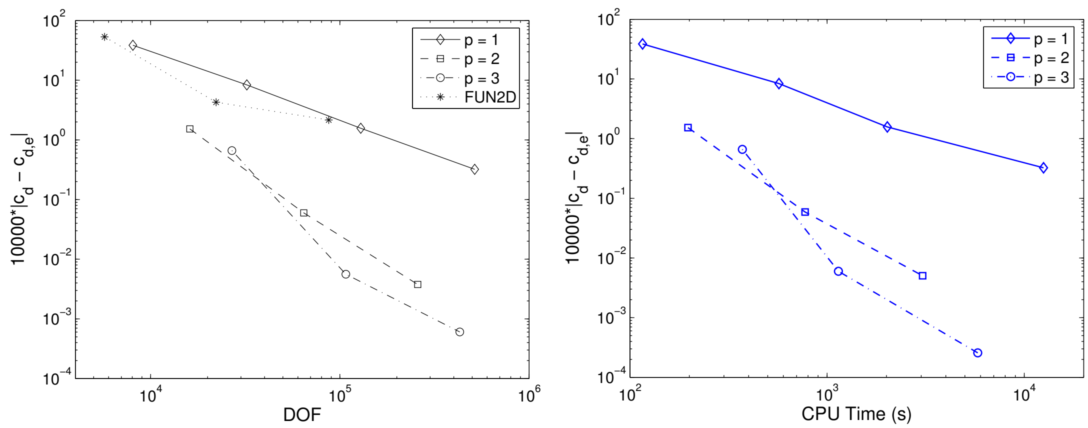


**Figure 1. Coarse NACA 0012 mesh, 672 elements.**

surface, a no-slip, adiabatic boundary condition was imposed. The airfoil was represented with piecewise cubic polynomials for all orders of solution approximation.

The drag error for each grid and polynomial order versus degrees of freedom (DOF) and CPU time is shown in Figure 2. The drag error is defined as the difference between the drag for a given case and the drag computed from the $p = 3$ solution on the 43008 element mesh. For comparison, results computed by FUN2D, which uses a node-centered finite volume algorithm, on the same meshes are shown in Figure 2(a).[57,58] The convergence of the FUN2D and $p = 1$ methods in terms of DOF is very similar. However, the $p = 2$ and $p = 3$ results are significantly better. For example, the drag for the 2688 element $p = 2$ solution ($6.5 \times 10^4$ DOF) is within 0.1 drag counts of the finest grid, $p = 3$ result, while the drag for the finest grid, $p = 1$ solution (43008 elements, $5.2 \times 10^5$ DOF) has an error of approximately 0.3 counts. Thus, at error levels of practical interest, higher-order solutions provide significantly better accuracy per DOF than $p = 1$ solutions on more refined meshes. However, this DOF comparison does not imply that the high-order solver outperforms FUN2D in terms of CPU time. While a CPU time comparison is presented in Figure 2(b), the FUN2D results from Figure 2(a) are not included because no attempt was made to optimize the performance of FUN2D or the current solver for the problem considered.

Figure 2(b) shows the drag error versus CPU time. The values plotted were obtained using a drag-based




(a) Drag error vs. DOF

(b) Drag error vs. CPU time

**Figure 2. Drag error results for $0 \leq p \leq 3$ for NACA 0012 at $M = 0.5$, $Re = 5000$, $\alpha = 0°$.**

stopping criterion. Specifically, the calculation was stopped when the change in the drag per iteration was less that 0.01 drag counts, $10000|c_d^{n+1} - c_d^n| < 0.01$, for three consecutive iterations. Clearly, the higher-order solutions produce smaller error in less time than the $p = 1$ solution. For example, to achieve a drag error of approximately 0.1 counts, the $p = 1$ solution would take approximately 100 times longer than either the $p = 2$ or $p = 3$ solutions.

Figure 3 shows the residual convergence for $p = 1$ and $p = 3$ on three meshes. The multigrid performance is seen to be largely independent of $p$ for the orders tested, however, a clear $h$ dependence is observed. For $p = 1$, on the 672 element mesh, the residual converges to $10^{-10}$ in approximately 15 multigrid iterations, while on the fine mesh, 36 iterations are required.

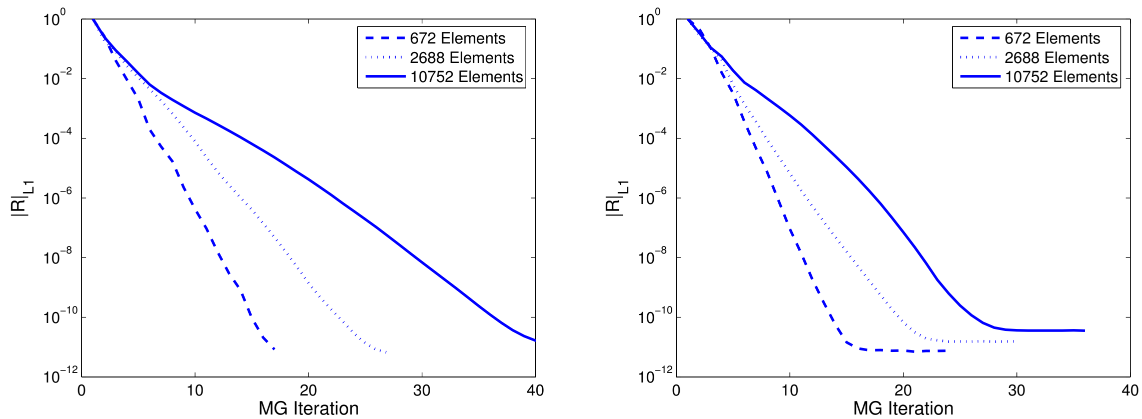
Figure 4 shows the performance of four different solution algorithms: element Jacobi with and without $p$-multigrid, and element line Jacobi with and without $p$-multigrid. The incorporation of the element line Jacobi smoother significantly improves performance, and $p$-multigrid with element line Jacobi smoothing is the most efficient solver.

While the higher-order DG solver described above is significantly more efficient for laminar airfoil flows than second-order ($p = 1$) discretizations, several challenges exist before the method can be applied to common aerospace applications. In particular,

- Shocks require a modification of the standard DG discretization. A variety of methods have been proposed based on shock-capturing stabilization as well as limiting. However, to date, the authors are unaware of any method that can robustly deal with shocks without affecting the accuracy in smooth regions of the flow.

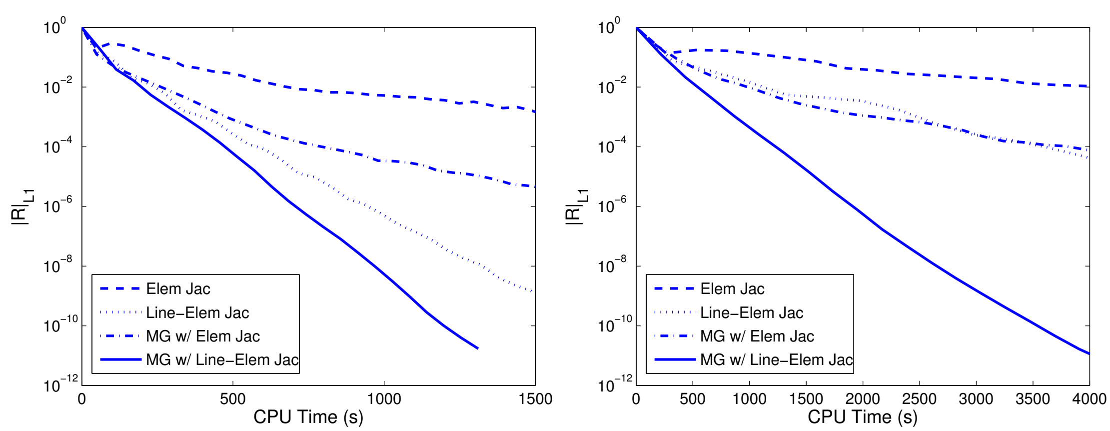
- Very little research has investigated higher-order finite element discretization of turbulence models.[43,44] The discretizations need to be extended and tested for a variety of RANS applications.

- Another difficulty with higher-order methods is the need for higher-order geometry representation. Without higher-order geometry, the solution accuracy cannot achieve optimal $O(h^{p+1})$ rates (assuming the flow is smooth).




(a) $p = 1$ (b) $p = 3$

**Figure 3. $p$-Multigrid residual convergence versus grid size for NACA 0012 at $M = 0.5$, $Re = 5000$, $\alpha = 0°$.**




(a) $p = 1$ (b) $p = 3$

**Figure 4. Solver comparison on 2688 element mesh for NACA 0012 at $M = 0.5$, $Re = 5000$, $\alpha = 0°$.**

## IV. Direct Interface to CAD

A common approach to define geometry for CFD analysis is through a surface definition such as IGES. Often, the surface representation is generated from a CAD model. However, this approach breaks the link with the engineer's original intent. Furthermore, IGES representations require significant human intervention to create something that is water-tight for subsequent use in mesh generation.

A CAD system is a natural manner for engineers to express their design intentions. By directly interfacing CFD to CAD, the time between concept and simulation can be greatly reduced. Furthermore, this level of automation would be critical for design optimization.

Another advantage of directly interfacing CFD to CAD is that the CAD model can serve as a common geometry description for multi-disciplinary analysis and design.[59] In addition, if the CAD model is constructed using a feature-based approach, then the different disciplines can select a level of featuring which is consistent with that discipline's requirements.

One solution for interfacing CFD with CAD is embodied by the CAPRI software.[60] CAPRI provides the user with a water-tight triangulation of the solid model and maintains the association of the triangulation with the solid model.[61,62] CAPRI has been used by several researchers to provide direct access to the underlying CAD model.[63–66] In particular, *Cart3D*[12,64,65] is notable for its ability to handle problems with significant geometric complexity and, except for its current limitation to inviscid flows, is a good example of the possibilities for CFD in the next generation.

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