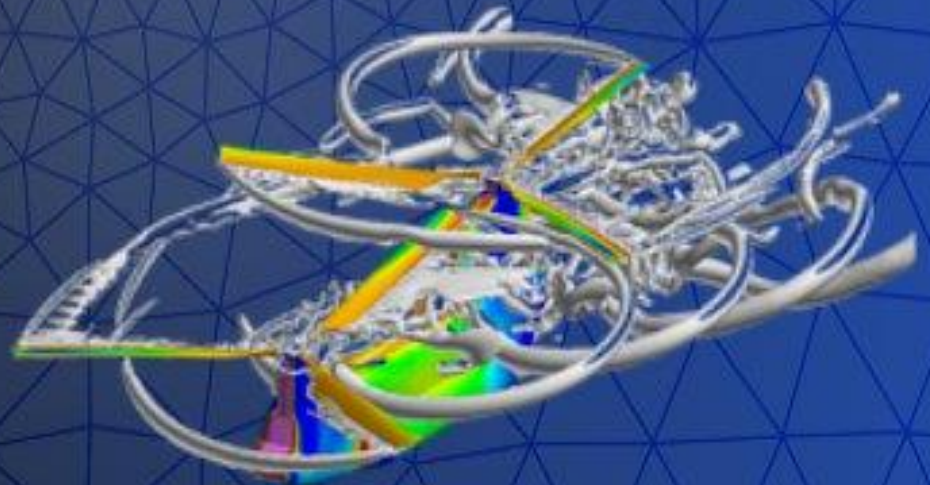


# CFD Vision 2030 Study

A Path to Revolutionary Computational  
Aerosciences



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# **CFD Vision 2030 Study: A Path to Revolutionary Computational Aerosciences**

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# 1 Executive Summary

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The ability to simulate aerodynamic flows using computational fluid dynamics (CFD) has progressed rapidly during the last several decades and has fundamentally changed the aerospace design process. Advanced simulation capabilities not only enable reductions in ground-based and in-flight testing requirements, but also provide added physical insight, enable superior designs at reduced cost and risk, and open new frontiers in aerospace vehicle design and performance. Throughout the evolution of physics-based simulation technologies in general, and computational fluid dynamics methods in particular, NASA's Aeronautics Research Mission Directorate has played a leading role in the development and deployment of these technologies. However, today the aerospace CFD community finds itself at a crossroads due to the convergence of several factors. In spite of considerable successes, reliable use of CFD has remained confined to a small but important region of the operating design space due to the inability of current methods to reliably predict turbulent-separated flows. At the same time, High Performance Computing (HPC) hardware is progressing rapidly and is on the cusp of a paradigm shift in technology that may require a rethinking of current CFD algorithms and software. Finally, during the last decade, government investment in simulation-based technology for aerospace applications has been significantly reduced and access to leading-edge HPC hardware has been constrained both in government and industry. Sustaining future advances in CFD and related multidisciplinary analysis and optimization tools will be critical for achieving NASA's aeronautics goals, invigorating NASA's space program, keeping industry competitive, and advancing aerospace engineering in general. The improvement of a simulation-based engineering design process in which CFD plays a critical role is a multifaceted problem that requires a comprehensive long-term, goal-oriented research strategy. The objective of this report is to develop such a plan, based on factual information, expert knowledge, community input, and in-depth experience.

This report represents the findings and recommendations of a multidisciplinary team that was assembled in response to a NASA Research Announcement (NRA) with the goal of formulating a knowledge-based forecast and research strategy for developing a visionary CFD capability in the notional year 2030. The diverse team members bring together deep expertise in the areas of aerodynamics, aerospace engineering, applied mathematics, and computer science, and the team includes members with extensive experience from industry, academia, and government. A multipronged strategy was adopted for gathering information and formulating a comprehensive research plan. Input from the broader international technical community was sought, and this was obtained initially through the development and compilation of an online survey that garnered more than 150 responses. As a

follow-up, a workshop was held with academic, industrial, and government participants from the general aerospace engineering community with a stake in simulation-based engineering. The results from the survey and workshop were synthesized and refined by the team, with considerable additions through internal discussions and feedback from sponsoring NASA officials. The overall project spanned a period of 12 months and resulted in a series of findings, a vision for the capabilities required in the year 2030, and a set of recommendations for achieving these capabilities.

## *Findings*

1. **NASA investment in basic research and technology development for simulation-based analysis and design has declined significantly in the last decade and must be reinvigorated if substantial advances in simulation capability are to be achieved.** Advancing simulation capabilities will be important for both national aeronautics and space goals, and has broad implications for national competitiveness. This will require advances in foundational technologies, as well as increased investment in software development, since problem and software complexity continue to increase exponentially.
2. **HPC hardware is progressing rapidly and technologies that will prevail are difficult to predict.** However, there is a general consensus that HPC hardware is on the cusp of a paradigm shift that will require significantly new algorithms and software in order to exploit emerging hardware capabilities. While the dominant trend is toward increased parallelism and heterogeneous architectures, alternative new technologies offer the potential for radical advances in computational capabilities, although these are still in their infancy.
3. **The use of CFD in the aerospace design process is severely limited by the inability to accurately and reliably predict turbulent flows with significant regions of separation.** Advances in Reynolds-averaged Navier-Stokes (RANS) modeling alone are unlikely to overcome this deficiency, while the use of Large-eddy simulation (LES) methods will remain impractical for various important applications for the foreseeable future, barring any radical advances in algorithmic technology. Hybrid RANS-LES and wall-modeled LES offer the best prospects for overcoming this obstacle although significant modeling issues remain to be addressed here as well. Furthermore, other physical models such as transition and combustion will remain as pacing items.
4. **Mesh generation and adaptivity continue to be significant bottlenecks in the CFD workflow, and very little government investment has been targeted in these areas.** As more capable HPC hardware enables higher resolution simulations, fast, reliable mesh generation and adaptivity will become more problematic. Additionally, adaptive mesh techniques offer great potential, but have

not seen widespread use due to issues related to software complexity, inadequate error estimation capabilities, and complex geometries.

5. **Revolutionary algorithmic improvements will be required to enable future advances in simulation capability.** Traditionally, developments in improved discretizations, solvers, and other techniques have been as important as advances in computer hardware in the development of more capable CFD simulation tools. However, a lack of investment in these areas and the supporting disciplines of applied mathematics and computer science have resulted in stagnant simulation capabilities. Future algorithmic developments will be essential for enabling much higher resolution simulations through improved accuracy and efficiency, for exploiting rapidly evolving HPC hardware, and for enabling necessary future error estimation, sensitivity analysis, and uncertainty quantification techniques.
6. **Managing the vast amounts of data generated by current and future large-scale simulations will continue to be problematic and will become increasingly complex due to changing HPC hardware.** These include effective, intuitive, and interactive visualization of high-resolution simulations, real-time analysis, management of large databases generated by simulation ensembles, and merging of variable fidelity simulation data from various sources, including experimental data.
7. **In order to enable increasingly multidisciplinary simulations, for both analysis and design optimization purposes, advances in individual component CFD solver robustness and automation will be required.** The development of improved coupling at high fidelity for a variety of interacting disciplines will also be needed, as well as techniques for computing and coupling sensitivity information and propagating uncertainties. Standardization of disciplinary interfaces and the development of coupling frameworks will increase in importance with added simulation complexity.

## ***Vision***

A knowledge-based vision of the required capabilities of state-of-the-art CFD in the notional year 2030 is developed in this report. The Vision 2030 CFD capability is one that:

- Is centered on physics-based predictive modeling.
- Includes automated management of errors and uncertainties.
- Provides a much higher degree of automation in all steps of the analysis process.
- Is able to effectively leverage the most capable HPC hardware of the day.
- Has the flexibility to tackle large-scale capability tasks in a research environment but can also manage large numbers of production jobs for database applications.

- Seamlessly integrates with other disciplinary codes for enabling complex multidisciplinary analyses and optimizations.

The Vision includes a much higher level of integration between advanced computational methods and improved ground-based and flight test techniques and facilities in order to best advance aerospace product development efforts and reduce technical risk in the future.

A number of Grand Challenge (GC) problems are used that constitute the embodiment of this vision of the required CFD capabilities in 2030, and cover all important application areas of relevance to NASA's aeronautics mission as well as important aspects of NASA's space exploration mission. Four GC problems have been identified:

1. Wall resolved LES simulation of a full powered aircraft configuration in the full flight envelope
2. Off-design turbofan engine transient simulation
3. Multidisciplinary Analysis and Optimization (MDAO) of a highly flexible advanced aircraft configuration
4. Probabilistic analysis of a powered space access configuration

These Grand Challenge problems are chosen because they are bold and will require significant advances in HPC usage, physical modeling, algorithmic developments, mesh generation and adaptivity, data management, and multidisciplinary analysis and optimization to become feasible. In fact, they may not be achievable in the 2030 time frame, but are used as drivers to identify critical technologies in need of investment and to provide benchmarks for continually measuring progress toward the long-term goals of the research program.

## ***Recommendations***

In order to achieve the Vision 2030 CFD capabilities, a comprehensive research strategy is developed. This is formulated as a set of recommendations which, when considered together, result in a strategy that targets critical disciplines for investment, while monitoring progress toward the vision. Two types of recommendations are made: a set of specific programmatic recommendations and a series of more general strategic recommendations. The programmatic recommendations avoid the identification of specific technologies and the prescription of funding levels, since these decisions are difficult at best given the long-range nature of this planning exercise. Rather, long-range objectives are identified through the vision and GC problems, and a set of six general technology areas that require sustained investment is described. A mechanism for prioritizing current and future investments is suggested, based on the periodic evaluation of progress toward the GC problems.

**Programmatic Recommendation 1:** NASA should develop, fund, and sustain a base research and technology (R&T) development program for simulation-based analysis and design technologies. The presence of a focused base R&T program for simulation technologies is an essential component of the strategy for advancing CFD simulation capabilities. This recommendation consists of expanding the current Revolutionary Computational Aerosciences (RCA) program and organizing it around six technology areas identified in the findings:

1. High Performance Computing (HPC)
2. Physical Modeling
3. Numerical Algorithms
4. Geometry and Grid Generation
5. Knowledge Extraction
6. MDAO

The physical modeling area represents an expansion of the current turbulence modeling area under the RCA program to encompass other areas such as transition and combustion, while the numerical algorithms area corresponds to a current emphasis in the RCA program that must be broadened substantially. The other areas constitute new, recommended thrust areas within the RCA program.

**Programmatic Recommendation 2:** NASA should develop and maintain an integrated simulation and software development infrastructure to enable rapid CFD technology maturation. A leading-edge in-house simulation capability is imperative to support the necessary advances in CFD required for meeting the 2030 vision. Maintaining such a capability will be crucial for understanding the principal technical issues and overcoming the impediments, for investigating new techniques in a realistic setting, and for engaging with other stakeholders. In order to be sustainable, dedicated resources must be allocated toward the formation of a streamlined and improved software development process that can be leveraged across various projects, lowering software development costs, and releasing researchers and developers to focus on scientific or algorithmic implementation aspects. At the same time, software standards and interfaces must be emphasized and supported whenever possible, and open source models for noncritical technology components should be adopted.

**Programmatic Recommendation 3:** NASA should utilize and optimize HPC systems for large-scale CFD development and testing. Access to large-scale HPC hardware is critical for devising and testing the improvements and novel algorithms that will be required for radically advancing CFD simulation capabilities. Although the current NASA paradigm favors computing for many small, production jobs (“capacity”) over larger, proof-of-concept jobs (“capability”), a mechanism must be found to make large-scale HPC hardware available on a regular basis for CFD and multidisciplinary simulation software development at petascale to exascale levels and beyond. This may be done through internal

reallocation of resources, sharing with other NASA mission directorates, leveraging other government agency HPC assets, or through any combination of these approaches.

**Programmatic Recommendation 4:** NASA should lead efforts to develop and execute integrated experimental testing and computational validation campaigns. Systematic numerical validation test datasets and effective mechanisms to disseminate validation results are becoming more important as CFD complexity increases. NASA is ideally positioned to lead such efforts by leveraging its unique experimental facilities in combination with its extensive in-house CFD expertise, thus contributing valuable community resources that will be critical for advancing CFD technology. The development of new experimental testing technologies and facilities is expected to play a continuing role not just in aerospace product development, but increasingly in computational method validation.

**Strategic Recommendation 5:** NASA should develop, foster, and leverage improved collaborations with key research partners and industrial stakeholders across disciplines within the broader scientific and engineering communities. In an environment of limited resources, achieving sustained critical mass in the necessary simulation technology areas will require increased collaborations with other stakeholders. Mutually beneficial collaborations are possible between NASA mission directorates, as well as with other US government agencies with significant ongoing investments in computational science. Tighter collaboration with industry, specifically in simulation technology areas, would also be beneficial to both parties and a joint Computational Science Leadership team is proposed to coordinate such collaborations. At the same time, investments must look beyond the traditional aerospace engineering disciplines to drive substantial advances in simulation technology, and mechanisms for engaging the wider scientific community, such as focused research institutes that engage the broader academic community, should be explored.

**Strategic Recommendation 6:** NASA should attract world-class engineers and scientists. The ability to achieve the long-term goals for CFD in 2030 is greatly dependent on having a team of highly educated and effective engineers and scientists devoted to the advancement of computational sciences. Mechanisms for engaging graduate and undergraduate students in computational science with particular exposure to NASA aeronautics problems must be devised. These include student fellowships, as well as visiting programs and internships, which may be facilitated through external institutes and centers.

## 2 Introduction

The rapid advance of computational fluid dynamics (CFD) technology during the last several decades has fundamentally changed the aerospace design process. Aggressive use of CFD is credited with drastic reductions in wind tunnel time for aircraft development programs<sup>1-4</sup>, as well as lower numbers of experimental rig tests in gas turbine engine development programs.<sup>5-6</sup> CFD has also enabled the design of high-speed, access-to-space, and re-entry vehicles in the absence of suitable ground-based testing facilities.<sup>7-9</sup> In addition to reducing testing requirements, physics-based simulation technologies such as CFD offer the added potential of delivering superior understanding and insight into the critical physical phenomena limiting component performance, thus opening new frontiers in aerospace vehicle design.<sup>10-11</sup>

Physics-based simulations in general, and CFD in particular, are front and center in any aerospace research program since these are crosscutting technologies that impact all speed regimes and all vehicle classes. This is evidenced in the National Research Council (NRC) commissioned decadal survey on aeronautics<sup>12</sup> which identifies five common themes across the entire aeronautics research enterprise, the first two being physics-based simulation and physics-based design tools. Similarly, these technologies affect all of the outcomes in the current National Aeronautics R&D Plan,<sup>13</sup> and continued advances in these technologies will be critical for meeting the stated outcomes.

Since the advent of scientific computing, NASA's Aeronautics Research Mission Directorate (ARMD) has played a leading role in the development and deployment of CFD technologies.<sup>14</sup> Successive external reviews of NASA Aeronautics programs during the last two decades by organizations such as the National Academy of Engineering (NAE) and others<sup>12</sup> have repeatedly praised the world-class status and leading-edge technical contributions of the simulation-based engineering tools developed under these programs. In fact, many algorithms, techniques, and software tools in use today within and beyond the aerospace industry can trace their roots back to NASA development or funding.

The development of computational aerodynamics has been characterized by a continual drive to higher fidelity and more accurate methods from the 1970s to the 1990s, beginning with panel methods, proceeding to linearized and nonlinear potential flow methods, inviscid flow (Euler) methods, and culminating with Reynolds-averaged Navier-Stokes (RANS) methods. These advances were arrived at through sustained investment in methodology development coupled with acquisition and deployment of leading edge High Performance Computing (HPC) hardware made available to researchers.<sup>15</sup> While Moore's law has held up remarkably well, delivering a million-fold increase in computational power during the last 20 years, there is also ample evidence that equivalent or greater increases in simulation capabilities were achieved

through the development of advanced algorithms within the same time frame.<sup>1,16-18</sup>

However, the last decade has seen stagnation in the capabilities used in aerodynamic simulation within the aerospace industry, with RANS methods having become the high-fidelity method of choice and advances due mostly to the use of larger meshes, more complex geometries, and more numerous runs afforded by continually decreasing hardware costs.<sup>19-23</sup> At the same time, the well-known limitations of RANS methods for separated flows have confined reliable use of CFD to a small region of the flight envelope or operating design space.<sup>24</sup> Simultaneously, algorithmic development has been substantially scaled back within NASA and access to leading-edge HPC hardware has been constrained, both at NASA and within industry.<sup>25</sup> In some sense, current CFD has become a commodity based on mature technology, suitable only for commodity hardware and reliable only for problems for which an extensive experience base exists.

Continued advances in physics-based simulation technologies in general, and CFD in particular, are essential if NASA is to meet its aeronautics research goals, as well as for successfully advancing the outcomes in the National Aeronautics R&D plan.<sup>13</sup> The required advances in fuel burn, noise, emissions, and climate impact will only be realized with vastly more sophisticated analysis of future configurations. Beyond Aeronautics, NASA's space missions rely heavily on computational tools developed within ARMD<sup>7-9, 26-30</sup> and superior designs at lower cost and risk will require radical advances in new CFD tools.<sup>31</sup> Additionally, the loss of the leadership role NASA ARMD once played in the development of simulation-based engineering technology has larger implications for the aerospace industry in particular, and national competitiveness in general.<sup>17,32,33</sup> Due to the long lead times and high risk involved, industry must rely on government agencies to develop and demonstrate new simulation technologies at large scale, after some investment in proof-of-concept at universities. In recent years, the National Science Foundation (NSF) and Department of Energy (DOE) have led investing in computational science-based research and in deploying leading-edge HPC facilities, although with a different focus based more on scientific discovery rather than engineering product design.<sup>16, 18, 34-36</sup> As noted by a blue-ribbon panel report convened by the NSF, simulation-based engineering is fundamentally different from science-based simulation and is in danger of being neglected under the current scenario, with important implications for national competitiveness.<sup>37, 38</sup>

Thus, there is a national imperative to reinvigorate the investment in physics-based engineering simulation tools in general, and in CFD in particular, and NASA is uniquely positioned to fill this role. In addition to enhancement of CFD technology, effective use of existing, and potentially new, ground-based testing facilities will be required to provide a complementary set of tools to best advance aerospace



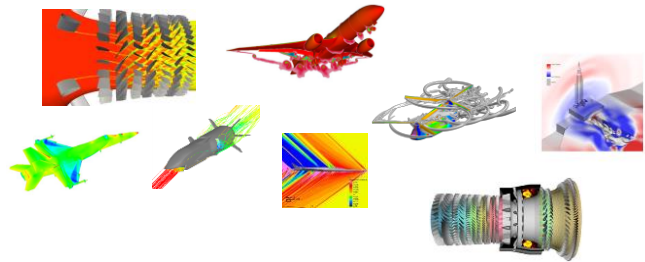
product development efforts and reduce technical risk in the future. Sustaining future advances in CFD and related multidisciplinary analysis and optimization tools along with strong support of ground-based and flight testing technologies and facilities will be key for achieving NASA next generation aeronautics goals, keeping industry competitive, invigorating NASA's space program, and advancing aerospace engineering. With investment, the resulting engineering design process would decrease risk, reduce time-to-market, improve products, and facilitate truly revolutionary aerospace vehicles through the ability to consider novel designs. Without such an investment, the engineering design process will look much the same in 2030 as it does today and act as a barrier to revolutionary advances in aerospace and other industries of national importance.

The improvement of a simulation-based engineering design process in which CFD plays a critical role is a multifaceted problem. Having relied on mature algorithms and ridden the wave of ever-decreasing commodity computer hardware costs, the CFD development community now finds itself poorly positioned to capitalize on the rapidly changing HPC architectures, which include massive parallelism and heterogeneous architectures.<sup>38-40</sup> New paradigms will be required to harness the rapidly advancing capabilities of new HPC hardware.<sup>41, 42</sup> At the same time, the scale and diversity of issues in aerospace engineering are such that increases in computational power alone will not be enough to reach the required goals, and new algorithms, solvers, physical models, and techniques with better mathematical and numerical properties must be developed.<sup>1,16-18</sup> Finally, software complexity is increasing exponentially, slowing adoption of novel techniques into production codes and shutting out production of new software development efforts, while simultaneously complicating the coupling of various disciplinary codes for multidisciplinary analysis and design.<sup>43</sup> The development of a long-range research plan for advancing CFD capabilities must necessarily include all these considerations, along with the larger goal of comprehensive advances in multidisciplinary analysis and optimization capabilities.

The objective of this study is to develop such a plan, based on factual information, expert knowledge, and the in-depth experience of the team and the broader community. The strategy begins by defining the required capabilities for CFD in the notional year 2030. By contrasting this vision with the current state, we identify technical impediments and formulate a technology development plan. This in turn is used to develop a research strategy for achieving the goals of the Vision 2030 CFD capability. The outcome of the research plan is a set of recommendations formulated to enable the successful execution of the proposed strategy.

### 3 Vision of CFD in 2030

Given the inherent difficulties of long-term predictions, our vision for CFD in 2030 is grounded on a desired set of capabilities that must be present for a radical improvement in CFD predictions of critical flow phenomena associated with the key aerospace product/application categories, including commercial and military aircraft, engine propulsion, rotorcraft, space exploration systems, launch vehicle programs, air-breathing space-access configurations, and spacecraft entry, descent, and landing (EDL).



This set of capabilities includes not only the accurate and efficient prediction of fluid flows of interest, but also the usability of CFD in broader contexts (including uncertainty quantification, optimization, and multidisciplinary applications) and in streamlined/automated industrial analysis and design processes. To complicate things further, CFD in 2030 must effectively leverage the uncertain and evolving environment of HPC platforms that, together with algorithmic improvements, will be responsible for a large portion of the realized improvements.

The basic set of capabilities for Vision 2030 CFD must include, at a minimum:

1. Emphasis on physics-based, predictive modeling. In particular, transition, turbulence, separation, chemically reacting flows, radiation, heat transfer, and constitutive models must reflect the underlying physics more closely than ever before.
2. Management of errors and uncertainties resulting from all possible sources: (a) physical modeling errors and uncertainties addressed in item #1, (b) numerical errors arising from mesh and discretization inadequacies, and (c) aleatory uncertainties derived from natural variability, as well as epistemic uncertainties due to lack of knowledge in the parameters of a particular fluid flow problem.
3. A much higher degree of automation in all steps of the analysis process is needed including geometry creation, mesh generation and adaptation, the creation of large databases of simulation results, the extraction and understanding of the vast amounts of information generated, and the ability to computationally steer the process. Inherent to all these improvements is the requirement that every step of the solution chain executes high levels of reliability/robustness to minimize user intervention.

### Critical Flow Phenomena Addressed in This Study

- |  |   |
|--|---|
| <ul style="list-style-type: none"> <li>• Flow separation: e.g., smooth-body, shock-induced, blunt/bluff body</li> <li>• Laminar to turbulent boundary layer flow transition/reattachment</li> <li>• Viscous wake interactions and boundary layer confluence</li> <li>• Corner/junction flows</li> <li>• Icing and frost</li> <li>• Circulation and flow separation control</li> <li>• Turbomachinery flows</li> <li>• Aerothermal cooling/mixing flows</li> <li>• Reactive flows, including gas chemistry and combustion</li> <li>• Jet exhaust</li> <li>• Airframe noise</li> <li>• Vortical flows: wing/blade tip, rotorcraft</li> </ul> | <ul style="list-style-type: none"> <li>• Wake hazard reduction and avoidance</li> <li>• Wind tunnel to flight scaling</li> <li>• Rotor aero/structural/controls, wake and multirotor interactions, acoustic loading, ground effects</li> <li>• Shock/boundary layer, shock/jet interactions</li> <li>• Sonic boom</li> <li>• Store/booster separation</li> <li>• Planetary retro-propulsion</li> <li>• Aerodynamic/radiative heating</li> <li>• Plasma flows</li> <li>• Ablator aerothermodynamics</li> <li>• Plasma flows</li> </ul> |
|--|---|

4. Ability to effectively utilize massively parallel, heterogeneous, and fault-tolerant HPC architectures that will be available in the 2030 time frame. For complex physical models with nonlocal interactions, the challenges of mapping the underlying algorithms onto computers with multiple memory hierarchies, latencies, and bandwidths must be overcome.
5. Flexibility to tackle capability- and capacity-computing tasks in both industrial and research environments so that both very large ensembles of reasonably-sized solutions (such as those required to populate full-flight envelopes, operating maps, or for parameter studies and design optimization) and small numbers of very-large-scale solutions (such as those needed for experiments of discovery and understanding of flow physics) can be readily accomplished.
6. Seamless integration with multidisciplinary analyses that will be the norm in 2030 without sacrificing accuracy or numerical stability of the resulting coupled simulation, and without requiring a large amount of effort such that only a handful of coupled simulations are possible.

Included in this desired set of capabilities is a vision for how CFD in 2030 will be used: a vision of the interaction between the engineer/scientist, the CFD software itself, its framework and all the ancillary software dependencies (databases, modules, visualization, etc.), and the associated HPC environment. A single engineer/scientist must be able to conceive, create, analyze, and interpret a large ensemble of related simulations in a time-critical period (e.g., 24 hours), without individually managing each simulation, to a pre-specified level of accuracy. There should be less emphasis on the mechanics of running and collecting the information, and more emphasis on interpreting and understanding the results of the work. Like the predictive nature of large-scale, finite-element-based, linear structural analyses that are assumed in the aerospace industry, information derived from computations of fluid flow must carry the same stamp of approval or, at least, a reasonable estimate of possible errors contained in the information provided. At the moment, CFD is not yet

sufficiently predictive and automated to be used in critical/relevant engineering decisions by the non-expert user, particularly in situations where separated flows are present.

Additionally, the Vision includes a much higher level of integration between advanced computational methods and improved ground-based and flight test techniques and facilities in order to best advance aerospace product development efforts and reduce technical risk in the future.

Finally, as part of our vision, we define a set of Grand Challenge (GC) problems (as shown in the graphic on the next page) that are bold and in fact may not be solvable in the 2030 timeframe, but are used as drivers to identify critical technologies in need of investment, and to serve as benchmarks for continually measuring progress toward the long-term development goals. These GC problems were chosen to embody the requirements for CFD in 2030, and cover all important application areas of relevance to NASA's aeronautics mission, as well as important aspects of NASA's space exploration mission. Details on the GC problems are presented in Section 6.

## 4 Current State

At present, CFD is used extensively in the aerospace industry for the design and analysis of air and space vehicles and components. However, the penetration of CFD into aerospace design processes is not uniform across vehicle types, flight conditions, or across components. CFD often plays a complementary role to wind tunnel and rig tests, engine certification tests, and flight tests by reducing the number of test entries and/or reducing testing hours.<sup>3-5</sup> But, in many circumstances, CFD provides the only affordable or available source of engineering data to use in product design due to limitations either with model complexity and/or wind tunnel capability, or due to design requirements that cannot be addressed with ground-based testing of any kind.<sup>8, 10, 31</sup> As a result, CFD technology development has been critical in not only minimizing product design costs, but also in enabling the design of truly novel platforms and systems.

## Grand Challenge Problems

**GC1** LES of powered aircraft configuration across the full flight envelope

**GC2** Off-design turbofan engine transient simulation

**GC3** MDAO of a highly-flexible advanced aircraft configuration

**GC4** Probabilistic analysis of a powered space access configuration



Generally, the design process is composed of three key phases: conceptual design, preliminary and detailed design, and product validation. The current usage of CFD tools and processes in all three of these design phases is summarized below.

**Conceptual Design.** CFD is often used in the early, conceptual design of products where it has been both previously calibrated for similar applications using data-morphing techniques, as well as for new configurations where little or no engineering data is available to guide design decisions. Simplified models are typically used during the conceptual optimization phase to allow reasonably accurate trades to be made between drag, fuel consumption, weight, payload/range, thrust, or other performance measures. Use of simplified models is necessary to allow often time-consuming optimization processes to be used in the overall design effort, but inherently places conservatism into the final design. This conservatism derives from the use of models that are too similar within the existing product design space, other geometric simplifications, or the use of low-fidelity CFD tools that trade off flow physics modeling accuracy for execution speed.

**Preliminary/Detailed Design.** Once a product development program is launched, CFD is a necessary and uniformly present tool in the detailed configuration design process. For example, CFD is indispensable in the design of cruise wings in the presence of nacelles for commercial airplanes, and for inlet and nozzle designs; wind tunnels are used to confirm the final designs.<sup>1,4</sup> In both military and commercial aircraft design processes, CFD is the primary source of data for aircraft load distributions and ground effect estimations.<sup>10</sup> Similarly, gas turbine engine manufacturers rely on CFD to predict component design performance, having reduced the number of single-component rigs substantially as CFD capability has become more mature.<sup>5,6</sup> Increasingly, multicomponent and multiphysics simulations are performed during the design cycle, but the long clock times often associated with these processes restricts their widespread adoption. For space exploration,

CFD is often used to gain important insight into flow physics (e.g., multiple plume interactions) used to properly locate external components on the surface of launch vehicles or spacecraft.<sup>9,27,29</sup> CFD is also increasingly providing substantial portions of the aero and propulsion performance database.<sup>7,9,30</sup> In many cases, wind tunnel data is used only to anchor the CFD data at a few test points to provide confidence in the CFD database. CFD is the primary source of data for the hypersonic flight regime when ground testing is limited or does not exist.<sup>8,44</sup>

**Product Validation and Certification.** As the product development process moves into the validation phase and certification testing, CFD is often used to confirm performance test results, assess the redesign of components that show potential for improved performance, and to answer any other questions that arise during product testing. Typically, product configurations evolve over the testing period based on a combination of measured results and engineering judgment bolstered by the best simulation capability available. In general, CFD modeling capability grows to capture the required scope and physics to answer the questions raised during testing. The expense of responding to often unplanned technical surprises—which results in more time on the test stand or in flight test, or changes in hardware—drives conservatism into aerospace designs and is a significant motivation for improving the accuracy and speed of CFD. If CFD is sufficiently accurate and fast, engineers can move from their traditional design space with greater confidence and less potential risk during testing.

For each of these design phases, the performance (in terms of numerical efficiency and solution accuracy) of CFD is of critical importance. A high-level view of the current state of CFD in several key technical areas is given below.

**High Performance Computing (HPC).** The effectiveness and impact of CFD on the design and analysis of aerospace products and systems is largely driven by the power and availability of modern HPC systems. During the last decades, CFD codes were formulated using message passing

(e.g., MPI) and thread (e.g., OpenMP) software models for expressing parallelism to run as efficiently as possible on current generation systems. However, with the emergence of truly hierarchical memory architectures having numerous graphical processing units (GPUs) and coprocessors, new CFD algorithms may need to be developed to realize the potential performance offered by such systems. Government labs, such as Oak Ridge National Lab (ORNL), Argonne National Lab (ANL), and the NASA Advanced Supercomputing (NAS) facility at NASA Ames Research Center, have often led the way with the acquisition and testing of new hardware. Much research on testing and tailoring of CFD algorithms takes place on these platforms with heavy participation from academia, national labs and to some extent industry as well. Government computing resources are also used to tackle large-scale calculations of challenge problems, such as the detailed direct numerical simulation (DNS) of spray injector atomization or high fidelity simulations of transition and turbulent separation in turbomachinery. However, because of the high cost of these leadership-class systems, industry and academia often purchase smaller commodity clusters utilizing similar types of processors when the latest hardware technology is fully demonstrated on CFD problems and other important applications.

**Turbulence Modeling.** Current practices for CFD-based workflows utilize steady Reynolds-average Navier-Stokes (RANS) with 1- or 2-equation turbulence models,<sup>46-48</sup> although hybrid unsteady RANS/LES methods are increasingly common for certain classes of simulations in which swirling and intentionally separated flows are dominant, such as combustors. Techniques to combine near-wall RANS regions and outer flow field, large-eddy simulation (LES) regions in these hybrid methods are immature. Many CFD design processes include an estimation of boundary layer transition, using a range of models, from purely empirical to coupled partial-differential equation (PDE) solutions of stability equations.<sup>49, 50</sup> Both approaches involve much empiricism, may be missing some modes of transition, and are evolving. As a result, no generalized transition prediction capability is in widespread use in Navier-Stokes CFD, and the default practice is to run the codes “fully turbulent”. Steady-state CFD accounts for a vast majority of simulations; unsteady flow predictions are inherently more expensive and not yet uniformly routine in the design process, with some exceptions.<sup>51</sup>

**Process Automation.** Current CFD workflows are often paced by the geometry preprocessing and grid generation phases, which are significant bottlenecks. In some cases, where the design effort involves components of similar configurations, specialized, automated processes are built that considerably reduce set-up time, execution of the CFD solver, and post-processing of results. This process to production capability of the CFD workflow only oc-

curs in areas where the design work is routine and the investment in automation makes business sense; single-prototype designs and novel configurations continue to suffer the pacing limits of human-in-the-loop workflows because the payoff for automating is not evident. This issue is not unique to the aerospace industry.

**Solution Uncertainty and Robustness.** In practice, CFD workflows contain considerable uncertainty that is often not quantified. Numerical uncertainties in the results come from many sources, including approximations to geometry, grid resolution, problem setup including flow modeling and boundary conditions, and residual convergence. Although NASA and professional organizations such as ASME and AIAA have created standards for the verification and validation of CFD and heat transfer analyses<sup>52-54</sup>, such techniques are not widely used in the aerospace industry. With a few notable exceptions, CFD is carried out on fixed grids that are generated using the best available practices to capture expected flow features, such as attached boundary layers.<sup>55</sup> Such approaches cannot reliably provide adequate resolution for flow features when locations are not known a priori, such as shocks, shear layers, and wakes. Although grid refinement is often seen as a panacea to addressing grid resolution issues, it is seldom done in practice (with the exception of a few workshop test cases) because uniform refinement is impractical in 3D. Adaptive mesh refinement strategies offer the potential for superior accuracy at reduced cost, but have not seen widespread use due to robustness, error estimation, and software complexity issues. Achieving consistent and reliable flow solver or residual convergence remains problematic in many industrial cases. Although many CFD codes are able to demonstrate convergence for a few simple problems, for many flows involving difficult flow physics and/or complex geometries such as an aircraft in high-lift configuration, many of the current solver techniques employed are not strong enough to ensure robust convergence.<sup>56</sup> Engineering judgment is required to interpret results that are not well converged, which introduces conservatism into decision-making. Furthermore, the use of steady-state flow solvers itself is in question for many flows of engineering interest.

**Multidisciplinary Analysis and Optimization (MDO).** Although the basic concepts of MDO are fairly well accepted in the community, the routine use of MDO methods is not, by any means, pervasive. At moderate levels of fidelity (commensurate with analyses conducted during the conceptual design phase), it is common industrial practice to perform coupled multidisciplinary analyses (MDA) of the most tightly integrated disciplines in a design. Aerostructural analyses, conjugate heat transfer calculations, and aero-acoustic simulations all tend to take place in aircraft, spacecraft, jet engine, and rotorcraft analysis and design processes. High fidelity CFD is not routinely used in such MDAs, although recent years have witnessed a signif-

icant rise in the coupling of state-of-the-art CFD with additional disciplines. While frameworks for the coupling of disciplinary analyses are widely available,<sup>57-60</sup> the ability to couple CFD with other high fidelity descriptions of participating disciplines is limited by the availability of coupling software and, more fundamentally, by a lack of general methodologies for accurate, stable, and conservative MDAs. The application of optimization techniques in industry is mostly limited to single-discipline simulations. Although conceptual design tools have long benefited from multidisciplinary optimization (MDO) approaches (with various modules at the lowest fidelity levels), high fidelity CFD-based optimizations are still rare. During the past decade, the development of advanced surrogate modeling techniques and the introduction of adjoint-based optimal shape design techniques have enabled the use of CFD in aerodynamic optimization of aircraft and gas turbine components. However, the use of optimization with multiple disciplines treated using high-fidelity methods is still within the realm of advanced research and is by no means a routine practice.

## 5 CFD Technology Gaps and Impediments

Given the current state of CFD technology, tools, and processes described above, necessary research and development to address gaps and overcome impediments in CFD technology are fundamental to attaining the vision for CFD in 2030 outlined earlier. Five key technical areas were identified during this Vision 2030 study and rose to the highest level of importance as identified from a user survey and workshop of a large international community of CFD researchers and practitioners. In the subsections below, the effective utilization of HPC is first considered. This includes both the implications of future computing platforms and the requirements imposed by potential emerging future programming paradigms to deal with exascale challenges. Next, we describe the desired level of capability (in 2030) for the prediction of unsteady, turbulent flows including transition and separation. We continue with a discussion of research topics in autonomous and reliable CFD simulation techniques that aim at providing both a high level of automation in the analysis process and the required algorithms (both for meshing and the solution process) to ensure confidence in the outcomes. Then, in order to derive useful information from the simulations, the discussion on smart knowledge extraction from large-scale databases and simulations considers the research required to automate the process of sifting through large amounts of information, often at a number of different geographic locations, and extracting patterns and actionable design decisions. Finally, we end with a discussion on multidisciplinary and multiphysics simulations that describes the research work required to perform seamless, accurate, and robust simulations of multiphysics problems in which CFD would be an integral part.

### 5.1 Effective Utilization of High-Performance Computing (HPC)

CFD in 2030 will be intimately related to the evolution of the computer platforms that will enable revolutionary advances in simulation capabilities. The basic framework for Vision 2030 CFD must map well to the relevant future programming paradigms, which will enable portability to changing HPC environments and performance without major code rework.<sup>41</sup> However, the specific architecture of the computing platforms that will be available is far from obvious. We can, however, speculate about the key attributes of such machines and identify key technology gaps and shortcomings so that, with appropriate development, CFD can perform at future exascale levels on the HPC environments in 2030.

Hybrid computers with multiple processors and accelerators are becoming widely available in scientific computing and, although the specific composition of a future exascale computer is not yet clear, it is certain that heterogeneity in the computing hardware, the memory architecture, and even the network interconnect will be prevalent. Future machines will be hierarchical, consisting of large clusters of shared-memory multiprocessors, themselves including hybrid-chip multiprocessors combining low-latency sequential cores with high-throughput data-parallel cores. Even the memory chips are expected to contain computational elements, which could provide significant speedups for irregular memory access algorithms, such as sparse matrix operations arising from unstructured datasets. With such a running target on the horizon, the description of 2030 CFD is grounded on a target supercomputer that incorporates all of the representative challenges that we envision in an exascale supercomputer. These challenges are certainly related to heterogeneity, but more concretely, may include multicore CPU/GPU interactions, hierarchical and specialized networks, longer/variable vector lengths in the CPUs, shared memory between CPU and GPUs, and even a higher utilization of vector units in the CPUs. Research must be conducted so that we are ready to tackle the specific challenges presented.

The wildcard in predicting what a leading edge HPC system will look like is whether one or more of several current nascent HPC technologies will come to fruition. Radical new technologies such as quantum computing, superconducting logic, low-power memory, massively parallel molecular computing, next generation “traditional” processor technologies, on-chip optics, advanced memory technologies (e.g., 3D memory) have been proposed but are currently at very low technology readiness levels (TRL). Many of these revolutionary technologies will require different algorithms, software infrastructures, as well as different ways of using results from CFD simulations.<sup>61</sup>

## CASE STUDY 1: Current Utilization of HPC at NASA

HPC utilization at NASA is almost entirely focused on capacity computing (running many, relatively small jobs) with little capability computing (running jobs utilizing a significant amount of a leadership class high performance computer). The largest NASA HPC system is Pleiades at the NASA Advanced Supercomputing (NAS) division. As of June 2013, this system is currently ranked 19<sup>th</sup> in the world in terms of its performance on the linear algebra benchmark LINPACK.<sup>1</sup> As of October 2013, Pleiades consists of:

- 11,136 nodes with Intel Xeon processors for a total of 162,496 cores
- 64 nodes with NVIDIA graphics processing units for a total of 32,768 cores
- 417 TB of total memory

From the NAS website, the theoretical peak performance of this configuration is quoted as 2.88 pFLOP/s and the demonstrated LINPACK rating is 1.24 pFLOP/s. By comparison, the current fastest system on the Top 500 list is Tianhe-2 at the National University of Defense Technology in China that has a theoretical peak performance of 54.9 pFLOP/s and a demonstrated LINPACK rating 33.9 pFLOP/s. The Top 10 HPC systems are provided in the embedded table, including Pleiades for comparison, and shows that Pleiades is a factor of 2 to 30 times slower than these Top 10 systems (in terms of the LINPACK performance). While Pleiades is within a factor of about 10 of the world's fastest HPC systems, it is rarely used at anywhere near its full capability. For example, a snapshot of the Pleiades job queue<sup>2</sup> (taken on October 24, 2013 at 2:00PM Eastern) shows the following utilization:

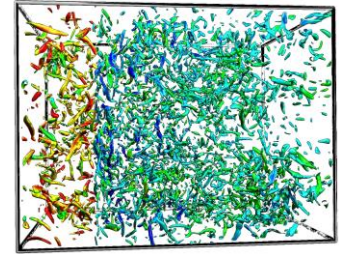
- 469 jobs running
- Average cores used per job: 457
- Maximum cores used per job: 5,000 (the only job running more than 1000 cores)

Thus, although the Pleiades system has approximately 160K CPU cores (and another 32K GPU cores), the average job size is less than 1K cores and Pleiades is therefore acting as a capacity facility. Further, the usage of Pleiades is over-subscribed with job queues often having delays numbering in the days, so that even in its role as a capacity facility, Pleiades is insufficient to meet NASA's needs.

Top 500 Ranking	System Site	LINPACK (pFLOP/s)	Theoretical Peak pFLOP/s)	Cores
1	Tianhe-2 (China)	33.9	54.9	3,120,000
2	Titan (USA: DOE)	17.6	27.1	560,640
3	Sequoia (USA: DOE)	17.2	20.1	1,572,864
4	K computer (Japan)	10.5	11.3	705,024
5	Mira (USA: DOE)	8.6	10.1	786,432
6	Stampede (USA: University of Texas)	5.2	8.5	462,462
7	JUQUEEN (Germany)	5.0	5.9	458,752
8	Vulcan (USA: DOE)	4.3	5.0	393,216
9	SuperMUC (Germany)	2.9	3.2	147,456
10	Tianhe-1A (China)	2.6	4.7	186,368
19	Pleiades (USA: NASA)	1.2	2.9	195,264

By comparison, the DOE has an HPC strategy that encompasses both capacity and capability computing. A key enabler of this strategy is the significant HPC resources at the DOE (for example, the DOE has 4 of the Top 10 supercomputer sites shown in the table: Titan, Sequoia, Mira, and Vulcan). This wealth of HPC resources allows the DOE to dedicate systems to both capacity and capability computing. For example, DOE leadership systems have job queue policies that (1) strongly favor large jobs that will use a significant fraction of a leadership system and (2) limit the potential that these systems are flooded by capacity computations. The DOE also has programs such as Innovative and Novel Computational Impact on Theory and Experiment (INCITE)<sup>3</sup> specifically designed to encourage capability computing. INCITE allocates up to 60% of the Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories to national and international research teams pursuing high-impact research that can demonstrate the ability to effectively utilize a major fraction of these machines in a single job. Utilization data for DOE's Leadership Facilities bears out the impact these policies have had on the pursuit of capability computing. For example, on DOE's Mira system, which is about four times larger than Pleiades, the average job size was 35K cores during the period from April through October 2013. The smallest job size during that time was 8K cores while the largest job size used essentially the entire system at nearly 800K cores. Comparisons can also be made between Pleiades and DOE's "Intrepid" system. Intrepid is the 58<sup>th</sup> fastest supercomputing site with 164K cores, a LINPACK performance of 0.46 pFLOP/s, and a

peak performance of 0.56 pFLOP/s. During the period from October 2011 through October 2013, Intrepid's average job size was 9K cores, with its smallest job being 256 cores, and largest job size used all 164K cores. Although Intrepid is a somewhat less capable system than Pleiades, the utilization patterns are in stark contrast. Further, for both Mira and Intrepid, the overall utilization is still high, with Mira's scheduled availability being utilized at 76% and Intrepid's at 87%.<sup>4</sup> A recent extreme example of capability computing using CFD is the 1.97M core simulation of shock interaction with isotropic turbulence (image shown) that was performed by combining the DOE's Sequoia and Vulcan systems.<sup>5,6</sup>



Looking toward CFD in the 2030s and beyond, the need for improved physics-based modeling in CFD is driving increasingly expensive simulations that will only be possible by leveraging leadership class HPC systems. Without NASA's leadership in the application of capability computing to CFD, the adoption of these technologies in the United States aerospace engineering industry will be hampered.

1 <http://www.top500.org/>

2 <http://www.nas.nasa.gov/hecc/resources/pleiades.html>

3 <http://www.doeleadershipcomputing.org/incite-program/>

4 Data courtesy of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

5 Bermejo-Moreno, I., Bodart, J., Larsson, J., Barney, B., Nichols, J., and Jones, S. "Solving the Compressible Navier-Stokes Equations on up to 1.97 Million Cores and 4.1 Trillion Grid Points." SC13, November 17-21 2013, Denver, CO, USA.

6 Larsson, J., Bermejo-Moreno, I., and S. K. Lele. "Reynolds- and Mach-Number Effects in Canonical Shock-Turbulence Interaction." *Journal of Fluid Mechanics*, 717:293-321, 2013.

We envision the leading edge HPC system in 2030 will have a peak capability of about 30 exaFLOPS when based on the evolution of current technologies. To achieve this anticipated hardware performance, and the required flow solver software enhancements to enable effective CFD on 2030 computing systems, a number of technology gaps and impediments must be overcome.

1. **Hardware system power consumption.** Current state-of-the-art computing systems consume too much power to be scaled up substantially, utilize structural components that are too large, and do not provide the level of computational and communication speed necessary. Development of advanced HPC hardware technologies with a special focus on power consumption and error protections and recovery is needed.
2. **Higher levels of software extraction.** The increased complexity of HPC exascale systems in 2030 will require higher levels of automation and the ability to hide this complexity from the subject matter experts. The whole software infrastructure stack does not scale to the level of complexity of future HPC systems and needs to be more resistant to errors. To overcome this gap, research into industrial strength implementations of the necessary middleware, especially operating systems, compilers, communication, and I/O libraries, as well as deployment and monitoring systems needs to continue.
3. **Advanced programming environments.** Another critical component in the development of the full future HPC ecosystem is the development of basic, highly scalable and error resistant algorithms, decomposable software architectures, and programming environments that allow scientific subject matter experts to express algorithms at the appropriate level of abstraction.
4. **Robust CFD code scalability.** As described earlier, an HPC system in 2030 will require tremendous levels of parallelization. Unfortunately, robust CFD flow solver scalability even on current multicore platforms is sorely lacking. Few applications can make efficient use of more than  $O(1,000)$  cores, although the largest machines today are available with  $O(1,000,000)$  cores.<sup>62</sup> In contrast, 20 years ago, production CFD codes ran routinely on the largest available shared-memory vector machines. To address these challenges new, extremely parallel CFD algorithms that balance computing and communication need to be developed. Furthermore, there needs to be investment in the development of CFD codes built on highly optimized libraries and middleware. In contrast, current CFD codes and related processes are rather monolithic today, making it difficult to change algorithms or implementations. A future CFD code and surrounding processes should be modular, allowing replacement of components with new components developed in academia or from commercial vendors easily and transparently. Such a modular approach would also enable coupling of MDA/O processes.
5. **Lack of scalable CFD pre- and post-processing methods.** Despite the deficiencies in current CFD solver scalability, the situation for the surrounding infrastructure of pre- and post-processing software is even worse. In order to streamline and accelerate the entire CFD workflow and design process, the development of basic scalable pre- and post-processing methods must be addressed. This includes geometry representation and mesh generation on the front end as well as visualization, database generation, and general knowledge extraction from large datasets on the back end.

6. **Lack of access to HPC resources for code development.** Another key issue is the lack of access to large-scale HPC resources as an integral part of software development. Consistent and reliable access to leading-edge HPC hardware is critical for devising and testing new techniques that enable more advanced simulations, as well as for demonstrating the impact that CFD technology enhancements can have on aerospace product development programs.<sup>11, 39</sup> Algorithmic choices and software implementation strategies are directly affected by the type of hardware made available during the software development process, and the stagnating scalability of current production CFD codes is at least partly attributable to the inability to test these codes consistently on large-scale HPC hardware. The resulting situation of scalability-limited simulation tools reduces demand for large-scale capability computing since few codes can take advantage of HPC hardware, while driving demand for throughput or capacity computing. Allocating a portion of HPC computing resources for highly scalable software development programs will be essential for pushing the boundaries of CFD simulation capabilities.<sup>45</sup>

## 5.2 Unsteady Turbulent Flow Simulations Including Transition and Separation

Perhaps the single, most critical area in CFD simulation capability that will remain a pacing item by 2030 in the analysis and design of aerospace systems is the ability to adequately predict viscous turbulent flows with possible boundary layer transition and flow separation present.<sup>23, 31, 63, 64</sup> While steady, fully turbulent attached flows can be predicted reasonably well with current RANS methods at all speed regimes,<sup>23, 65, 66</sup> all types of separated flows are still difficult to predict. In particular, smooth body separation remains very hard to simulate accurately and efficiently for high-speed (buffet-limited) stall, low-speed high-lift, inlets at crosswind conditions, engine simulations and compressor stall, flows at the edges of the design envelope, and for maneuvering flight with moving control surfaces. In general, two critical components of flow physics need to be modeled accurately: the exact location of separation as controlled by boundary-layer physics and the feedback from the separated region to the boundary layer.

Based on feedback from the CFD survey and the follow-up workshop held as part of this study, it is clear that the majority of the engineering and scientific community believes that RANS-based turbulence models, in conjunction with the expanded use of hybrid RANS-Large Eddy Simulation (LES) methods, will be the norm in 2030. This sentiment was confirmed from discussions at the workshop: all of the

invited speakers in the session on turbulence predicted the continued use of RANS, including one and two-equation models, as opposed to the more complex Reynolds-Stress Transport models. They also predicted the extensive use of hybrid methods. However, LES-dominant methods for the range of engineering problems of interest (specifically for higher Reynolds numbers) will likely not be feasible based on current estimates of HPC computing performance in 2030 using standard CFD approaches (see “Case Study 2: LES Cost Estimates and 2030 Outlook” below).

In the area of viscous turbulent flows with transition and separation, a number of technology gaps and impediments must be overcome to accurately model these flows in the 2030 timeframe. Specifically, they are:

1. **Lack of a theoretically based, hybrid RANS-LES turbulence simulation capability.** Ideally, unsteady flow simulations using advanced turbulence models (e.g., DES, full LES) should be used to resolve the key turbulent length scales that drive development and propagation of flow separation. There has been progress in the representation of post-separation physics with the use of hybrid RANS-LES, or in general, turbulence-resolving methods (i.e., at least the part of the domain that is solved in LES mode).<sup>67, 68</sup> In contrast, however, the prediction of pre-separation physics is still provided by RANS models, which have seen nearly stagnant development for 20 years.<sup>48</sup> Unfortunately, hybrid methods are currently cost-prohibitive for routine use on realistic configurations at Reynolds numbers of interest in aerospace, at least in the thinner regions of the boundary layer such as near the wing attachment line. Another key impediment in fielding a robust hybrid RANS-LES capability is the changing nature of the interface between RANS and LES regions. For hybrid methods to be routinely used, a seamless, automatic RANS-to-LES transition in the boundary layer is urgently required.<sup>69</sup>
2. **Availability and convergence of complex turbulence models in practical codes.** A recurring issue in using elaborate RANS models with second moment closures (e.g., Reynolds Stress Transport methods) for practical applications is both their availability in widely used flow solvers (e.g., FUN3D, OVERFLOW) and their notoriously poor convergence characteristics for flow simulation involving complex geometries and/or complex flow physics.<sup>70</sup> The key impediments are the complexity of the models themselves manifesting in myriad variations, inadequate attention to numerics during design of the models, and the lack of powerful solution techniques in these codes that may be needed to solve the flow and turbulence model equations.<sup>71</sup>



## CASE STUDY 2: LES Cost Estimates and 2030 Outlook

The predictions of when LES will be available in a reasonable turnaround time for engineering use have been performed by numerous researchers. Here, we focus on wall-modeled LES (WMLES) in which the anisotropic near-wall region is modeled in some manner such that the LES is responsible only for the larger, more isotropic outer flow. In 1979, Chapman estimated that such wall-modeled LES would be possible in the 1990s for practical aerodynamic applications.<sup>1</sup> This clearly has not been realized in practice and one key factor in the optimistic predictions of Chapman was an underestimation of the computational work required for LES. Since that time, Spalart, et al. in 1997<sup>2</sup> and 2000<sup>3</sup> revised the computational cost estimates and predicted that full-wing LES would not be available for engineering use until 2045. Most recently, Choi and Moin<sup>4</sup> revisited Chapman's estimate applying the analysis of Spalart to show that the required resolution for wall-modeled LES in the turbulent portion of a boundary layer flow (i.e., after transition) scales asymptotically with Reynolds number, that is the number of grid points  $N \sim Re_L$  (Chapman had estimated  $N \sim Re_L^{2/5}$ ).

A potential concern is that these estimates ignore the cost of the laminar and transitional region of the boundary layer. In fact, because this region is significantly thinner than the turbulent boundary layer (even though it is generally a much smaller fraction of the chord), the computational cost may be non-negligible. To be precise, we follow Spalart, et al. 1997 and count the number of cubes of volume  $\delta^3$ , where  $\delta$  is the boundary layer thickness. We consider both the laminar (including transition) and turbulent region of a boundary layer on a unit aspect ratio NACA 0012 wing. The flow is modeled using the 2D coupled integral boundary layer method of Drela<sup>5</sup> with transition estimated using an  $e^N$  method ( $N_{crit} = 9$ ). The table below shows that the number of cubes in the laminar region is 10 to 100 times larger than in the turbulent region. Thus, we conclude that a key issue in the application of WMLES will be the modeling of the laminar and transitional region.

$Re_c$	$N_{cubes}^{lam}$	$N_{cubes}^{turb}$	$N_{cubes}^{(Total)}$
1e6	1.1e6	1.3e4	1.1e6
1e7	1.1e7	1.5e5	1.1e7
1e8	9.1e7	3.1e6	9.4e7

We can estimate the performance of WMLES on HPC in 2030. We base this estimate on existing second-order accurate finite volume and finite difference discretizations with explicit time integration. While clearly other options exist, in particular higher-order methods, this combination is representative of the class of algorithms currently being applied throughout aerospace CFD on LES and DES simulations. Thus, we are making estimates based solely on how increased computational power will impact the ability to perform WMLES simulations. Specifically, we make the following assumptions:

- The mesh is an isotropic refinement of the boundary layer cubes with  $n$  points in each direction (and thus  $n^3$  unknowns in a single cube). In this example, we choose  $n=20$ .
- The timestep of the explicit method is equal to  $h_{min} / a_\infty$  where  $h_{min} = \delta_{min} / n$  and  $a_\infty$  is the freestream speed of sound.
- The number of floating point operations per timestep per point is  $C_{iter}$ . In this example, we choose  $C_{iter}=1250$ .
- The time integration is performed over  $C_T$  convective timescales. In this example, we choose  $C_T=100$ .

The table below shows the petaFLOP/s required to achieve a 24-hour turnaround for Mach 0.2 flow around a unit aspect-ratio geometry (estimates for high aspect ratio wings can be obtained by scaling by the desired aspect ratio). We note that the FLOP cost scales with approximately  $Re_L^{1.3}$ , which is due to  $\sim Re_L$  for gridding requirements and  $Re_L^{1/3}$  for timestep requirements. Estimates for wall-resolved LES<sup>4</sup> show gridding requirements that scale with  $Re_L^{13/7}$  which gives FLOP costs scaling with  $Re_L^{2.5}$ .

$Re_c$	$N_{dof}$	$N_{iter}$	FLOP	PFLOP/s
1e6	9.0e9	4.6e7	5.2e20	6
1e7	8.5e10	1.5e8	1.6e22	180
1e8	7.5e11	4.6e8	4.3e23	5,000

We can then compare these estimates to existing HPC capability as well as estimated capability in 2030. At present, the world's top HPC machine is Tianhe-2, a supercomputer developed by China's National University of Defense Technology, with a theoretical peak performance of 55 PFLOP/s (and an actual achieved performance of 34 PFLOP/s on the Linpack benchmark). Thus, by today's capability, wall-modeled LES is feasible in a 24-hour turnaround time at Reynolds number of about 1 million on unit-aspect ratio geometries using existing algorithms. Looking ahead to 2030, the leadership class HPC machine is estimated to have a theoretical peak performance of about 30 exaFLOP/s (see Appendix A). Thus, by 2030, we could expect to perform these types of calculations on the leadership HPC machine.

Additional conclusions based on these results are:

- For the higher aspect ratios that are more relevant to external flows, the costs will be an order of magnitude larger and thus out of the reach of even 2030 leadership HPC machines at the high Reynolds numbers of interest.
- At lower Reynolds numbers, the cost differences between wall-modeled and wall-resolved LES disappear. Thus, for lower Reynolds number applications, e.g., in some components of turbomachinery, wall-resolved LES is feasible on leadership class machines today.<sup>6</sup>
- As additional complexities are introduced, e.g., the full geometric complexity of a turbomachinery or a high-lift configuration, the cost will increase further.
- The cost estimate assumes that the laminar and transition regions are simulated using the same resolution (per cube) as in the turbulent region, i.e., the transition process is simulated. If the transition process could instead be modeled so that the grid resolution was essentially that required for steady laminar boundaries, then the cost of the laminar and transition region would become negligible compared to the turbulent region and reduces the above cost estimates by a factor of 10 to 100.
- The wall modeling for this type of LES is a current weakness that could limit the reliability of using this approach for separation prediction.
- While these types of LES calculations may be feasible on leadership class HPC machines, engineering CFD calculations are not often pursued at this level of parallelism. Rather, engineering CFD calculations tend to be performed with 1,000s and rarely 10,000s of compute nodes. Thus, to realize these capabilities will require effort to exploit existing and future HPC performance.
- The potential impact of algorithmic work could be significant. For example, a 10-fold improvement due to algorithmic performance (e.g., through adaptivity, or higher-order discretizations, or improved solution algorithms) could bring these 24-hour calculations down to a few hours. Further, this could relieve some of the pressure on wall modeling and transition modeling by facilitating increased grid resolution (or improved accuracy at less cost), and head toward wall-resolved LES.

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4. Choi, H., and Moin, P., "Grid-point requirements for large eddy simulation: Chapman's estimates revisited," *Phys. Fluids* **24**, 011702 (2012)
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3. **Effects of grid resolution and solution scheme in assessing turbulence models.** A key gap in the effectiveness of current and future turbulence models is the effect of grid resolution and solution scheme on both the accuracy and convergence properties of the models. Studies show that adequate grid resolution is required to capture the full range of turbulence structures in models ranging from simple eddy-viscosity formulations to full LES and DNS simulations.<sup>55</sup> Additionally, choice of solution scheme may be important when using marginal grid resolution for complex geometries. Much work has been performed on building-block geometries,<sup>23,65</sup> but real-world cases are now too complex to assess full grid convergence.<sup>56</sup>
4. **Insufficient use of foundational validation/ calibration datasets to drive physics-based improvements to turbulence prediction.** Key experimental datasets are critically important in the ongoing development and refinement of the full range of turbulence models from RANS to LES. Typical impediments include test cost, large number of cases needed, and instrumentation limitations. Moreover, many existing datasets are often not effectively exploited to use all available data in assessing and improving models.
5. **Insufficient use of real-world experiments to validate turbulence models.** In addition to building-block exper-

iments, more specific test data from complex, integrated flow fields using geometries that are more representative of complex aerospace systems is needed. Impediments include balancing test cost and model complexity, difficulty in designing experiments, geometry deviations, measurement detail, and accuracy of CFD.

6. **Robust transition prediction capability.** Boundary layer transition is not well predicted (if at all) in CFD practice, impacting wind tunnel to flight scaling, laminar flow prediction and control, turbomachinery design, and hypersonic transition/heating analysis, among others. Transition modeling for lower Reynolds number applications is particularly lacking, with specific impact on high bypass ratio turbomachinery and for the lower Reynolds number vehicles being designed today. Currently,  $e^n$  methods are difficult to use. However, there have been some novel and promising developments in transition prediction methods (e.g., the Langtry-Menter correlation-based model),<sup>50</sup> but these partial-differential equation (PDE) based methods (as opposed to  $e^n$  techniques) must be calibrated for a wide range of flow regimes and problems of interest, and should be viewed as in-development and somewhat risky. Still, these methods are being improved and are propagating into both government and commercial CFD codes<sup>72</sup> even as they (currently) do not account for the cross-flow mode of

transition. Solid research is needed both on the PDE and  $e^{\text{p}}$  tracks, with emphasis on both accuracy and ease of coupling with RANS codes.

7. **Lack of explicit collaboration among turbulence researchers.** There is a general lack of close coordination between turbulence modelers and researchers both in the aerospace field itself (scattered amongst academia, industry, and government), and between researchers in aerospace and related fields. In order to generate the new ideas necessary to address the key issues of flow separation and transition, it is imperative that a more concerted effort be undertaken to connect members of the aerospace turbulence community to others in weather prediction, bio-fluids, and hydrodynamic fields.

### 5.3 Autonomous and Reliable CFD Simulation

Today, most standard CFD analysis processes for the simulation of geometrically complex configurations are onerous, both in terms of cycle time and process robustness. Even for simpler configurations that are typically analyzed during the conceptual design phase, full automation is essential in order for a conceptual designer to effectively exploit the capacity of high performance computers and physics-based simulation tools. Based on feedback from the engineering and scientific communities as determined through our CFD Vision 2030 survey and workshop, the key issues related to CFD automation and reliability can be categorized into the broad areas of mesh generation and adaptivity, discretizations, solvers and numerics, and error control and uncertainty quantification.

#### *Mesh generation and adaptivity*

Today, the generation of suitable meshes for CFD simulations about complex configurations constitutes a principal bottleneck in the simulation workflow process. Often the mesh generation phase constitutes the dominant cost in terms of human intervention, and concerns about the cost and reliability of mesh generation were raised repeatedly in the survey and workshop. However, since a computational mesh is merely a means to enable the CFD simulation, ultimately the mesh generation process should be invisible to the CFD user or engineer. Given a suitable geometry representation and a desired level of solution accuracy, a fully automated meshing capability would construct a suitable mesh and adaptively refine this mesh throughout the solution process with minimal user intervention until the final accuracy levels are met. This process allows the user to focus on the final solution without concern for the construction and maintenance of the underlying mesh. Achieving this vision of fully automated meshing requires overcoming various important current impediments.

1. **Inadequate linkage with CAD.** Configuration geometry definitions required by mesh generation software are generally provided by computer-aided design

(CAD) packages. However, there is currently no single standard for representing surface or solid geometries within CAD tools, complicating efforts to fully automate the link between mesh generation and geometry definition. Furthermore, many existing CAD geometry definitions are poorly suited for CFD analyses, either due to insufficient accuracy (non water-tight geometries often adequate for manufacturing purposes), or due to excessive detail not essential for the CFD analysis. This results in the need to incorporate specialized post-processing tools such as shrink-wrapping in the former case, and/or de-featuring techniques in the latter case. At the same time, additional information such as slope and curvature or even higher surface derivatives may be required for the generation of curved mesh elements suitable for use with higher-order accurate CFD discretizations.<sup>73,74</sup> Finally, for adaptive meshing purposes, tight coupling between the CFD software and geometry definition is required to enable low-overhead, on-demand, geometry surface information queries within the context of a massively parallel computing framework.<sup>75</sup>

2. **Poor mesh generation performance and robustness.** Significant human intervention is often required in the mesh generation process due to lack of robustness. This is evidenced by the inability of current mesh generation software to consistently produce valid high-quality meshes of the desired resolution about complex configurations on the first attempt. Additionally, many current mesh generation algorithms (e.g., advancing-front methods) do not scale appropriately on parallel computer architectures, and most mesh generation software is either run sequentially, or using a small number of computer cores or processors. On the other hand, CFD solver technology has demonstrated very good scaling on massively parallel machines,<sup>76-78</sup> and is demanding ever larger meshes, which the mesh generation community is finding increasingly difficult to deliver due both to memory and time constraints using desktop commodity hardware. During the last decade or more, developments in mesh generation software came from third-party commercial vendors and NASA investment in this area has essentially evaporated. However, fundamental advances in computational geometry and other areas will be key to improving the reliability, robustness, and parallel scalability of mesh generation capabilities, particularly as larger simulations using finer meshes about more complex geometries are sought. Additionally, paradigm shifts in meshing technology (i.e., cut cell methods, strand grids, meshless methods) may lead to revolutionary advances in simulation capabilities.<sup>79-82</sup>

#### *Discretizations, Solvers, and Numerics*

The core of an autonomous and reliable CFD capability must rely on efficient and robust discretization and solution

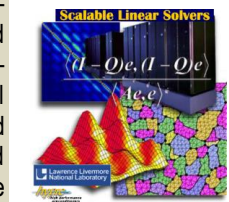
strategies. Discretizations must be tolerant of localized poor mesh quality while at the same time be capable of delivering high accuracy at low cost. Solution techniques must be scalable, efficient, and robust enough to deliver converged solutions under all reasonable conditions with minimal user intervention. One of the principal concerns raised throughout our survey and workshop was the high level of expertise and human intervention often required for performing and understanding CFD analyses, with a consensus that a principal requirement for relieving this dependency will require added investment in basic numerical methods research. Current gaps and impediments with numerical methods include:

1. **Incomplete or inconsistent convergence behavior.** Most current CFD codes are capable of producing fully converged solutions in a timely manner for a variety of simple flow problems. However, most often these same tools are less reliable when applied to more complex flow fields and geometries,<sup>56,85</sup> and may fail, or require significant user intervention to obtain adequate results. There are many possible reasons for failure, ranging from poor grid quality to the inability of a single algorithm to handle singularities such as strong shocks, under-resolved features, or stiff chemically reacting terms. What is required is an automated capability that delivers

### CASE STUDY 3: Scalable Solver Development

The development of optimal solvers has been central to the success of CFD methods since the early days of numerical simulation, for both steady-state and time-implicit problems. Optimal solvers are defined as methods that are capable of computing the solution to a problem with  $N$  unknowns in  $O(N)$  operations. Because the number of unknowns in industrial CFD problems is most often very large ( $10^6 < N < 10^9$ ), optimal solvers offer the potential for orders of magnitude increase in solution efficiency compared to simple iterative solvers, which most often scale as  $O(N^2)$  or higher.

Multigrid methods constitute the most successful and widely used optimal solvers for CFD problems. These methods were developed for CFD applications at an early stage, with considerable NASA investment. In the late 1970s, joint NASA collaborative work with academic leaders in multigrid solver technology produced some of the first successful multigrid solvers for potential flow methods<sup>1</sup>, followed by efficient multigrid solvers for the Euler equations<sup>2</sup>, and the Navier-Stokes equations. The success was such that multigrid methods were implemented and used in virtually all important NASA CFD codes, including TLNS3D, CFL3D, OVERFLOW, and more recently FUN3D. Multigrid methods have become essential solver components in commercial production codes such as Fluent and STARCCM+, and have received particular attention within the DOE where they are used in various large-scale production codes. Despite their early success, many impediments remain for successfully extending these solvers to larger and more complex problems. While most early NASA investment focused on geometric multigrid for structured meshes, extending these solvers to complex geometry CFD problems or even abstract matrix inversion problems requires the development of algebraic multigrid methods (AMG). At the same time, improvements to current multigrid strategies are required if these methods are to scale effectively on emerging massively parallel HPC hardware. Although NASA investment in further research on multigrid methods has stalled since the early 1990s, considerable research has been directed toward developing more optimal AMG solvers designed for use on petascale and exascale hardware within the DOE. For example, the Scalable Linear Solver group at Lawrence Livermore National Laboratory has developed parallel AMG technology and related methods such as Smoothed Aggregation techniques that maintain optimal solver qualities while delivering vastly improved scalability on massively parallel machines. Current capabilities include the demonstration of the solution of a problem involving over  $10^{12}$  degrees of freedom with good scalability on over 100,000 cores.<sup>3</sup> Although these solvers are publicly available, they have not drawn the interest of the aerospace CFD community, and will likely require considerable investment to modify and extend to production aerospace CFD problems.



Multigrid method developments are often reported at dedicated multigrid specialist conferences. For example, the first successful multigrid solution of the Euler equations was reported at the 1983 Copper Mountain Multigrid Methods conference.<sup>2</sup> This conference series was traditionally well attended by NASA participants and, as recently as 1996, the conference proceedings were edited and published by NASA Langley<sup>4</sup>. However, during the last decade there has been virtually no NASA presence at these conferences. This has been accompanied by a significant decline of scalable solver papers published in AIAA venues, while NASA CFD codes have remained confined to the same multigrid technology that was developed in those early years.

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hands-off solid convergence under all reasonable anticipated flow conditions with a high tolerance to mesh irregularities and small-scale unsteadiness. Reaching this goal necessarily will require improvements in both discretizations and solver technology,<sup>86</sup> since inadequate discretizations can permit unrealizable solutions, while temperamental solvers may be unable to reach existing valid solutions. Although incremental improvements to existing algorithms will continue to improve overall capabilities, the development of novel robust numerical techniques such as monotone, positivity-preserving, and/or entropy-preserving schemes<sup>87,88</sup> and their extension to complex problems of industrial relevance offers the possibility of radical advances in this area.

- 2. Algorithm efficiency and suitability for emerging HPC.** In previous decades, NASA has invested heavily in numerics and solver technology, and it is well documented that equivalent advances in numerical simulation capability have been enabled through the development of more efficient algorithms compared to advances in HPC hardware.<sup>1,16-18</sup> However, during the last decade, algorithmic investment has been dramatically curtailed, with the result that the many flow solvers in use today were developed more than 20 years ago and are well known to be suboptimal. Because solver optimality is an asymptotic property, as larger simulations are attempted, the potential benefits of better solvers grow exponentially, possibly delivering orders of magnitude improvement by the exascale computing timeframe. At the same time, the drive to more complex flows (including more complex turbulence models, stiff chemically reacting terms, or other effects) and tightly coupled multidisciplinary problems will require the development of novel techniques that remain stable and efficient under all conditions. Finally, existing numerical techniques were never conceived with massive parallelism in mind, and are currently unable to capitalize on the emerging massively parallel and heterogeneous architectures that are becoming the mainstay of current and future HPC. In order to improve simulation capability and to effectively leverage new HPC hardware, foundational mathematical research will be required in highly scalable linear and nonlinear solvers not only for commonly used discretizations but also for alternative discretizations, such as higher-order techniques.<sup>89</sup> Beyond potential advantages in improved accuracy per degree of freedom, higher-order methods may more effectively utilize new HPC hardware through increased levels of computation per degree of freedom.

### ***Error control and uncertainty quantification***

Errors in current CFD simulations are not well understood or well quantified, including errors due to spatial and temporal discretization, incomplete convergence, and the physical models and parameters they embody. The lack of error

quantification raises the risk that engineering decisions are based on inaccurate and/or uncertain results. The Vision 2030 survey highlighted the need for improvements in error quantification. Furthermore, in terms of reliable and automated CFD simulations, discretization error estimation is a key ingredient for the realization of a solution adaptive process. Current error control and uncertainty quantification gaps and impediments include:

- 1. Limited use of existing error estimation and control methods.** Significant progress has been made in the estimation and control of discretization errors, in particular in terms of output-based techniques.<sup>90-93</sup> However, while these techniques were demonstrated by multiple groups for steady 2D RANS<sup>94</sup> and 3D inviscid flows,<sup>83</sup> the applications to 3D RANS and unsteady flows were limited, in particular for complex geometries. These more complex applications have been severely impeded by the inadequacies of 3D anisotropic and time-dependent adaptive meshing, as well as by poor robustness of current discretization and solution algorithms (i.e., to be able to solve flow and adjoint equations on potentially poor quality meshes during the adaptive process).
- 2. Inadequacy of current error estimation techniques.** While discretization error estimation techniques for outputs have improved during the past 10 years, these techniques do have fundamental limitations that could influence their application to increasingly complex problems. In particular, output-based error estimation techniques are based on linearizations about existing (approximate) solutions and as a result can have significant error when the flows are under resolved (even in the case of a linear problem, the techniques generally only provide error estimates and are not bounds on the error). Furthermore, for unsteady, chaotic flows (which will be a key phenomenon of interest as turbulent DES and LES simulations increase in use moving forward) linearized analysis will produce error estimates that grow unbounded with time (due to the positive Lyapunov exponent for chaotic flows).<sup>95,96</sup> In these situations, existing output-based methods will be swamped by numerical error, rendering the sensitivity information meaningless. This issue will affect not only error estimation but also design optimization moving forward.
- 3. Limited use of uncertainty quantification.** The consideration of uncertainty due to parametric variability as well as modeling error raises significant challenges. Variability and uncertainty of inputs (boundary and initial conditions, parameters, etc.) to fluid dynamic problems are largely unquantified. Even if estimates are available and/or assumed, the propagation of these uncertainties poses a significant challenge due to the inherent cost, the lack of automation and robustness of the solution process, and the poor utilization of high performance com-

puting. Even more challenging is the quantification of modeling error. This will likely require significantly more expensive methods (e.g., based on Bayesian approaches).<sup>97</sup> While uncertainty quantification is being investigated in the broad research community, most notably through DOE and NSF led programs,<sup>98</sup> the engineering community, and the aerospace community in particular, have had minimal investments to address these issues.

#### 5.4 Knowledge Extraction and Visualization

An integral part of effectively using the advanced CFD technology envisioned in 2030 is the way in which the very large amount of CFD-generated data can be harvested and utilized to improve the overall aerodynamic design and analysis process. The resulting utilization of this data would include insight into pertinent flow physics, use with aerodynamic or multidisciplinary optimization, and generation of effective databases for a myriad of purposes, including control law development, loads assessment, flight/performance simulation, etc.

A number of technology gaps and impediments in the area of knowledge extraction for large-scale CFD databases and simulations must be overcome to efficiently analyze and utilize CFD simulations in the 2030 time frame.

1. **Effective use of a single, high-fidelity CFD simulation.** As high-performance computing (HPC) systems become faster and more efficient, a single unsteady CFD simulation using more complicated physical models (e.g., combustion) to solve for the flow about a complete aerospace system (e.g., airplane with full engine simulation, space vehicle launch sequence, aircraft in maneuvering flight, etc.) using a much higher number of grid points (~10 to 100 billion) will become commonplace in the 2030 time frame. Effective use (visualization and in-situ analysis) of these very large, single, high-fidelity CFD simulations will be paramount.<sup>99</sup> Similarly, higher-order methods will likely increase in utilization during this time frame, although currently the ability to visualize results from higher order simulations is highly inadequate. Thus, software and hardware methods to handle data input/output (I/O), memory, and storage for these simulations (including higher-order methods) on emerging HPC systems must improve. Likewise, effective CFD visualization software algorithms and innovative information presentation (e.g., virtual reality) are also lacking.
2. **Real-time processing and display of many high-fidelity CFD simulations.** By the year 2030, HPC capabilities will allow for the rapid and systematic generation of thousands of CFD simulations for flow physics exploration, trend analysis, experimental test design, design space exploration, etc. The main goal, therefore, is to collect, synthesize, and interrogate this large array of computational data to make engineering decisions in

real time.<sup>39</sup> This is complicated by a lack of data standards which makes collection and analysis of results from different codes, researchers and organizations difficult, time consuming and prone to error. At the same time, there are no robust, effective techniques for distilling the important information contained in large collections of CFD simulation data into reduced-order models or meta-models that can be used for rapid predictive assessments of operational scenarios, such as the correlation of flow conditions with vehicle performance degradation or engine component failures, or assessments of engineering tradeoffs as required in typical design studies.<sup>100</sup>

3. **Merging of high fidelity CFD simulations with other aerodynamic data.** With wind tunnel and flight-testing still expected to play a key role in the aerospace system design process, methods to merge and assimilate CFD and multidisciplinary simulation data with other multi-fidelity experimental/computational data sources to create an integrated database, including some measure of confidence level and/or uncertainty of all (or individual) portions of the database, are required. Currently, the merging of large amounts of experimental and variable fidelity computational data is mostly carried out through experience and intuition using fairly unsophisticated tools. Well founded mathematically and statistically based approaches are required for merging such data,<sup>101-103</sup> for eliminating outlier numerical solutions, as well as experimental points, and for generally quantifying the level of uncertainties throughout the entire database in addition to at individual data points.<sup>104</sup>

#### 5.5 Multidisciplinary/Multiphysics Simulations and Frameworks

We also assume that CFD capabilities in 2030 will play a significant role in routine, multidisciplinary analysis (MDA) and optimization (MDO) that will be typical of engineering and scientific practice. In fact, in 2030 many of the aerospace engineering problems of interest will be of a multidisciplinary nature and CFD will have to interface seamlessly with other high-fidelity analyses including acoustics, structures, heat transfer, reacting flow, radiation, dynamics and control, and even ablation and catalytic reactions in thermal protection systems. With increasingly available computer power and the need to simulate complete aerospace systems, multidisciplinary simulations will become the norm rather than the exception. However, effective multidisciplinary tools and processes are still in their infancy.

Limitations on multidisciplinary *analyses* fall under various categories including the setup and execution of the analyses, the robustness of the solution procedures, the dearth of formal methodologies to guarantee the stability and accuracy of coupled high-fidelity simulations, and the lack of

existing standards for multidisciplinary coupling. The result tends to be one-off, laborious, and nonstandard interfaces with other disciplines with dubious accuracy and stability. Multidisciplinary *optimizations* inherit all of these limitations and suffer from additional ones of their own, including the inability to produce accurate discipline and system-level sensitivities, the lack of quantified uncertainties in the participating models, the lack of robustness in the system-level optimization procedures, as well as very slow turnaround times.

The vision for 2030 MDA/O involves the seamless setup and routine execution of both multidisciplinary analyses and optimizations with

- Rapid turnaround (hours for MDA and less than a day for MDO).
- User-specified accuracy of coupled simulations.
- Robustness of the solution methodology.
- Ability to provide sensitivity and uncertainty information.
- Effective leveraging of future HPC resources.

For this vision to proceed forward, the development of multidisciplinary standards will be necessary, as well as the creation of coupling frameworks that facilitate the multidisciplinary interactions envisioned here. Moreover, key research challenges in multidisciplinary coupling, computation of system-level sensitivities, management of uncertainties in both the analyses and optimizations, hierarchical decomposition of the optimization problems, and both automation and standardization processes will need to be overcome.

More specifically, a number of technology gaps and impediments must be tackled to enable truly multidisciplinary analyses and optimizations in the 2030 timeframe. In this report, we focus on the requirements that affect 2030 CFD. Although, by extension, we also discuss some more general gaps and impediments that are likely to affect our vision.

**1. Robustness and automation of CFD analyses in multidisciplinary environments.** To ensure that 2030 CFD can be an integral part of routine multidisciplinary, multiphysics simulations, the manpower cost required to set up and execute such calculations must be drastically reduced. Firstly, the setup of high-fidelity multidisciplinary analyses must be largely automated including all operations involving surface and volume grid transfers and interpolations, grid deformations and/or re-generation, information exchanges, and mappings to HPC environments. Secondly, the execution of multiphysics simulations that involve Vision 2030 CFD must include appropriate measures to ensure the robustness of the solution procedure, protecting against coupled simulation failure and including the on-demand availability of all necessary modules in the CFD chain so that CFD failure modes are protected.

Such automation and robustness characteristics provide the foundation for more complex problems that require the solution of multidisciplinary simulations.

- 2. The science of multidisciplinary coupling at high fidelity.** Exchanges of information between Vision 2030 CFD and other disciplinary solvers with which CFD will need to interact will require assurances of both accuracy and stability. Such properties often require the satisfaction of conservation principles to which close attention must be paid.<sup>105</sup> Moreover, within the context of nonlinear phenomena and unsteady flows, the proper interfacing between CFD and other codes requires significant effort and can be hard to generalize. The development of libraries and procedures that enable high fidelity, accurate, and stable couplings, regardless of the mesh topologies and characteristic mesh sizes must be pursued. Such software may also need to be cognizant of the discretization details of the CFD solver. Ultimately, solvers using discretizations of a given accuracy (in space and in time), when coupled to other solvers, must ensure that the accuracy of the component solvers is preserved and that the coupling procedure does not give rise to numerical errors that may manifest themselves through solution instabilities.<sup>106</sup>
- 3. Availability of sensitivity information and propagation of uncertainties.** Vision 2030 CFD is expected to interact with other solvers (for different disciplines) in multidisciplinary analyses and optimizations. In 2030, the state of the art is presumed to include the quantification of uncertainties (UQ), at the system level, arising from uncertainties in each of the participating disciplines. In order to facilitate both optimization and UQ at the system level, Vision 2030 CFD must be able to provide sensitivities of multiple derived quantities of interest with respect to large numbers of independent parameters at reasonable computational cost. Novel techniques for the propagation of uncertainties will need to be embedded into 2030 CFD for more comprehensive treatment of UQ problems. Moreover, the support for system-level sensitivity information and UQ will demand the availability of derivative and UQ information related to outputs of CFD that may be utilized by other solvers. Ensuring that these capabilities are present in our Vision 2030 CFD will permit advanced analyses, optimizations, and UQ to be carried out.
- 4. Standardization and coupling frameworks.** Owing to the multitude of disciplinary solvers available for coupling with 2030 CFD, the uncertainty regarding the actual code structure, HPC solver architecture, and internal solution representation, it is fundamental to ensure that multidisciplinary simulation standards (such as the CGNS standard<sup>107</sup> created for CFD) are created so that a variety of solvers can participate in multidisciplinary analyses and optimizations. Beyond the typi-

cal codification of the inputs and outputs of a particular physical simulation, standards for MDAO may need to include sensitivities, uncertainties, and overall descriptions of the parameterization (possibly including the geometry itself) and the optimization problem. To enable tight coupling of diverse disciplines and codes, the data standards need to extend to include memory resident information and coding structures.<sup>57,59,60</sup>

## 6 Technology Development Plan

To achieve our vision of CFD in 2030 and directly address the key CFD technology shortcomings and impediments that currently limit the expanded use of CFD methods within the aerospace analysis and design process, a comprehensive CFD development plan has been developed and is presented in this section. In order to place future technology developments within the context of our Vision for 2030 CFD, we first describe in more detail a number of Grand Challenge (GC) problems that embody the goals for CFD in 2030. Next, a comprehensive roadmap that depicts key technology milestones and demonstrations needed to support the GC simulations is introduced and described. An integrated research plan is then proposed. Finally, an overall research strategy with specific recommendations for executing the plan to advance the state of the art in CFD simulation capability is provided.

### 6.1 Grand Challenge Problems

The intent of the GC problems is to drive the identification and solution of the critical CFD barriers that would lead to a desired revolutionary CFD capability. We purposely have chosen GC problems that are bold, recognizing that they may not be routinely achievable by 2030, but, if achieved, would represent critical step changes in engineering design capability. To this end, the GC cases are chosen to encompass the CFD capabilities required to design and analyze advanced air and space vehicles and systems in 2030, and represent important application areas of relevance to the various NASA aeronautics and space missions. Details on each of the four GC problems are given below.

#### *Grand Challenge Problem 1:*

**LES of a powered aircraft configuration across the full flight envelope.** This case focuses on the ability of CFD to simulate the flow about a complete aircraft geometry at the critical corners of the flight envelope including low-speed approach and takeoff conditions, transonic buffet, and possibly undergoing dynamic maneuvers, where aerodynamic performance is highly dependent on the prediction of turbulent flow phenomena such as smooth body separation

and shock-boundary layer interaction. Clearly, HPC advances alone will not be sufficient to solve this GC problem and improvements in algorithmic technologies or other unforeseen developments will be needed to realize this goal. Progress toward this goal can be measured through the demonstration of effective hybrid RANS-LES and wall-modeled LES simulations with increasing degrees of modeled versus resolved near-wall structures with increasing geometric complexity. Fully optimized flow solvers running on exascale computing platforms will also be critical.

#### *Grand Challenge Problem 2:*

**Off-design turbofan engine transient simulation.** This case encompasses the time-dependent simulation of a complete engine including full-wheel rotating components, secondary flows, combustion chemistry, and conjugate heat transfer. This GC will enable virtual engine testing and off-design characterization including compressor stall and surge, combustion dynamics, turbine cooling, and engine noise assessment. Similar to GC 1, demonstration of advances in accurate prediction of separated flows, complex geometry, sliding and adaptive meshes, and nonlinear unsteady flow CFD technologies will be required to achieve this goal. In addition, advances in the computation of flows of widely varying time scales, and the predictive accuracy of combustion processes and thermal mixing, will be necessary.

#### *Grand Challenge Problem 3:*

**MDAO of a highly flexible advanced aircraft configuration.** The increased level of structural flexibility that is likely to be present in future commercial aircraft configurations (of the N+3 and N+4 types envisioned by NASA and its partners) dictates a system-level design that requires the tight coupling of aerodynamics, structures, and control systems into a complete aero-servo-elastic analysis and design capability. This GC problem focuses on the multidisciplinary analysis and optimization of such configurations including explicit aeroelastic constraints that may require a time-accurate CFD approach. In addition to the aero-servo-elastic coupling, this GC includes the integration of other disciplines (propulsion and acoustics) as well as a full mission profile. The ultimate goal is to demonstrate the ability (in both MDA and MDAO) to perform CFD-based system-level optimization of an advanced configuration that requires both steady and unsteady high-fidelity models.



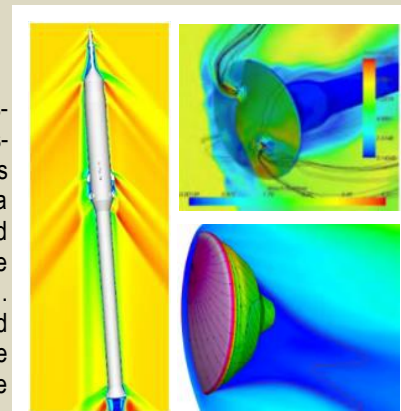
## CASE STUDY 4: Impact of CFD Tool Development on NASA Science and Space Exploration Missions

Traditionally, the development of physics-based simulation tools for aerospace vehicle analysis and design has been the responsibility of NASA's Aeronautics Research Mission Directorate (ARMD), with an emphasis on solving ARMD's aeronautics goals. However, NASA's science and space exploration missions rely heavily on simulation tools. CFD has played a critical role in virtually all recent past and present NASA space vehicle programs, including Space Shuttle return to flight,<sup>1</sup> entry-descent and landing (EDL) predictions for the entire series of Mars landings,<sup>2</sup> support for the recent Constellation Program<sup>3</sup> and, more recently, for the Multipurpose Crew Vehicle (MPCV) and the Space Launch System (SLS) programs. Throughout many of these efforts, limitations in numerical simulation tools for space vehicle design were uncovered, requiring expensive contingency planning. For example, the Ares I development, which employed a combination of wind-tunnel testing and CFD methods for aerodynamic database generation, found that CFD was often less reliable and more expensive than experimental testing, resulting in limited use of CFD principally in specific regions of the flight envelope where testing was not feasible.<sup>4</sup> Similar conclusions were drawn by engineers developing the MPCV Orion aerodynamic database.

In a recent yearly review of NASA's Aerosciences State-of-the-Discipline, NASA's technical fellow for Aerosciences has assessed the ability of the discipline to support NASA's missions, and identified these top three technical challenges:

- Prediction of unsteady separated flows
- Aero-plume interaction prediction
- Aerothermal predictions

Accurate prediction of unsteady separated flow is critical in the design of launch vehicle systems, where buffet and aeroacoustic fluctuating pressures in the transonic regime during ascent can result in high vibrational environments. Currently, launch vehicle buffet environments are obtained almost exclusively through wind tunnel testing and correlation with empirical data at considerable expense and uncertainty, resulting in overly conservative structural mass and reduced payload to orbit. Advanced simulation techniques such as DES are beginning to be explored but have been found to be expensive and to require further refinement and validation. Similarly, quantifying the aeroacoustic environment in launch vehicle design due to separated flows and aero-plume interactions is an important consideration for flight qualification of vehicle electronic components and passenger safety. Previous vehicle programs such as Ares I have incurred considerable expense for the experimental determination of aeroacoustic environments, while investigations by NASA have determined that current CFD techniques are inadequate for the prediction of launch vehicle



aeroacoustic environments.<sup>5</sup> However, the largest payoff in launch vehicle design would come from the use of CFD as a dynamic flight simulation capability, rather than a static aerodynamic database generation tool, as is currently the case, although little effort is being targeted toward this area. Accurate prediction of separated flows is also an important consideration for spacecraft EDL, which is compounded by the need for accurate aerothermal predictions, which in turn are hindered by the need for reliable transition prediction and the inclusion of other multiphysics considerations such as radiation and ablator performance. Accurate simulation of the aero-plume interactions of the reaction-control systems for bluff body re-entry is another area where the development of accurate simulation capabilities could reduce cost and uncertainties associated with complex experimental campaigns. Finally, the design and validation of spacecraft decelerators, including high-speed parachutes and deployable decelerators would benefit enormously from the development of a reliable, nonempirical simulation capability, although this represents a complex nonlinear aero-structural problem with massive flow separation that is well beyond current capabilities.

Clearly, there is a need for better simulation tools within NASA's science and space exploration missions, as well as within aeronautics itself. Furthermore, many of the technological barriers are similar in both areas, such as the inability to accurately simulate separated flows and transition and the need to harness the latest HPC hardware, while other issues are more critical to the space mission such as aero-plume and aerothermal prediction capabilities. To overcome these deficiencies, increased coordination will be required between NASA's science and space exploration programs, which are driving these requirements, and NASA aeronautics, where much of the expertise for simulation method development resides. In the place of the current approach, which relies on the periodic assessment of existing simulation tools, a longer term outlook that invests in new simulation capability development for specific space programmatic objectives must be adopted.

1 Gomez, R. J., Aftosmis, M. J., Vicker, D., Meakin, R. L., Stuart, P. C., Rogers, S. E., Greathouse, J. S., Murman, S. M., Chan, W. M., Lee, D. E., Condon, G. L., and Crain, T., *Columbia Accident Investigation Board (CAIB) Final Report*. Vol. II, Appendix D.8. Government Printing Office, 2003.

2 Edquist, K. T., Dyakonov, A. A., Wright, M. J., and Tang, C. Y., "Aerothermodynamic Design of the Mars Science Laboratory Backshell and Parachute Cone," AIAA paper, 2009-4078.

3 Abdol-Hamid, K. S., Ghaffari, F., and Parlette, E. B., "Overview of the Ares-I CFD Ascent Aerodynamic Data Development and Analysis based on USM3D," AIAA paper, 2011-15, 49<sup>th</sup> AIAA Aerospace Sciences Meeting and Exhibit, Orlando, FL, January 2011.

4 Malik, M. R. and Bushnell, D., (eds.), "Role of Computational Fluid Dynamics and Wind Tunnels in Aeronautics R&D," NASA TP 2012-217602, September 2012.

5 "Independent Assessment of External Pressure Field Predictions Supporting Constellation Program Aeroacoustics (ITAR)," NASA Engineering and Safety Center Report NESC-RP-07-040, September 2013.

### **Grand Challenge Problem 4:**

**Probabilistic analysis of a powered space access configuration.** The goal of this case is to provide a complete description of the aerothermodynamic performance, including reliable error estimates and quantified uncertainty with respect to operational, material, and atmospheric parameters, for a representative space vehicle throughout its flight envelope. This capability will enable reliability predictions and vehicle qualification in light of limited availability of ground-based test facilities. Demonstration of advances in combustion modeling, off-design performance, adaptive and dynamic overset meshing, unsteady flow, hypersonic flow, CFD reliability, and reliability and uncertainty quantification is required.

Required research toward meeting these GCs is identified in six areas, namely HPC, physical modeling, numerical algorithms, geometry/grid generation, knowledge extraction, and MDAO, and is used to formulate the overall research plan. In order to evaluate the progress of each individual area of the research plan, technical milestones and demonstrations are formulated with notional target dates. While these provide a measure of progress in the individual technology roadmap domains, the capability of these combined technologies toward meeting the stated GC problems must also be evaluated periodically and used to prioritize research thrusts among the various technology areas.

## **6.2 Technology Roadmap**

The CFD technology roadmap (presented in Figure 1) is a complete and concise view of the key research technologies and capabilities that must be developed, integrated into production CFD tools and processes, and transitioned to the aerospace CFD user community to achieve our vision of CFD in 2030. The individual elements on the roadmap were identified based on the results of the CFD user survey, detailed technical discussions held during the Vision 2030 CFD workshop, and from interactions among our team members.

Key technology milestones, proposed technology demonstrations, and critical decision gates are positioned along timelines, which extend to the year 2030. Separate timelines are identified for each of the major CFD technology elements that comprise the overall CFD process. The key milestones indicate important advances in CFD technologies or capabilities that are needed within each technology element. Technology demonstrations are identified to help verify and validate when technology advances are accomplished, as well as to validate advances toward the simulations of the GC problems identified above. The technology demonstration (TD) entries are linked by black lines in instances when a given TD can be used to assess CFD advances in multiple areas. Critical strategic decision gates are identified where appropriate to represent points in time where specific research,

perhaps maturing along multiple development paths, is assessed to establish future viability and possible change in development and/or maturation strategy. Each individual timeline is colored by Technology Readiness Level (TRL) in three levels: low (red), medium (yellow), and high (green). The TRL scale is used to indicate the expected overall maturity level of each technology element at a specific point in time. In general, many of the critical CFD technologies are currently at a relatively low TRL level, but with proper research and development, mature to a high TRL level by 2030. Some of the CFD technologies must be sequentially developed and, therefore, it is not expected that all technologies will be at a high TRL in 2030. Specific details of the development plan for each technology element are given below.

**High Performance Computing (HPC).** As mentioned previously, advances in HPC hardware systems and related computer software are critically important to the advancement of the state of the art in CFD simulation, particularly for high Reynolds turbulent flow simulations. Based on feedback from the user survey and from discussions during the CFD workshop, we envision HPC technology advancing along two separate paths.

Ongoing development of exascale systems, as mentioned earlier, will continue through 2030, and represents the technology that will most likely provide the large increase in throughput for CFD simulation in the future.<sup>42,108</sup> However, novel technologies, such as quantum computing or molecular computing, offer a true paradigm shift in computing potential and must be carefully considered at strategic points in the overall development plan, even though the technology is at a very low TRL level today. In order to properly address the HPC challenge, three specific thrusts must be supported. Firstly, current simulation software must be ported to evolving and emerging HPC architectures with a view toward efficiency and software maintainability. Secondly, investments must be made in the development of new algorithms, discretizations, and solvers that are well suited for the massive levels of parallelism and deep memory architectures anticipated in future HPC architectures.<sup>39,41</sup> Finally, increased access to the latest large-scale computer hardware must be provided and maintained, not only for production runs, but also for algorithmic research and software development projects, which will be critical for the design and validation of new simulation tools and techniques.<sup>11, 45</sup> We propose several key milestones that benchmark the advances that we seek: modification of NASA and related CFD codes to efficiently execute on hierarchical memory (GPU/co-processor) systems by 2020, initial evaluation of exascale performance on a representative CFD problem, and a demonstration of 30 exaFLOP performance for one or more of the proposed GC problems in the 2030 time frame.



Concurrently, we stress the importance of closely observing advances in revolutionary HPC technologies, such as superconducting logic, new memory technologies, alternatives to current Complementary Metal Oxide Semiconductor (CMOS) technologies with higher switching speeds and/or lower power consumption (specifically for graphene, carbon nanotubes, and similar developments), quantum computing and molecular or DNA computing. Because these technologies are in their infancy, we foresee decision gates in 2020, 2025, and 2030 to establish the ability of these systems to solve a relevant model problem<sup>61</sup> (i.e., typical of a Poisson problem for PDE-based problems). Implicit in this strategy is the need to provide access to experimental hardware on a continual basis and to explore radical new approaches to devising CFD simulation capabilities. If, at any of these decision points, the technology clearly shows its expected potential, we recommend increased investment to accelerate the use of these machines for CFD applications.

A review of current HPC trends and a forecast of future capabilities are given in Appendix A.

**Physical Modeling.** Advances in the physical modeling of turbulence for separated flows, transition, and combustion are critically needed to achieve the desired state of CFD in 2030.<sup>1,23,24,31,39,63,64</sup> For the advancement of turbulent flow simulation, we propose three separate tracks for research: RANS-based turbulence treatments; hybrid RANS/LES approaches where the entire boundary layer is resolved with RANS-based models, and the outer flow is resolved with LES models; and LES, including both Wall-Model (WMLES) and Wall-Resolved (WRLES). Details on each of the three development tracks and for transition and combustion modeling, are given below. Additionally, a longer term high-risk effort should investigate radically new approaches to physical modeling.

RANS-based turbulence models continue to be the standard approach used to predict a wide range of flows for very complex configurations across virtually all aerospace product categories.<sup>23,30,56,66,85</sup> As a result, the TRL level for these methods is high. They are easy to use, computationally efficient, and generally able to capture wall-bounded flows, flows with shear, flows with streamline curvature and rotation, and flows with mild separation. For these reasons, as well as the fact that RANS models will remain as an important component in hybrid RANS/LES methods, their use will continue through 2030. An advanced formulation of the RANS-based approach, where the eddy viscosity formulation is replaced with the direct modeling of the Reynolds stresses, known as the Reynolds Stress Transport (RST) method,<sup>109</sup> in principle will be able to capture the onset and extent of flow separation for a wider range of flows.<sup>110</sup> Currently, RST models lack robustness and are occasionally less accurate than standard RANS models. Solid research is needed in advancing RST models to production capability. To this end,

we envision continued investment in RST models to 2020, including careful implementation, verification, and validation of the most promising variants of these models into research and production CFD codes, including hybrid RANS/LES codes. In the 2020 time frame, a comprehensive assessment of the ability of these models to predict flow separation would be enabled to determine whether or not further investment is warranted.

Hybrid RANS/LES methods show perhaps the most promise in being able to capture more of the relevant flow physics for complex geometries at an increasingly reasonable computational cost.<sup>68,111</sup> From the user survey, the majority of survey participants ranked the continued development of hybrid RANS/LES methods as the top priority in the area of turbulence modeling. However, as mentioned previously, several issues still exist. First, the prediction of any separation that is initiated in the boundary layer will still require improvements in RANS-based methods. Second, a seamless, automatic RANS-to-LES transition in the boundary layer is needed to enhance the robustness of these methods. Continued investment in hybrid RANS/LES methods to specifically address these two critical shortcomings will be required. Additionally, more effective discretizations and solvers designed specifically for LES type problems must be sought. When combined with advances in HPC hardware, these three developments will enable continued reduction in the RANS region as larger resolved LES regions become more feasible. It is fully anticipated that hybrid RANS/LES methods will become viable in production mode by the 2030 timeframe for problems typical of the proposed GCs. Ultimately, progress will be measured by the degree to which the RANS region can be minimized in these simulations and the added reliability they provide in predicting complex turbulent-separated flows.

Application of LES to increasingly complex flows is a very active research area.<sup>112</sup> At present, the TRL level of this technology is relatively low. As discussed in Case Study 2, cost estimates of WRLES show scaling with Reynolds number of about  $Re_L^{2.5}$  while WMLES is about  $Re_L^{1.3}$ , with the costs being the same at approximately  $Re_L$  of  $10^5$ . For the typically higher Reynolds numbers and aspect ratios of interest to external aerodynamics, WRLES will be outside of a 24-hour turnaround even on 2030 HPC environments unless substantial advances are made in numerical algorithms. However, WRLES is potentially feasible in 2030 for lower Reynolds numbers and is a reasonable pursuit for many relevant aerospace applications including many components of typical aerospace turbomachinery.<sup>113</sup> Further, the development of WRLES directly benefits WMLES in that the basic issues of improved HPC utilization and improved numerics are essentially the same for both. WMLES, however, requires additional development of the wall-modeling capability<sup>114</sup> that is currently at a very low TRL. As such, we recommend investments in LES with emphasis on (1) improved utilization of HPC including developments of numerical algorithms that can more effectively utilize future HPC environments, and

(2) improved wall-modeling capability necessary for reliable WMLES. To this end, we envision waypoints to assess technology maturation: a technology demonstration of LES methods for complex flow physics at appropriate Reynolds numbers around 2020, and a GC problem involving complex geometry and complex flows with flow separation in 2030. Here, as for hybrid RANS/LES models, reductions in the wall modeled region ultimately leading to WRLES will be continuously sought through 2030 and beyond.

Transition modeling is also a key area of investment, as an effective transition model would benefit RANS, hybrid RANS/LES, and LES (by relieving mesh requirements in the laminar and transition regions). Thus, an additional research thrust must be devoted toward the development of reliable and practical transition models that can be incorporated in the turbulence models being matured along each of the development tracks. The transition prediction method should be fully automatic, and be able to account for transition occurring from various mechanisms such as Tollmien–Schlichting waves, cross-flow instabilities, Görtler vortices, and nonlinear interactions associated with bypass transition.

In the area of turbulent reactive flows, investment needs to continue toward the development of a validated, predictive, multiscale combustion modeling capability to optimize the design and operation of evolving fuels for advanced engines. The principal challenges are posed by the small length and time scales of the chemical reactions (compared to turbulent scales), the many chemical species involved in hydrocarbon combustion, and the coupled process of reaction and molecular diffusion in a turbulent flow field. Current combustion modeling strategies rely on developing models for distinct combustion regimes, such as non-premixed, premixed at thin reaction zone, and so forth. The predictive technology should be able to switch automatically from one regime to another, as these regimes co-exist within practical devices. Furthermore, research should continue into methods to accelerate the calculation of chemical kinetics so that the CFD solution progression is not limited by these stiff ordinary differential equations (ODEs). The deep research portfolios of DOE and the US Air Force can be leveraged to further these modeling needs.

In addition to the above thrusts, a small portion of the research portfolio should be devoted to the investigation of radically novel approaches to physical modeling that may offer revolutionary changes in modeling capabilities. As an example, renormalization group theory<sup>115,116</sup> has been proposed as a general framework for turbulence and other multiscale physical modeling, although revolutionary advances have not materialized specifically for turbulence modeling. Nevertheless, advances in multiscale modeling such as systematic upscaling (SU)<sup>106,117</sup> offer the possibility for step changes in physical modeling capability, and should be pursued in a measured manner, similar to the proposed investments in radical HPC technologies.

**Numerical Algorithms.** The development of novel numerical algorithms will be critical to achieving the stated CFD 2030 goals. Indeed, the proposed GCs are sufficiently ambitious that advances in HPC hardware alone during the next 20 years will not be sufficient to achieve these goals. As demonstrated in Case Study 2, even for LES of relatively simple geometries, leadership class HPC hardware in 2030 will be needed for 24-hour turnaround if existing algorithms are used. Thus, to tackle the proposed GCs, orders of magnitude improvement in simulation capabilities must be sought from advances in numerical algorithms.<sup>1,39</sup> The focus of investment must be on discretizations and solvers that scale to massive levels of parallelism, that are well-suited for the high-latency, deep memory hierarchies anticipated in future HPC hardware, and that are robust and fault tolerant.<sup>41</sup> A well balanced research program must provide for incremental advances of current techniques (e.g., extending the scalability of current CFD methods to the exascale level whenever possible), while at the same time investing in the fundamental areas of applied mathematics and computer science to develop new approaches with better asymptotic behavior for large-scale problems and better suitability for emerging HPC hardware.

Discretization techniques such as higher-order accurate methods offer the potential for better accuracy and scalability, although robustness and cost considerations remain.<sup>89</sup> Investment must focus on removing these barriers in order to unlock the superior asymptotic properties of these methods, while at the same time pursuing evolutionary improvements in other areas such as low dissipation schemes,<sup>118-120</sup> flux functions, and limiter formulations. Simultaneously, novel nontraditional approaches, such as Lattice-Boltzmann methods<sup>121,122</sup> or other undeveloped schemes, should be investigated for special applications. Improved linear and nonlinear solvers must be developed, and here as well, the focus must be on highly scalable methods that are designed to be near optimal for the large-scale, time-implicit unsteady CFD and MDAO simulations anticipated in the future. These may include the extension of well-known matrix-based techniques, Krylov methods,<sup>123</sup> highly parallel multigrid methods,<sup>124</sup> or the development of completely novel approaches such as systematic upscaling methods.<sup>117</sup> Furthermore, these methods must be extensible to tightly coupled multidisciplinary problems. Investment in discretizations and solvers must also consider the potential of these methods to operate on dynamically adapting meshes, to enable optimization procedures, and to incorporate advanced uncertainty quantification capabilities. In many cases, adjoint technology<sup>125,126</sup> will be required from the outset for all of these capabilities, but the potential of other more advanced technologies such as second-order gradients (Hessians)<sup>127,128</sup> should be investigated as well. Longer term, high-risk research should focus on the development of truly enabling technologies such as monotone or entropy stable schemes<sup>87,88</sup> in combination with innovative solvers on large-scale HPC hardware. The technology

roadmap envisions the demonstration of improved robust and scalable solvers in the 2015-2017 timeframe, for both second-order and higher-order accurate methods. The demonstration of complete configuration-grid convergence technology in the 2020 time frame relies on the use of robust higher-order discretizations combined with improved scalable solvers and adaptive h-p refinement. Toward the 2030 time frame, it is anticipated that novel entropy stable formulations will begin to bear fruit for industrial simulations.

With regard to uncertainty quantification, a new thrust in the area of probabilistic large-scale CFD for aerospace applications should be initiated. This program can build on the significant advances already made in this area by other government agencies,<sup>98</sup> but provide the focus required for leveraging these technologies for aerospace applications.<sup>129,130</sup> An initial thrust in this area should focus on enabling current aerospace CFD tools with well-known uncertainty quantification techniques, such as sensitivity analysis and propagation methods using adjoints and forward linearizations, non-intrusive polynomial chaos methods, and other reduced-order model formulations.<sup>131,132</sup> Additionally, a concerted effort should be made to characterize important aerospace uncertainties and to make these available to the general research community for enabling relevant UQ research in these areas. Improved error estimation techniques must be investigated and developed, given the known deficiencies of current approaches (including adjoint methods). This will require a foundational program in the mathematics of error estimation and its application to CFD software. Finally, longer term research must focus on statistical approaches such as Bayesian techniques for quantifying more accurately modeling and other nonlinear error sources.<sup>97</sup> The technology roadmap includes an early target date of 2015 for the characterization of typical aerospace uncertainties in order to stimulate work in this area. Improved error estimation techniques will be gradually brought into the simulation capabilities and the state of these estimates will be assessed in the 2018 time frame. Comprehensive uncertainty propagation techniques including discretization error, input and parameter uncertainties in production-level CFD codes should be targeted for 2025, while the development of more sophisticated stochastic and Bayesian approaches will continue through the 2030 timeframe.

**Geometry and Grid Generation.** Substantial new investment in geometry and grid generation technology will be required in order to meet the Vision CFD 2030 goals. In general, this area has seen very little NASA investment during the last decade, although it remains one of the most important bottlenecks for large-scale complex simulations. Focused research programs in streamlined CAD access and interfacing, large-scale mesh generation, and automated optimal adaptive meshing techniques are required. These programs must concentrate on the particular aspects required to make mesh generation and adaptation less burdensome and, ultimately, invisible to the CFD process, while developing tech-

nologies that enable the capabilities that will be required by Vision 2030 CFD applications, namely very large scale ( $0(10^{12})$  mesh points) parallel mesh generation, curved mesh elements for higher order methods,<sup>73,74</sup> highly scalable dynamic overset mesh technology,<sup>77,133</sup> and in-situ anisotropic adaptive methods for time-dependent problems. It is important to realize that advances in these areas will require a mix of investments in incremental software development, combined with advances in fundamental areas such as computational geometry, possibly with smaller components devoted to high risk disruptive ideas such as anisotropic cut-cell meshes,<sup>80</sup> strand mesh ideas,<sup>81</sup> and even meshless methods.<sup>82</sup> Additionally, because significant technology currently resides with commercial software vendors, particularly for CAD interfaces and access, involving these stakeholders in the appropriate focused research programs will be critical for long-term success. Innovative approaches for achieving such partnerships must be sought out, such as the formation of consortiums for the definition and adoption of standards or other potential issues such as large scale parallel licensing of commercial software. The technology development roadmap envisions the demonstration of tight CAD coupling and production adaptive mesh refinement (AMR) in the 2015-2017 time frame, followed by maturation of large-scale parallel mesh generation in the 2020-2025 time frame, and leading ultimately to fully automated in-situ mesh generation and adaptive control for large-scale time-dependent problems by 2030.

**Knowledge Extraction.** Petascale and exascale simulations will generate vast amounts of data and various government agencies such as the NSF and DOE have instituted major programs in data-driven simulation research.<sup>134,135</sup> In order to make effective use of large scale CFD and MDAO simulations in aerospace engineering, a thrust in data knowledge extraction should be initiated. Ideally, this should contain three components, a visualization component, a database management component, and a variable fidelity, data integration component. Methods to process and visualize very large-scale unsteady CFD simulations in real time, including results from higher-order discretizations, are required to support the advanced CFD capabilities envisioned in 2030. Although many of the current efforts in maturing visualization technology are being led by commercial vendors who continue to supply enhanced capabilities in this area, more fundamental research to directly embed visualization capabilities into production CFD tools optimized for emerging HPC platforms is needed to achieve real-time processing.<sup>99</sup> Moreover, the CFD capability in 2030 must provide the analyst with a more intuitive and natural interface into the flow solution to better understand complex flow physics and data trends and enable revolutionary capabilities such as computational steering, which could be used, as an example, for real-time virtual experiments or virtual flight simulation.<sup>136,137</sup> Foreseeing the capability of generating large databases with increasing computational power, techniques for rapidly integrating these

databases, querying them in real time, and enhancing them on demand will be required, along with the ability to provide reliable error estimates or confidence levels throughout all regions of the database.

Finally, integrating high fidelity simulation data with lower fidelity model data, as well as experimental data from wind tunnel tests, engine test rigs, or flight-test data will provide a powerful approach for reducing overall risk in aerospace system design.<sup>101</sup> Techniques for building large-scale flexible databases are in their infancy, and range from simple software infrastructures that manage large numbers of simulation jobs to more sophisticated reduced-order models,<sup>138</sup> surrogate models, and Kriging methods.<sup>102,103</sup> The objective of a research thrust in this area should be to apply existing techniques to current CFD simulation capabilities at a large scale, while simultaneously performing foundational research in the development of better reduced-order models and variable fidelity models that are applicable to aerospace problems and can support embedded uncertainty quantification strategies. The technology roadmap envisions the demonstration of real-time analysis and visualization of a notional  $10^{10}$ -point unsteady CFD simulation in 2020, and a  $10^{11}$ -point simulation in 2025. These technology demonstrations would be an integral part of the GC problems designed to benchmark advances in other CFD areas. The development of reduced-order models and other variable fidelity models will entail long-term research and will likely remain an active research topic past the 2030 time frame. However, the technology roadmap envisions the periodic assessment of the state-of-the-art in these areas at 5 to 10 year intervals, with investment directed toward demonstrating promising approaches on large-scale aerospace applications.

**Multidisciplinary Design and Optimization.** The ability to perform CFD-based multidisciplinary analysis (MDA) and analysis/optimization (MDO) relies on the availability of future capabilities that need to be developed between now and 2030. Pervasive and seamless MDAs (that can be routinely exercised in industrial practice for configuration studies, e.g., full aero-thermo-elastic/aeroacoustic simulations of entire airframe/propulsion systems including shielding) will require the development of accepted standards and APIs for disciplinary information and the required multidisciplinary couplings (such as with acoustics, combustion, structures, heat transfer, radiation). A concerted effort is envisioned that results in a set of standards available to the community around 2016. In parallel with this effort, it will also be necessary to develop high-fidelity coupling techniques that guarantee the accuracy and stability of high fidelity, tightly coupled MDAs,<sup>106</sup> while ensuring that the appropriate conservation principles are satisfied with errors below acceptable thresholds. This capability, together with the coupling software that includes such information transfers must be available around 2018. Together, the standards and the coupling techniques/software would enable demonstrations of two-way coupled MDAs with the best and most robust existing CFD

solvers of the time, and guaranteeing coupling fidelity by the year 2020. Such demonstrations can focus on multiple aerospace problems of interest, including aircraft aero-structural/aeroelastic analyses, aircraft aero-acoustics, rotorcraft aero-structural and aero-acoustic couplings, unsteady combustion, re-entry aerothermodynamics and material response, and the like. Initially, such routine MDAs would focus on portions of an entire vehicle (around 2020) and would transition to the treatment of the entire system around 2025. A number of capabilities also must be developed in order to enable MDO with and without the presence of uncertainties (robust and reliability-based design). A major research component that is likely to span a significant period (from 2015 to 2025) is the work needed to endow industrial-strength CFD solvers with both gradient calculation and uncertainty quantification capabilities for use in multidisciplinary optimization. Some of this work has been described in the “Numerical Algorithms” section. For the gradient/ sensitivity analysis capability, we envision that the CFD solver will be able to compute this information for full unsteady flows for the turbulence models available at the time. Finally, all these new capabilities must come together on a series of MDO grand-challenge demonstrations in the 2030 timeframe.

## 7 Recommendations

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In order to effectively execute the CFD development plan described above and achieve the goals laid out in the vision of CFD in 2030, a comprehensive research strategy and set of recommendations are presented. This research strategy calls for the renewed preeminence of NASA in the area of computational sciences and aerodynamics, and calls for *NASA to play a leading role in the pursuit of revolutionary simulation-based engineering.*

Aerospace engineering has had a long history of developing technology that impacts product development well beyond the boundaries of aerospace systems. As such, NASA is a critical force in driving technology throughout aerospace engineering directly by fulfilling its charter to “*preserve the role of the United States as a leader in aeronautical and space science technology.*”<sup>139</sup> Computational methods are a key example of this broad impact, as NASA has historically been a leader in the development of structural finite-element methods, computational fluid dynamics, and applications of HPC to engineering simulations. The criticality of engineering-based simulation to the competitiveness of the United States and the lack of sustained federal support have been highlighted previously by the NSF<sup>37</sup> and elsewhere.<sup>17,32</sup>

NASA’s effort must be targeted toward research and technology development that can make revolutionary impacts on simulation-based engineering in the aerospace sciences. In particular, the current state of CFD is such that small, incremental improvements in existing capability have not had

revolutionary effects. In an environment of constrained resources, this will require that NASA evaluate its activities with a critical eye toward supporting those efforts whose impact could be revolutionary.

To ensure that the technology plan and roadmap are as effective as possible, we propose specific recommendations in three broad areas: enhancement of the current Revolutionary Computational Aerosciences (RCA) program, important programmatic considerations, and key strategic initiatives that taken together will help achieve the goals of our vision of CFD in 2030.

## 7.1 Development of a Comprehensive Revolutionary Computational Aerosciences Program

**Recommendation 1:** *NASA should develop, fund and sustain a base research and technology (R&T) development program for simulation-based analysis and design technologies.*

Physics-based simulation is a crosscutting technology that impacts all of NASA aeronautics missions and vehicle classes, as evidenced by the common themes in the NAE Decadal survey report.<sup>12</sup> In addition, technologies developed within NASA's Aeronautics Research Mission Directorate impact many other aspects of the missions of various other NASA directorates. Yet, until recently, there has been no systematic program for developing simulation technologies, and all advances in simulation and CFD methods had to be justified by potential short-term impacts on one of the existing programs, or were done in response to critical simulation failures observed through the course of a program. This leads to the preference for small improvements to existing software, with the result that most current software is more than 20 years old, and the initiation of any new software project cannot be supported. Furthermore, investment in developing revolutionary simulation technologies is out of the question within such a program structure due to the long fruition time required and distant impact on existing programs. Yet without a focused base R&T development program, CFD will likely remain stagnant. Other international government agency aeronautic programs (such as DLR and ONERA) contain a base R&T component that is used to advance simulation technologies<sup>140,141</sup> and certainly the new NASA Revolutionary Computational Aerosciences (RCA) program is a step in the right direction. However, NASA must ensure this program is strengthened, maintained, and expanded to cover investment in the critical elements required for advancing CFD and other physics-based simulation technologies as outlined in our research roadmap.

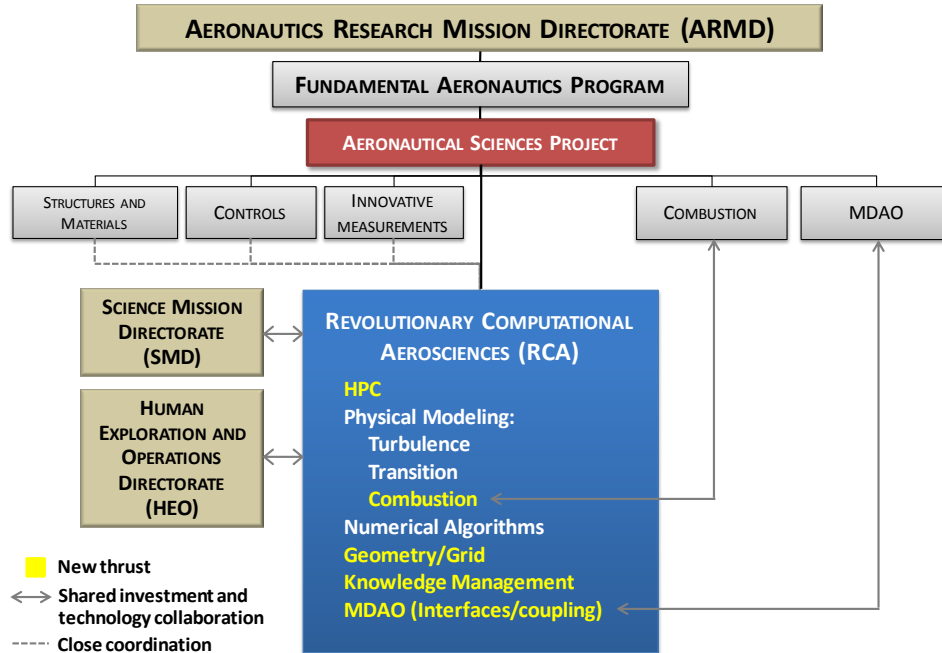
An integrated research plan is required for the fulfillment of the technology development roadmap and eventual demonstration of the GC problems. At present, the current RCA

program within the Aeronautical Sciences Project of the Fundamental Aeronautics Program (FAP) is too narrow in scope to address all the required technology areas in this report. Thus, we recommend broadening and enhancing the RCA program in several ways. The Aeronautical Sciences Project encompasses various subtopics including the RCA program, but also other areas such as materials, controls, combustion, innovative measurements, and MDAO.

We recommend that all components of subtopics focused on computational simulation technologies be coordinated with the RCA program. For example, numerical simulation of combustion is an important technology that would be ill served by being isolated from the developments achieved under the RCA program. Thus, we suggest joint oversight of the numerical modeling aspects of combustion between the RCA program and the combustion program. Similarly, significant components of MDAO related to solver technology and interfacing CFD with other disciplines will benefit from close interaction with the RCA program. Next, we recommend that the RCA program be structured around the six technology areas that we have outlined in this report, namely HPC, Physical Modeling, Numerical Algorithms, Geometry/Grid Generation, Knowledge Extraction, and MDAO. Currently, the RCA program contains technology thrust areas specifically in Numerical Algorithms and Turbulence modeling. Thus, the recommended structure represents a logical extension of the current program, achieved by extending the turbulence modeling technical area to a physical modeling technical area (i.e., adding transition modeling and combustion modeling), coordinating the relevant MDAO thrusts within the broader Aerosciences program, and adding the other required technology areas. Additionally, collaboration in computational methods between RCA and the Controls and the Structure and Materials programs should be encouraged, while CFD validation thrusts can be expected to benefit from collaboration with the Innovative Measurements program. This new programmatic structure is illustrated in Figure 2.

In the preceding section, each technical area is described in detail and the required research thrusts for advancing each area is provided. Naturally, individual research thrusts affect multiple technical areas, which in turn affect the ability to meet various milestones and progress toward the GC problems. However, for programmatic reasons it is desirable to have each individual research thrust reside within a single technology area. The success of this strategy relies on good communication and interaction between the different technology areas over the life of the program. A concise view of the proposed research program structure, including all technology areas and research thrusts is given in Figure 3.





**Figure 2. Proposed Enhanced Revolutionary Computational Sciences Program**

HPC	PHYSICAL MODELING	NUMERICAL ALGORITHMS
<ol style="list-style-type: none"> <li>Increasing access to leading-edge HPC hardware</li> <li>Porting of current and future codes to leading-edge HPC</li> <li>Radical emerging HPC technologies</li> </ol>	<ol style="list-style-type: none"> <li>RANS turbulence modeling</li> <li>Hybrid RANS-LES modeling               <ol style="list-style-type: none"> <li>Improved RANS component</li> <li>Seamless interface</li> </ol> </li> <li>LES (wall-modeled and wall-resolved)</li> <li>Transition</li> <li>Combustion</li> <li>Radically new modeling approaches</li> </ol>	<ol style="list-style-type: none"> <li>Advances in current algorithms for HPC</li> <li>Novel discretizations               <ol style="list-style-type: none"> <li>Higher-order methods</li> <li>Low dissipation/dispersion schemes</li> <li>Novel approaches (foundational)</li> </ol> </li> <li>Solvers               <ol style="list-style-type: none"> <li>Linear and non-linear scalable solvers</li> <li>Enhancements for MDAO and UQ</li> </ol> </li> <li>UQ               <ol style="list-style-type: none"> <li>Define aerospace uncertainties</li> <li>Leverage known techniques</li> <li>Improved error estimation techniques</li> <li>Statistical approaches</li> </ol> </li> </ol>
GEOMETRY AND GRID GENERATION	KNOWLEDGE MANAGEMENT	
<ol style="list-style-type: none"> <li>CAD access and interfaces</li> <li>Large scale parallel mesh generation</li> <li>Adaptive mesh refinement</li> <li>Curved mesh elements for higher-order methods</li> </ol>	<ol style="list-style-type: none"> <li>Visualization</li> <li>Data-base management</li> <li>Variable fidelity models</li> </ol>	
	MDAO	
	<ol style="list-style-type: none"> <li>Interfaces and standards</li> <li>Accurate and stable coupling techniques</li> <li>UQ support and sensitivities (system-level)</li> </ol>	

**Figure 3. Proposed New Revolutionary Computational Sciences (RCA) Program Structure**

The overall program goals are driven by the GC problems, which embody the vision of what CFD should be capable of achieving with balanced investment over the long term, and provide a means for maintaining program direction and measuring progress. While advances in all technology areas will be critical for achieving the GC problems, certain areas are described in less detail than others (e.g., knowledge ex-

traction, combustion, MDAO), and this is partly due to the focus on CFD technology in the current report. As can be seen, the proposed research program contains a balanced mix of near-term and long-term research thrusts. The overall program is also highly multidisciplinary and draws on advances in disciplines at the intersection of aerospace engineering, physics of fluids, applied mathematics, computational geom-

etry, computer science and statistics. Successful execution of the program will require devising appropriate mechanisms for leveraging expertise in these diverse fields. By its very nature, the formulation of a comprehensive research program of this type results in an exhaustive list of research thrusts that need to be addressed, and clearly prioritization of these individual thrusts must be performed within a limited budget environment. The prioritization of research thrusts and the prescription of funding levels must be an ongoing process and is certainly beyond the scope of this report. However, consistent mechanisms for making such decisions must be instituted. We propose the use of periodic workshops (e.g., at 5-year intervals) convened to measure progress toward the GC problems, that can be used to identify the most critical technologies in need of investment, evaluate the success of previous investments, and prioritize future investments.

## 7.2 Programmatic Considerations

**Recommendation 2:** *NASA should develop and maintain an integrated simulation and software development infrastructure to enable rapid CFD technology maturation.*

To reach the goals of CFD in 2030, research and technology development must effectively utilize and leverage in-house simulation expertise and capabilities with focused attention to HPC infrastructure, software development practices, interfaces, and standards.

### **Maintain a World-Class In-House Simulation Capability.**

To support broad advances in CFD technology, NASA's simulation capability should be, in many aspects, superior to the capabilities that reside with academic and industrial partners and in the commercial software vendor arena. NASA's in-house simulation code development is driven by the need to support NASA missions and must apply to all important application regimes of relevance to the NASA ARMD mission including fixed- and rotary-wing external aerodynamics, turbomachinery flows, combustion, aeroacoustics, and high speed flows, as well as applications of relevance to NASA's science and space exploration missions. While NASA has excelled in many of these areas (notably fixed- and rotary-wing external aerodynamics, and space vehicle entry, descent and landing [EDL]), there are other areas such as turbomachinery, combustion, and icing where it is believed that NASA's capabilities are no longer on the cutting edge. Maintaining an in-house capability is crucial for understanding the principal technical issues and overcoming impediments, for investigating new techniques in a realistic setting, for supporting NASA's own missions, and for engaging with other stakeholders. Whether technology transfer is ultimately achieved through the development of production level software that is adopted by industry, technology spin-offs to commercial software companies, or simply through realistic demonstrations on industrial problems with accompanying publications, has been the subject of much discussion for many years within NASA and the broader community, and

remains beyond the scope of this report. However, what is evident is that without such an internal competence, NASA will be severely handicapped in any attempts to advance the state of the art in physics-based simulation technologies. Additionally, this recommendation is targeted to a broader audience at NASA than simply ARMD: given the deep reliance on simulation-based engineering for all mission directorates and the fact that an agency-wide coordination mechanism exists, efforts to develop world-class, in-house simulation capabilities should be cooperatively pursued.

**Streamline and Improve Software Development Processes.** CFD software development at NASA has a checkered history. Many of the most successful codes in use today have their roots in the inspiration and the devotion of a single or small number of researchers. In some sense, this reflects one of the strengths of NASA's workforce and work environment that, in the past, accorded significant scientific freedom. However, despite their successes, many of these codes are still maintained by a small number of developers who struggle to keep up with the increasing demands of bug fixes, application support, and documentation that comes with increased usage.

Today, it is well recognized that software development must be a team effort due to increasingly complex software.<sup>41 43</sup> While some NASA software projects (such as FUN3D) have successfully transitioned to a team effort model,<sup>142</sup> there remains no formal structure for supporting software development issues such as regression testing, porting to emerging HPC architectures, interfacing with pre- and post-processing tools, general application support, and documentation. Most commercial software companies staff entire teams devoted to these types of activities, thus freeing the developers to pursue technology development and capability enhancements. CFD software efforts at DLR<sup>143,144</sup> and ONERA,<sup>145,146</sup> for instance, are known to provide continual support for dedicated software engineering tasks, while various US government projects such as the Department of Defense (DOD) Computational Research and Engineering Acquisition Tools and Environments – Air Vehicles (CREATE-AV) program have set up similar capabilities including an elaborate application support structure.<sup>60</sup> Furthermore, if individual NASA codes are to be applied to diverse areas such as external aerodynamics, internal turbomachinery flows, combustion, LES and aeroacoustics, support of this type will be essential since no single individual can cover such a wide range of disciplines. While there are continual cost pressures to reduce the number of CFD codes being supported, mandatory use of a single code for all applications is overly constraining and even unfeasible in many cases for new technology development, since newly developed algorithms may be ill-suited for retrofitting into existing codes due to their data structures and inherent assumptions. Thus, the creation of a formal software support structure could provide relief and continuity to developers of established production codes while also facilitating and lowering the development costs of potentially prom-

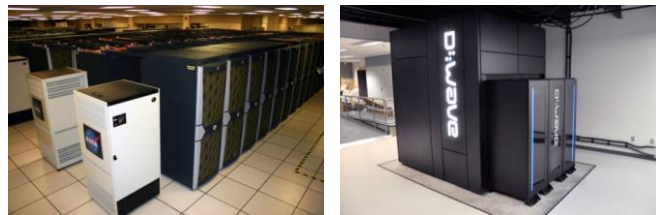
ising new software efforts designed either for research investigations or production CFD and MDAO. Moreover, this approach has the potential for cost savings due to reduction in duplication of efforts between individual software development projects. Ideally, these software components would be open-source and freely distributed within the United States and abroad. This would mark a significant departure from current NASA software practices, but could be achieved by isolating any sensitive capabilities in closed source software, as is regularly done at the US Department of Energy (DOE).

**Emphasize CFD standards and interfaces.** Many of the impediments outlined in this report relate to the difficulty in accessing or exchanging information between various software components, such as CAD data for grid generation; AMR, post-processing data; or exchange of information between different components of a multidisciplinary problem. In many cases, the development of standardized interfaces can be used to greatly relieve these problems and facilitate further advances in CFD. As a government agency, NASA is uniquely positioned to spearhead the development and adoption of international standards and interfaces in various areas of CFD and MDAO. In particular, this is an activity that may not require significant funding in dollar terms, but will require identifying and organizing key stakeholders, developing a consensus among them, and continuing the advocacy and support of developed standards and interfaces. At the same time, it is important to note that frameworks and standardization can lead to significant constraints and may not be the best solution in all cases. Thus, a large part of such an effort must involve determining under what conditions standardization is appropriate, and then developing sufficiently flexible standards and building a consensus among all stakeholders.

**Recommendation 3:** NASA should make available and utilize HPC systems for large-scale CFD development and testing.

Access to leading-edge HPC hardware is critical for devising and testing new techniques that enable more advanced simulations,<sup>39,41</sup> for demonstrating the impact that CFD technology enhancement can have on aerospace product development programs,<sup>11,45</sup> and for addressing the GC problems defined previously. As described in Case Study 1, NASA's HPC hardware is used primarily for throughput (capacity) computing rather than capability. Although hardware parallelism has increased dramatically during the last several decades, the average size of NASA CFD jobs remains well below 1,000 cores, even though the NASA Advanced Supercomputing (NAS) division flagship system contains over 160,000 CPU cores and is ranked 19<sup>th</sup> in the top 500 HPC installations worldwide.<sup>62</sup> Other large HPC installations regularly allocate significant fractions of their

resources toward enabling leading-edge petascale or higher simulation capabilities.<sup>45</sup> Lack of access to large-scale HPC hardware on a regular and sustainable basis within NASA has led to stagnating simulation capabilities. To remedy this situation, NASA, and in particular the NASA Advanced Supercomputing (NAS) division, should make HPC available for large-scale runs for CFD research and technology development. Use of HPC for large-scale problems will drive demand by enabling testing of more sophisticated algorithms at scale, making users more experienced and codes more scalable since many issues are only uncovered through large-scale testing. However, this approach is complicated by the fact that ARMD only controls a fraction of NASA's HPC resources. This will require advocating the benefits of large-scale computing within NASA, either for modifying the current HPC usage paradigm, or for sharing resources between NASA directorates (e.g., Science Mission Directorate, Human Exploration and Operations) with an interest in more radical simulation capabilities. NASA ARMD must also leverage other national HPC facilities and enter into a discussion with the NSF, DOE and any other agencies for providing access to these systems on a regular basis for NASA objectives that overlap with these agency priorities<sup>147,148</sup>. Furthermore, NASA should remain at the forefront in new HPC



technologies through the use of test platforms made available to the research community. The recently installed D-Wave Two quantum computer<sup>149</sup> at NASA Ames is a good example of this, but it does not appear to be part of a concerted effort to track and test HPC developments.

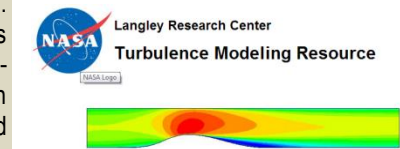
**Recommendation 4:** NASA should lead efforts to develop and execute integrated experimental testing and computational validation campaigns.

During the past decade, workshops to assess CFD predictive capabilities have been effective in focusing attention in key areas important to the aerospace community such as drag prediction,<sup>23</sup> high-lift prediction,<sup>56</sup> and aeroelasticity,<sup>85</sup> to name a few (see accompanying Case Study). In most cases, the workshops involve CFD simulation of challenging flow physics on realistic geometries. If available, experimental data is used to anchor the CFD predictions. However, with the exception of the Common Research Model (CRM) model development<sup>150</sup> and transonic test campaign,<sup>151</sup> workshops typically rely on pre-existing experimental datasets that often have an incomplete set of test data available, quality control issues, or a combination of both. Moreover, in many cases,

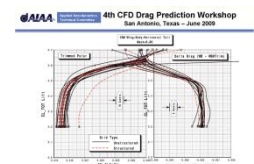
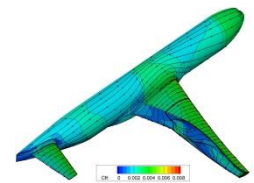
## CASE STUDY 5: Community Verification and Validation Resources

As numerical simulation capabilities become more complex, verification and validation (V&V) efforts become more important but also more difficult and time consuming. Verification is defined as the determination of whether a model is implemented correctly, whereas validation is defined as the determination of how well the model represents physical reality. One approach to reduce this burden and encourage higher V&V standards and usage is through the development of community resources for V&V. As a government agency, NASA is uniquely positioned to serve as the integrator and steward of such community resources.

An excellent example of community V&V resources can be found in the NASA Turbulence Modeling Resource web site.<sup>1</sup> The site is hosted by NASA, and the effort is guided by the Turbulence Model Benchmarking Working Group (TMBWG), a working group of the Fluid Dynamics Technical Committee of the AIAA, with contributions from NASA, academia, and industry. The objective of the site is to provide a central resource for turbulence model verification, which includes a precise definition of commonly used turbulence models including different model variants, and a set of verification test cases with supplied grids and sample results using different CFD codes, including grid convergence studies. By providing a sequence of progressively highly refined meshes, many of the verification test cases (principally in 2D) establish fully grid converged results for different CFD codes, providing a benchmark by which other codes can be measured to verify correct implementation of the model and consistency of the discretization. These are important prerequisites for applying implemented models to more complex cases with confidence. At present, the site provides descriptions for 11 turbulence models, and provides four verification test cases for which the most popular models have been tested with more than one CFD solver. The site also provides experimental data for a variety of 2D and 3D test cases in order to facilitate model validation.



During the last decade, the community workshop approach has emerged as a viable model for the validation of individual numerical simulation tools, as well as for the assessment of the entire state of the art in specific simulation capabilities. One of the original workshop series, the Drag Prediction Workshop (DPW), was initiated in 2001<sup>2</sup> and has since held five workshops.<sup>3</sup> The first workshop in 2001 was a grass-roots effort, which included substantial NASA participation, and focused mostly on comparison of CFD results for transport aircraft transonic cruise drag prediction, with secondary emphasis on comparison to available published experimental data. Over the years, the importance of high quality experimental data was increasingly recognized, leading to greater NASA involvement and investment, resulting in the design, fabrication and testing of the common research model (CRM), supported by NASA, including industry input, and conceived specifically for CFD validation purposes.<sup>4</sup> Throughout this period, the DPW series has firmly established the importance of discretization error as a dominant error source (often larger than turbulence modeling error) for accurate CFD prediction of aircraft forces and moments. The DPW series has emphasized the need for careful grid convergence studies, resulting in the establishment and documentation of best practices for grid generation and grid convergence studies. Each individual workshop has provided a contemporary evaluation of the state of the art in CFD force and moment prediction, while the entire workshop series has enabled the assessment of continual improvements in the state of the art over more than 10 years. Reduced workshop result scatter can be correlated with evolving methodologies, increased grid sizes, and advancing computational power. The workshop series has also served to clearly identify the successes and deficiencies of current RANS methods, with particular emphasis on the rapid degradation of RANS predictive capabilities with increasing amounts of flow separation. Finally, the workshop series resulted in a large database of publicly available geometries, grids, and CFD results against which new software development programs can benchmark for more effective V&V.



The success of the DPW has spawned other workshops in related areas, such as the High-Lift Prediction Workshop Series (HiLiftPW)<sup>5</sup> and the Aeroelastic Prediction Workshop (AePW).<sup>6</sup> A common feature of these workshop series, and other community V&V resources such as the NASA Turbulence modeling Resource web site, is that they combine the efforts of government, academia, and industry to promote advances in the state of the art, benefiting the community at large. However, in all cases, NASA involvement and investment has served as a key driver without which most of these endeavors would not be sustainable.

1 <http://turbmodels.larc.nasa.gov/>

2 Levy, D. W., Zickuhr, T., Vassberg, J., Agrawal, S., Walls, R. A., Pirzadeh, S., and Hensch, M. J., "Data Summary from First AIAA Computational Fluid Dynamics Drag Prediction Workshop," *AIAA Journal of Aircraft*, 2003, Vol.40.10.2514/1.1684

3 <http://aaac.larc.nasa.gov/tsab/cfdlarc/aiaa-dpw/>

4 Vassberg, J., Dehaan, M., Rivers, M., and Wahls, R. A., "Development of a Common Research Model for Applied CFD Validation Studies," 26th AIAA Applied Aerodynamics Conference, 2008, 10.2514/6.2008-6919

5 <http://hiliftpw.larc.nasa.gov/>

6 <https://c3.nasa.gov/dashlink/static/media/other/AEPW.htm>

the geometry definition of the tested configuration must be refurbished for CFD grid generation purposes. To help achieve the vision of CFD in 2030, an integrated approach involving well designed, ground-based (and perhaps flight<sup>152</sup>) experiments to provide high quality datasets directly coupled with CFD technology and application code verification and validation is required. This could be used in support of both CFD workshops, and the solution of GC problems, would help focus and solidify technology development in multiple areas, and establish best practices. Moreover, with physics-based computational modeling continuing to expand, the need for systematic numerical validation test datasets and an effective mechanism to disseminate the results of the validation results are becoming paramount. NASA has both a full range of experimental test facilities in which to collect high-quality data, as well as the computational tools and processes in which to benchmark CFD capabilities. For this reason, NASA should pursue a leadership role in developing complementary experimental and computational datasets to help guide CFD technology development.

### 7.3 Strategic Considerations

***Recommendation 5:** NASA should develop, foster, and leverage improved collaborations with key research partners and industrial stakeholders across disciplines within the broader scientific and engineering communities.*

**Leverage other government agencies and stakeholders (US and foreign) outside of the aerospace field.** Currently, NASA ARMD's interaction with other government entities is almost exclusively focused on agencies that have a major stake in the national aeronautics enterprise such as the Federal Aviation Administration (FAA), United States Air Force (USAF), and others. However, in the last decade, computational science has had important visibility at the national level, through various competitiveness thrusts,<sup>17,32</sup> and has become an important focus for various agencies such as the DOE, NSF and the National Institute of Standards and Technology (NIST).<sup>153</sup> Therefore, it is natural for NASA ARMD, which performs the bulk of the R&T in computational science for the agency, to seek out and establish meaningful collaborations with these traditionally non-aerospace focused agencies. However, such collaborations have been sorely lacking. For example, various multi-agency studies and white papers are frequently published on the topic of exascale computing,<sup>41,42,108</sup> but surprisingly NASA has not been a participant in these multiagency discussions. With its limited budget, and dim prospects for improved research budgets, NASA ARMD cannot afford to "go it alone" and hope to make substantial progress in the important areas of computational science and simulation technology that are so important to advancing the agency's mission in various directorates. Creative strategies must be devised to leverage funding and resources with other stakeholders with similar objectives, because the current approach has been shown to pro-

duce a stagnating capability in the environment of shrinking budgets during the last decade. These creative strategies can involve a wide range of partners from different directorates within the agency, such as Space Exploration and Science, to other agencies such as NSF and DOE, and in terms of hardware, software, and research results. As an example, the lack of access to HPC for NASA researchers could be addressed through a potential collaboration with DOE to obtain guaranteed slices of time on their leadership class machines through a formal program that could be negotiated at an interagency level, for example through the Networking and Information Technology Research and Development (NITRD) Program.<sup>147,148</sup> In addition, many of the DOE- and DOD-sponsored advances in HPC were derived from investments in fundamental research that could be effectively leveraged by more direct NASA participation in the setup, running, and partial sponsoring of these efforts. Finally, Memorandums Of Understanding (MOUs) and other vehicles for interacting with foreign government agencies should be considered whenever possible.

**Improve collaboration with industry.** NASA has been at the forefront of CFD technology for decades and was responsible for introducing much of the CFD technology used in industry today. At the same time, in collaboration with universities, industry has addressed additional CFD technology needs that are unique and essential to their business success. These include increased emphasis in the areas of physics-based modeling, rapid complex geometry and grid capabilities, managing the generation of CFD-based aerodynamic design matrices, improving accuracy and robustness, and integrating CFD databases with experimental data and other disciplines. The result has been a substantial reduction in physical testing but not uniformly across all products or flow regimes. Continued advances are required to address full-flight envelope predictions and propulsion system operating conditions, reduce design cost and cycle time, reduce ground and flight-testing, and enable product certification through analysis. Accelerated maturation of CFD technologies for all aerospace applications (e.g., external aerodynamics, turbomachinery, space) could be better achieved with expanded three-way collaboration between industry, NASA, and academia, beyond the current collaborations in physical testing at NASA facilities and research through NASA Research Announcements (NRAs). While industry is in a unique position to provide requirements and assess the value and impact of various CFD technologies on the aerospace industry, NASA is best positioned to coordinate and advance CFD technologies required for maintaining competitiveness and leadership. As mentioned above, many of these technologies require substantial advances in physical modeling (e.g., turbulence, transition, and combustion) and numerics (e.g., stability, accuracy, uncertainty quantification, gradient estimation, adjoint methods). These are traditional NASA strengths and should be re-emphasized. Further, NASA is also in a unique position to coordinate the definition of standards for

data, codes, and databases that would enable more rapid generation of next generation tools, and interfaces to industrial scale CFD applications. Similarly, critical areas that have mostly been left to industry (e.g., complex geometry representations, grid generation and 3D visualization) could also benefit from a renewed focus by NASA, perhaps in a closer partnership with both the aerospace industry and other industries that are similarly challenged, such as the automotive industry. Finally, we advocate the creation of a NASA-Industry Computational Science (CS) leadership team, which will be tasked with the mission of identifying joint CS projects oriented toward addressing the four GC problems presented in Section 6. We believe that projects with 3-year cycles accompanied by gate reviews from independent parties would facilitate and ensure maturation and transition of relevant technology to industry.

**Emphasize basic funding in applied math and computer science.** In order to advance the state-of-the-art of CFD, advances must also be sought in related disciplines such as applied mathematics and computer science. We have referred to

these throughout the report, invoking such areas as computational geometry for grid generation, applied mathematics for linear and nonlinear solver development, and computer science issues related to HPC. The specific areas of CFD, as well as the broader area of MDAO, are components of the general field of computational science. CFD lies at the intersection of applied math, computer science, and an application science area (in this case, aerodynamics), or more broadly, aerospace engineering.<sup>1,39</sup> It is notable that at other government agencies, such as the NSF, a significant portion of funding for computational fluid dynamics comes from the mathematical and physical sciences program, while numerical solver groups at various DOE labs are staffed largely by scientists with degrees in applied math and/or computer science. The aerospace CFD and MDAO community is notoriously insular, with most researchers having an aerospace engineering background, publishing in AIAA or similar venues, and with scant presence in regular computational science meetings hosted by the Society for Industrial and Applied Mathematics (SIAM), the Institute of Electrical and Electronics

## CASE STUDY 6: Sponsored Research Institutes

Currently NASA relies on a mix of internal development and external funding with academic and industrial partners through NASA Research Announcements (NRA) to advance its research goals. However, additional mechanisms must be sought to more fully engage the broader scientific community especially for computational science problems, which are both crosscutting and multidisciplinary. Sponsored research institutes have been used in many areas of science and engineering to further such goals. These institutes can take on various forms and funding models, ranging from fully self-supporting autonomous institutes such as the Southwest Research Institute (SWRI),<sup>1</sup> university-based institutes, multi-stakeholder institutes, and government-agency based institutes. The nature, size, and funding model of these institutes must be considered based on the objectives of the sponsoring agency or stakeholders.

The objective of a computational science based institute for NASA aeronautics would be to provide a centralized focal point for the development of crosscutting disciplines, to engage the broader scientific community, and to execute a long-term research strategy with sufficient autonomy to be free of NASA mission directorate short-term concerns. Under these conditions, the self-supporting research institute model such as SWRI is not appropriate due to the short-term pressures to continually raise research funding, and the difficulties in maintaining agency-related focus, given the diverse and changing composition of a competitively funded research portfolio. University-based institutes have been used successfully by a variety of funding agencies, and are the preferred mechanism for agencies with no internal facilities of their own, such as the National Science Foundation (NSF). During the last two decades, the NSF has set up a number of High Performance Computing (HPC) centers at universities across the United States, as well as various scientific institutes such as the Institute for Mathematics and its Applications (IMA) at the University of Minnesota.<sup>2</sup> Mission agencies such as the DOE and NASA have also followed this model occasionally, for example through support for the previous DOE ASCI centers, NASA's previous support of the CTR at Stanford University,<sup>3</sup> and current DOE support for the PSAAP centers.<sup>4</sup> Although many of these institutes have been highly successful, such a model may not be optimal for the considered objectives, since focused investment at specific universities is not an ideal mechanism for engaging the broader community, while at the same time geographical separation between sponsor and university can be a detriment to collaboration.

A number of multi-stakeholder and agency co-located research institutes with aerospace-focused computational science objectives were used with generally favorable outcomes. CERFACS,<sup>5</sup> located in Toulouse, France, is a research organization that aims to develop advanced methods for the numerical simulation of a wide range of large scientific and technological problems. CERFACS is organized as a private entity with shareholders, which include government agencies ONERA, CNES, Meteo France, and corporate sponsors EADS, SAFRAN, TOTAL, and Electricite de France (EDF). The shareholders fund the majority of research performed at CERFACS and, as a result, jointly own research results and intellectual property. The institute employs approximately 150 people, of which 130 are technical staff including physicists, applied mathematicians, numerical analysts, and software engineers. The institute is organized around inter-



disciplinary teams that focus on the core fundamental area of numerical methods for parallel computing, combined with more applied focus areas in aerodynamics, gas turbines, combustion, climate, environmental impact, data assimilation, electromagnetism and acoustics and multidisciplinary code coupling. The CERFACS model is interesting because it brings together common computational science problems from different areas such as aeronautics, space, weather/climate modeling, and combustion, and includes combined government-industrial sponsorship.

The C<sup>2</sup>A<sup>2</sup>S<sup>2</sup>E institute<sup>6</sup> at DLR in Braunschweig Germany provides a model that is more focused on the development of computational science for specific aeronautics applications. The institute is jointly funded by DLR, Airbus, and the German State of Lower Saxony (Niedersachsen). The objective of the institute is to be an “interdisciplinary center of excellence in numerical aircraft simulations.” The institute was conceived as a major new aerospace simulation center under the DLR Institute of Aerodynamics and Flow Technology in Braunschweig, with the objective of providing a campus-like environment that brings together world-renowned experts and guest scientists to stimulate top-level research in the field of numerical simulation. Another function of the institute is to provide high-end computer simulation and visualization hardware and capabilities. C<sup>2</sup>A<sup>2</sup>S<sup>2</sup>E employs approximately 50 technical staff with expertise in applied mathematics, computer science, and aerospace engineering.

In past years, NASA has used field-center co-located institutes such as ICASE at NASA Langley, ICOMP at NASA Glenn, and RIACS at NASA Ames as vehicles for long-term research and to better engage the broader scientific community. Arguably, the most successful of these was ICASE, which was created in 1972 and was supported for 30 years. The goal of ICASE was to perform long-term research in computational science and broadly related fields that was relevant to NASA’s aeronautics mission. The institute was rather small, with an average fluctuating total of 30 people of which approximately 25 were researchers, and with a robust visitor program of 50 to 70 people per year. Institute funding consisted of a mix of long-term core and short-term task funding from NASA, in approximately a 60/40 ratio, with a total budget of about \$2M in the 1990s. While task funding was obtained directly from the supporting NASA center (Langley), experience had shown that it was important for the core funding to be obtained from NASA Headquarters directly, in order to shield the institute from the shorter term pressures and objectives of the supporting NASA center. A key to success was to be aware of long-term NASA goals, but also to acquire in-depth knowledge of broader interdisciplinary research performed at other research centers and universities both within the United States and internationally. A central purpose of the visitor program was to keep abreast of emergent technologies that the institute should be investing in to meet NASA’s long-term needs. Although shorter term in nature, task funding provided critical mass for the institute, lowering administrative costs, while at the same time tying the institute more closely to the needs of the NASA center, and thus enabling a better long-term vision. However, pressure to grow the institute through increased task funding needed to be resisted for the institute to retain its long-term focus. The institute was structured as a private nonprofit entity, managed by an outside umbrella organization.

The above examples illustrate how differently structured research institutes can be used to achieve multidisciplinary and longer term research goals. In most cases, it is not the direct level of funding that determines the success of the institute; rather, it is the establishment of a structure that enables engagement of the broader scientific community and provides a long-term focus aligned with the sponsoring agency or stakeholder goals, while shielding the institute from shorter term pressures and objectives.

1 <http://www.swri.org/>

2 <http://www.ima.umn.edu/>

3 <http://nnsa.energy.gov/aboutus/ourprograms/defenseprograms/futurescienceandtechnologyprograms/asc/univpartnerships/psaap>

4 <http://ctr.stanford.edu/>

5 <http://www.cerfacs.fr/>

6 [http://www.dlr.de/as/en/desktopdefault.aspx/tabid-4083/6455\\_read-9239/](http://www.dlr.de/as/en/desktopdefault.aspx/tabid-4083/6455_read-9239/)

Engineers (IEEE), and the Association for Computing Machinery (ACM). This trend can be noted as well in the various survey reports compiled for the national aerospace enterprise, such as the NAE decadal surveys<sup>12</sup> and the National Aerospace R&D plans,<sup>13</sup> which repeatedly refer to specific aerospace capabilities that must be developed through numerical simulation, without acknowledging the role developments in other related fundamental disciplines play in meeting these objectives. This should be contrasted with numerous reports issued by the DOE and NSF and other computational science-based studies that emphasize the needed investment in areas at the intersection of applied math, computational science and application science disciplines.<sup>16,18,37,106</sup> An essential component for advancing state-of-the-art CFD will require that the research portfolio be expanded beyond pure aeronautics and fluid mechanics disci-

plines into these related fundamental areas. However, given its limited budget, NASA ARMD can ill afford to start new programs in these areas. Rather, the course of action should focus on specific areas with potentially high payoff that are unique to the NASA mission, as well as increased leveraging of ongoing activities within other government programs in the United States and abroad. At a minimum, NASA should establish a presence at the important computational science meetings hosted by SIAM, IEEE, and ACM to keep abreast of developments in these areas.

**Develop and foster collaborations with other disciplines through the creation of research institutes.** As mentioned above, investments in applied math and computer science will be critical for achieving specific advances in CFD. Likewise, advances in MDAO will require investments in

key disciplines outside of traditional aerodynamics. However, the current makeup of NASA and the broader aerospace community is such that it will be difficult to obtain the required multidisciplinary expertise from within. Furthermore, it will likely be difficult to ensure relevance of investments in these more distantly related fields for maximum impact in aeronautics.

In general, NASA relies on a mix of internal development and external funding of academia and industry through NASA Research Announcements (NRAs). However, other mechanisms are needed to engage scientists in other related disciplines. In the past, NASA relied on semi-academic institutes such as the Institute for Computer Applications in Science and Engineering (ICASE), the Institute for Computational Mechanics in Propulsion (ICOMP), the Research Institute for Advanced Computer Science (RIACS) set up at various NASA centers, and the Center for Turbulence Research (CTR) at Stanford University, to foster collaboration in specific, related disciplines and to engage the broader national and international scientific community in problems of relevance to the NASA aeronautics mission. During the last decade, larger institutes such as the National Institute of Aerospace (NIA) and the Ohio Aerospace Institute (OAI) were created and absorbed some of these functions. However, these institutes, which serve many purposes, are not devoted to specifically advance computational science issues and were not conceived to focus principally on NASA's longer term requirements, (although they could be modified to include such aspects). It is noteworthy that the small, semi-academic institute model has been replicated at various other US national labs, such as the Center for Nonlinear Studies (CNLS) at Los Alamos National Laboratory (LANL) and the Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory (LLNL), as well as in Europe at the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) in France and the Center for Computer Applications in AeroSpace Science and Engineering (C<sup>2</sup>A<sup>2</sup>S<sup>2</sup>E) in Germany, with great success. Indeed, some of these centers include industrial funding in their model, further tying the institute to important stakeholders. One of the keys to the success of these institutes is that they are able to establish a facility and create a climate that fosters collaborations among government researchers and leading academics with the goal of advancing computational science and modeling of physics. The freedom that is afforded to the researchers while aligning broadly with the mission of the organization serves as a magnet for attracting the best talent from around the world, while ensuring relevance of the research. NASA should re-examine the role such institutes have played in the overall long-term success of computational methods within the agency and develop a new initiative to create an institute devoted to the advancement of both CFD and MDAO for NASA aeronautics, science, and space exploration mission directorate problems (see accompanying Case Study). The goal of the institute

would be to broaden NASA interactions with the wider scientific community and to foster long-term collaborations with experts in important complementary fields. To be effective, the institute will require critical mass, sustained core funding over the long term, and the development of a reputation for excellence. One approach to building up this facility would be to start with seed funding for a sustained summer visitor program that would grow in size over several years, and which can be complemented with a small group of internal researchers or longer term visitors.

**Recommendation 6:** *NASA should attract world-class engineers and scientists.*

The ability to achieve the long-term goals for CFD in 2030 is greatly dependent on having a team of highly educated and effective engineers and scientists devoted to the advancement of computational sciences. This is particularly critical within NASA given the demographics of the current workforce.

Opportunities to stabilize and expand CFD and simulation personnel in the future should be pursued to enable a renewed leadership role in CFD development including researchers and developers with diverse backgrounds (physical modeling, numerical algorithms, applied mathematics, computer science, software development, and various aerospace engineering application domains). Attracting this future generation of leaders will present challenges. To be successful, several suggestions are presented here. NASA currently has several fellowship programs in key areas throughout the agency, but none are specifically devoted to computational science. A NASA-focused fellowship program similar to the Department of Energy's Computational Science Graduate Fellowship (DOE-CSGF)<sup>154</sup> should be considered. In addition, having opportunities for longer term visits (e.g., summer or other) for students will also be important to continually attract the best aerospace talent: this is best achieved through formal visit programs with specific computational-science goals, managed either directly through NASA or through supported research institutes. Finally, attempts to capture future generations of computational engineers and scientists can benefit from providing visiting students with the opportunity to meaningfully contribute to grand-challenge efforts that capture their imagination and are closely aligned with their values (environmental impact of commercial aviation, personal air vehicle, larger degrees of autonomy/UASs, and the sizable interest in high-speed vehicles including supersonics, hypersonics, and re-entry).





## 8 Conclusions

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Despite considerable past success, today there is a general feeling that CFD development for single and multidisciplinary aerospace engineering problems has been stagnant for some time, caught between rapidly changing HPC hardware, the inability to predict adequately complex separated turbulent flows, and the difficulties incurred with increasingly complex software driven by complex geometry and increasing demands for multidisciplinary simulations. In this report, we have provided a knowledge-based vision of what future CFD capabilities could be, and indeed must be, in order to radically advance the aerospace design process and enable a new generation of more capable aerospace vehicles. This vision was used to identify important barriers and impediments, which in turn were used to formulate a long-term technology development plan. These findings were obtained with broad community input, including a formal survey, a community workshop, as well as through numerous informal interactions with subject matter experts. This information was distilled into a programmatic structure and a set of recommendations that are expected to be important for advancing the state-of-the-art CFD in particular and multidisciplinary simulations in general, while also achieving the Vision. Although some outcomes of this study point to specific technological solutions, many recommendations are simple and self-evident: robust support for basic simulation technologies, better access to leading-edge HPC hardware, better internal collaborations between aeronautics and space drivers, better coordination with other large computational science programs, and the need for innovative strategies to advance the research agenda in a resource-constrained environment.

Many current large government agency programs in computational science can trace their roots to reports that originated from communities of experts, from the grassroots upwards, often based on input from community workshops, commissions, or private and public panels and testimonies. We have followed such a model in this work, with the realization that many such endeavors are not successful on their first attempt, but often require years of gestation. However, the broad community input, general consensus, and wide range of expert opinions coupled with a diverse experience base from academia, government, and industry that have contributed to this report make it a significant advocacy document. To ultimately be successful, periodic reviews of CFD technology development like this must be undertaken to continually drive the state of the art forward.

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# APPENDIX A. High Performance Computing Trends and Forecast for 2030

## Introduction

Computational Fluid Dynamics (CFD) codes utilize High Performance Computing (HPC) systems, so understanding where HPC technology might be in the 2030 timeframe is an important component of creating a vision for CFD codes in 2030. Of course, forecasting where HPC technologies will be in the future requires a significant amount of extrapolation, which is especially hard in such a fast changing area as HPC. The fastest current systems can perform more than 10 petaFLOPS (1 petaFLOPS is  $10^{15}$  floating point operations per second) and the HPC community is working toward systems capable of  $10^{18}$  FLOPS (exaFLOPS), which are expected sometime between 2018 and 2023. Some work is even looking at  $10^{21}$  FLOPS (zetaFLOPS). However, reaching that level of performance is unlikely without radically new technologies.

A common, though controversial, measure of HPC systems is the total number of floating point operations a given system can perform in a second while solving a large linear system of equations using Gaussian elimination; this is the HP LINPACK benchmark. Twice a year a list of the top 500 systems in the world against which those numbers are measured is published by the Top500 organization. The current list (June 2013) is topped by the Tianhe-2 system, developed by China's National University of Defense Technologies, which achieved 33.86 petaFLOPS (quadrillions of calculations per second) on the LINPACK benchmark [Top500.org]. Here, we will estimate only the peak floating-point performance in terms of the maximum number of operations that can be performed per second. We note that the performance of many applications, including CFD applications, may be more accurately estimated by using sustained memory bandwidth,<sup>1</sup> for the purposes of this summary, we assume that other aspects of system performance, such as memory latency and bandwidth and integer operation performance, are provided in a similar ratio to today's systems. This is a significant assumption and should be borne in mind when considering the predictions outlined in this summary.

A significant measure of a processor is the feature size of its components. The smaller the features, the more elements can be placed in the same area, and hence the more powerful a processor becomes. Feature size also has a direct

impact on power consumption, and heat generation, with smaller sizes being better. Thus, forecasting feature sizes of future processors is very important. Unfortunately, the industry has not always been good in that forecasting, which is one reason why predicting where HPC technology will be in 2030 is particularly hard. For example, in 2005, the International Technology Roadmap for Semiconductors (ITRS) forecasted a 22-nm gate length by 2008; that is, the structures in a modern processor were forecast to have features with sizes around 22 nm. However, in 2008 the forecast date moved to 2011 and in 2011, it moved again to 2012. A similar slip occurred for other (smaller) gate lengths (see Figure 4). Note that the forecasts of the ITRS combine inputs from all major chip manufacturers, equipment suppliers, and research communities and consortia, so it represents the combined wisdom of the industry. Nevertheless, as Figure 4 shows, forecasting a key feature of even this basic component of processors is hard. The figure points out that Moore's "Law" is really just an observation about engineering progress and offers no guarantee. There are serious concerns about the longevity of this law, especially when trying to extrapolate to 2030.

To come to our final predictions of a HPC system in 2030 we go through a two-step process. We start with a prediction about a practical exascale system, likely in the 2020-2023 time frame. To help with the forecasting, we incorporate some thoughts about the predictions made for a petascale system around 2000, and how they panned out. In the second step, we further extrapolate from this base to 2030.

To help create a vision for a CFD Code in 2030, it is important to describe three different classes of HPC systems

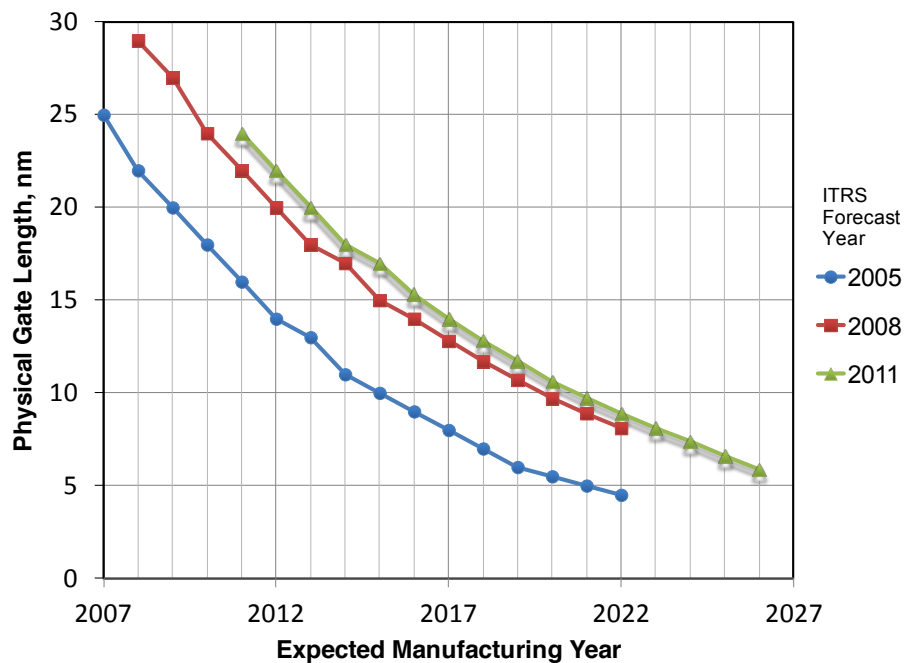


Figure 4. Changing Predictions About Semiconductor Sizes

that are of importance for the CFD community. First are the leadership class systems that reside at National Laboratories or other government agencies, such as NASA. These will be used to solve the hardest, most challenging problems that break new ground and drive basic understanding about flow phenomena and how to simulate them. The second class of systems is the type of systems large industrial companies like Boeing, Pratt & Whitney, or Airbus use. These are in general one to two orders of magnitude smaller than the leadership class systems. For example, Airbus entered a system at number 29 in the June 2011 Top500 list, with a capability about 33 times smaller than the number one system on that list. Finally, the third class of systems consists of HPC systems that would be used by smaller companies, or individual departments of larger companies. These are again one to two orders of magnitude smaller than the systems in the second class.

It is likely that similar technologies will be used by all of these classes of systems, with the performance scaling roughly with the size (number of nodes) of the system. The reason that the performance is not strictly proportional to system size is that the performance of the interconnect that ties all of the computing elements together does not scale with the size of the system, requiring either more advanced technologies at larger scale or providing lower overall performance at scale.

Another critical component of HPC capability in 2030 is the advances in software infrastructure and programming methodologies that will be necessary to take advantage of these future HPC systems. The ultimate purpose for these systems is to solve the most pressing problems in academia and industry. In particular, industrial users pursue this technology because of the large impact on future product designs, and the ability to avoid or minimize the use of other, more costly methods such as wind tunnels or other types of physical tests.

### ***Petascale Predictions and What Happened***

Here we consider the predictions that were made in the 1990s about the first petascale systems: which of them proved true and which of them proved false.

The following statements are from “Enabling Technologies for PetaFLOPS Computing” (1995):

1. “The software for the current generation of 100 GF machines is not adequate to be scaled to a TF...”
2. “The petaFLOPS computer is achievable at reasonable cost with technology available in about 20 years [2014].”
3. “Software technology for [Massively Parallel Processors] MPP’s must evolve new ways to design software that is portable across a wide variety of computer architectures. Only then can the small but important MPP sector of the computer hardware market leverage the massive investment that is being applied to commercial software for the business and commodity computer market.”

4. “To address the inadequate state of software productivity, there is a need to develop language systems able to integrate software components that use different paradigms and language dialects.”

Of these predictions, only number 2, a statement about computer hardware, proved true, as systems with a peak performance of a petaFLOP were delivered in 2008 and achieved sustained performance in 2012.<sup>2</sup> It is notable that in 1995, it was predicted that the clock speed of a processor would be 700MHz—well under what was achieved by commodity processors, but exactly the speed of the processors in the IBM BlueGene/L system—a clock speed chosen as the optimal one for performance at a given power. Also notable is that programming for a petascale system was expected to need new approaches, with nine overlapping programming models, including shared memory, message passing, data parallel, distributed shared memory, functional programming, object-oriented programming, and evolution of existing languages, considered essential.

Observe that while the predictions about hardware were reasonable, those about software (1, 3, and 4) were not supported by quantitative data and turned out to be far too pessimistic. This is not to say that there is not a software productivity problem, but that it has not prevented the use of petascale systems, several of which are now in operation and are successfully performing computations in science and engineering. Given this experience, great care must be taken in making assumptions about what software might work (if not easily) and what is truly inadequate for exascale systems and beyond.

### ***Exascale Background***

An exascale system is one capable of  $10^{18}$  operations per second, roughly 100 times as fast as the most powerful systems today. Several factors suggest that an exascale system will not just be a simple evolution of today’s petascale systems:

1. *Clock rates.* Clock rates for commodity logic have plateaued, in large part because of leakage currents. This implies that increasing performance will be tied to increasing parallelism, as has been true since about 2006. It is unlikely that a new technology will be available by 2023 to provide an alternative with faster clock rates. Rapid Single Flux Quantum (RSFQ), a technology using superconducting devices, could provide 250GHz gates, but bringing that technology to sufficient maturity, including density and cost, is unlikely within 10 years. With a sustained investment, it might be available by 2030, but we still view this as unlikely to be a mature technology by 2030.
2. *Power consumption.* Current petascale systems are consuming on the order of 10-20 megawatts (about 1 MW/PF), so scaling current technology would require 1 gigawatt for an exascale system (announced targets are

between 20 and 60 MW for an exascale system). Contributors to power consumption include:

- a. Processor Speed – slower processors are more power efficient (to a point); this implies even greater concurrency to reach a given level of performance. Processors may be in the 1 to 20 GHz range, with the most likely range being 1 to 5 GHz.
  - b. Complex computing elements—features used to improve scalar performance, such as speculation, caches, and out-of-order execution—all have low power efficiency for the compute benefit they deliver. Processing elements are likely to be simpler and optimized for particular computing patterns. For example, there may be separate scalar, vector, and stream computing elements. GPUs already exploit the advantages of being specialized.
  - c. Memory, based on the current DRAM architecture, consumes a surprising amount of power. As a result (and combined with the need for increased parallelism), there is likely to be both much less memory per processing element and much less memory total; for example, an exascale system may have only 10 PB of memory.
  - d. Moving data anywhere takes power, even within a “node” (e.g., between local memory and the nearest processing units). This will argue for much greater data locality in the choice of algorithms and their implementation.
3. *Fault tolerance and resiliency.* This is a tricky subject and there is a great deal of misinformation about it. A common analysis is to take the failure rates of today’s systems (particularly commodity cluster systems) and extrapolate to a system built with the same parts but 100 to 1,000 times as large, based on the number of processing elements expected in an exascale system. However, failure rates are more dependent on the number of parts (e.g., chips), not gates, and experience with some of the largest systems, such as the IBM Blue Gene systems, bears this out. Parts intended for the commodity market may accept higher rates of faults than what is acceptable for a large-scale, reliable exascale system. Having said that, there are reasons why an exascale system may have a higher rate of faults. For example, some techniques being proposed to reduce power consumption may raise the rate of failures.
4. *Performance regularity and scalability.* Because of the extreme degree of parallelism required, scalability will be a major issue. Approaches that work with 1,000 or even 10,000 nodes may fail to perform well on an exascale system. In addition, several approaches under consideration suggest that the performance of the compute elements may be less predictable than it is now (e.g., using dynamic frequency adjustment to improve power efficiency). As a result, algorithms will not be able to decompose work based on any assumption about

uniform performance or work. Adaptivity will be required in the algorithms and implementations.

5. *Latency tolerance.* References to all memory, both local and remote, will take 100s to 10,000s of cycles. For remote references, much of this is speed-of-light delays, and can only be solved by making the entire machine physically smaller, which is unlikely in the next 10 years. For more local references, this is a result of the memory hardware. Most novel memory techniques that may increase available memory size and/or reduce power consumption, also increase the latency for memory accesses. In fact, latencies of hundreds of cycles are common today in microprocessors, but much of this is hidden from the programmer through the use of memory caches and prefetch hardware.

### *Sample Exascale Architecture*

An exascale computer might look something like this:

Each node contains 16 1-GHz simple scalar processors, each with an integrated, 1,000 core streaming processor (also 1 GHz). At the memory interface is another 1,000 core streaming processors (but with more limited operations, also at 1 GHz). This gives 128 TFLOPS per node (assuming fused multiply-adds, 2 per cycle). 10,000 of these nodes bring you to 1 exaFLOPS. The interconnect may be a combination of electrical and optical (chosen to provide power-efficient bandwidth) using high-radix routers, similar to what is used in the Blue Waters Supercomputer at NCSA. It may also be a 3D torus (between the nodes), but allowing each link to be used concurrently, as in the IBM Blue Gene/P systems.

Note the reliance on “stream” processing; you can think of this as a distributed memory vector processor, where virtually all of the work must be suitable for the vector/stream processing elements (those 1,000-core components). Today’s graphics processing units, as well as Intel’s Xeon Phi (MIC) chips, can be considered examples of stream processors.

Bisection bandwidth relative to peak performance is likely to be much smaller than in today’s systems. However, there may be support for some critical global operations, such as a nonblocking allreduce or nonblocking barriers. These global operations might be underappreciated, but might be particularly useful for special cases, for example for distributed termination detection.

Other systems will have a different balance, for example, more scalar (or short vector) compute units, more nodes but with less parallelism per node. Operation mixes may be different, e.g., more support for integer operations at the expense of floating point, or specialized integer units. (Such a different approach is shown in Table 1 in the prediction for an exascale system in 2023). However, it is very unlikely that an exascale system would look much like an IBM Blue Gene, Cray XE/XK, or IBM Productive, Easy-to-use, Reliable Computing System (PERCS), which is officially known as Power 775.<sup>3</sup> From a functional standpoint, an exascale sys-

tem is likely to have heterogeneous functional elements, each optimized to different styles of computing. The closest current systems are GPU clusters, such as RoadRunner at Los Alamos National Laboratory with IBM PowerXCell accelerators, Titan at Oak Ridge National Laboratory with NVIDIA GPUs, or Stampede at the Texas Advanced Computing Center with Intel Xeon Phi (MIC) coprocessors. However, an exascale system will be much more tightly integrated; it will not have accelerators and coprocessors as loosely connected to the rest of the system, as is the case in current offerings. An all-accelerator/coprocessor-like system is possible but unlikely (consider the above sample system, but with no scalar processors). Exascale systems may well have CPU-like and accelerator/coprocessor-like elements on the same chip as described in the first paragraph.

### ***Programming in Exascale***

Programming languages take many years to develop. It is very unlikely that a new programming model will be developed in time for the first exascale systems. What is possible and even likely is that higher-level, special-purpose languages will be developed to help write efficient code for these systems. Applications will be a mix of current programming models (C/C++/Fortran), combined with Message Passing Interface (MPI) and OpenMP, possibly Unified Parallel C (UPC) and Co-Array Fortran (CAF), now partially integrated into Fortran 2008, combined with specialty languages for particular computation styles, like Compute Unified Device Architecture (CUDA) or OpenCL, algorithm and data-structure specific code writing systems like the Tensor Contraction Engine (TCE),<sup>4</sup> and runtimes implementing other programming techniques (e.g., Intel's Thread Building Blocks (TBB) for intranode parallelism and CHARM++ for general parallelism). Further developments to improve the programming of accelerators and coprocessors through directive-based concepts as defined in OpenACC and future versions of OpenMP will play an important role, especially since they are addressing some of the portability concerns of software developers. Finding the right balance between general programming language support and more limited but less complex tools sufficient to achieve performance will be an important part of any exascale application development. Such special features may include higher level programming models for the "stream" or vector computing elements or support for software and/or algorithm assisted fault tolerance.

There have been efforts to develop new approaches for programming high-performance computing systems. The DARPA High Productivity Computing System (HPCS) project had a goal of a tenfold increase in productivity through a combination of new programming languages and new hardware capabilities. While interesting research came out of the language efforts (particularly Cray's Chapel and IBM's X10 languages), these have yet to provide users with viable alternatives to existing models. Outside of a few specialized areas, the adaptation of partitioned global address space (PGAS)

languages such as UPC is very low. The reality is that creating a truly new language is a long-term project, and is unlikely to be completed before the first exascale systems appear. More likely is the evolution and enhancement of existing languages, including extensions to MPI (e.g., MPI-3 now provides access to shared memory regions) and to existing programming languages (e.g., OpenACC is a small extension to C/C++ and Fortran). There is an opportunity to develop new programming systems for 2030, but only if work starts soon on the necessary research.

### ***Other Issues***

File input/output (I/O) is another issue. Many of the same issues apply (power, latency, smaller ratio of space/FLOP). Current approaches based on blocking I/O to a single file per process will not be effective. At the scale of these future systems, it will probably be necessary to have a subset of processors perform I/O for groups of processors, preferably in parallel to the computation. This is another example of specialization, this time at the software level.

Finally, while an exascale system can act as 1,000 petascale systems (or a million terascale systems), this is unlikely to be an efficient use of the system. Simple approaches to ensemble calculations that can be executed serially on a collection of much smaller systems do not constitute an exascale calculation (regardless of their scientific importance).

### ***HPC in 2030***

To extrapolate computer performance to 2030, we have made the following assumptions. These are for a conservative design, and provide a likely minimum performance level for 2030:

1. The 2012 International Technology Roadmap for Semiconductors (ITRS), which has predictions out to 2026, can be extended to 2030.
2. Computer organization will be similar to current systems that integrate multiple processor types, but with greater degrees of integration. Specifically, we postulate that a system will contain nodes that integrate a fast scalar processor, a stream processor, and processing in memory (PIM).
3. Processing elements have a constant number of devices and the size of a chip is roughly constant. Thus, the number of processing elements per chip increases with the square of the ratio of gate feature size.
4. The many engineering challenges required to achieve the ITRS targets will be met.

Table 1 shows estimated performance in 2012, 2020, 2023, and 2030. This estimate is consistent with current leading systems; both IBM Blue Gene/Q and Cray XK7 systems achieve around 20 PetaFLOPS peak. The estimate for 2023 is consistent with some current DOE estimates, providing a little more than 1 exaFLOPS. By assuming a significant increase in processor density, we estimate that performance

**Table 1. Estimated Performance for Leadership-class Systems**

Year	Feature size	Derived parallelism	Stream parallelism	PIM parallelism	Clock rate GHz	FMA's	GFLOPS (Scalar)	GFLOPS (Stream)	GFLOPS (PIM)	Processor per node	Node (TFLOP)	Nodes per system	Total (PFLOPS)
2012	22	16	512	0	2	2	128	1,024	0	2	1	10,000	23
2020	12	54	1,721	0	2.8	4	1,210	4,819	0	2	6	20,000	241
2023	8	122	3,873	512	3.1	4	3,026	12,006	1,587	4	17	20,000	1,330
2030	4	486	15,489	1,024	4	8	31,104	61,956	8,192	16	101	20,000	32,401

Feature size is the size of a logic gate in a semiconductor, in nanometers. Derived parallelism is the amount of concurrency, given processor cores with a constant number of components, on a semiconductor chip of fixed size. Stream and PIM parallelism are the number of specialized processor cores for stream and processor-in-memory processing, respectively. FMA is the number of floating-point multiply-add units available to each processor core. From these values, the performance in GigaFLOPS is computed for each processor and node, as well as the total peak performance of a leadership-scale system.

between 16 to 32 exaFLOPS may be achievable by 2030. Note that there are many assumptions in this estimate, and many yet unsolved engineering problems must be overcome to maintain the targets in the ITRS roadmap. In addition, we have assumed lower clock rates in the stream and processor-in-memory elements, reflecting a different optimization point for speed and energy use.

It is important to note that these predictions are sensitive to a number of hard-to-forecast values. For example, energy and power dissipation problems could reduce the number of processing units that can be assembled into a single system, reducing total performance.<sup>5</sup> Conversely, new 3D fabrication and packaging could increase the density of components, allowing even greater parallelism. The major conclusion that should be drawn from this table is that current trends will yield significantly faster systems than we have today, but not ones that are as fast as the past 20 years of development would suggest.

Another important feature of an HPC system in this time frame we expect to see are even more levels of memory than we currently have. Current systems have up to three levels of cache, and then main memory. Systems with accelerators have additional memory attached to the accelerator. In 2030, main memory itself might be composed of different levels, with portions being very fast, but small, and other portions larger and slower. Combined with the concept of processing in memory, that is, having some computing capability embedded within the memory subsystem, this will lead to an even more complex overall system.

***Programming a 2030 HPC system***

Software has a much longer lifespan than hardware, and as pointed out earlier, the expectation is that there will be only evolutionary changes to the programming model in the 2020-2023 timeframe. For 2030, the likelihood that some major, revolutionary changes to the programming models will occur is higher because of the extra development time. It is important to point out that this is not a guarantee, as many programming languages and models have shown a surprising level of sustainability. In addition, as we pointed out in the discussion on the validity of petascale projections, software

advances are much tougher to predict than hardware advances.

Future programming models will be driven by dealing with locality, whether they are new or extensions of existing programming models. Programmers need to be able to express locality and relationships between data abstractly. NVIDIA’s CUDA programming language is an example of a newer programming model that forces programmers to deal directly and explicitly with locality. This illustrates the need for the expression of locality while also showcasing the need for ways to express this information about locality more abstractly and portable.

As discussed above, we pointed out that the memory system will probably become much more complex, both with the introduction of processing in memory (PIM) as well as with more levels of memory architectures. While some of this complexity will be hidden from the developers, a lot of it will not. The developers need to be able to express what computing should be done by the slower processing elements inside the memory subsystem, and what needs to be done by the fast scalar processor or the streaming elements. The processing elements within the memory subsystem will have significantly higher bandwidth to memory. One of the easiest uses to imagine of this processing is to perform calculations for prefetching of data (gather), and scatter the results of calculations back into the final locations in the memory subsystem. Because of the processing power and bandwidth envisioned in the memory subsystems, these can be significantly more complex than possible within the processors, which will be especially useful for software with complex memory access patterns, for example, unstructured CFD codes.

We do not believe that there will ever be a programming model that completely hides the complexity of the underlying HPC system from the programmer while achieving the necessary performance. Nevertheless, we do think that great advances can be made to allow the programmer better to express her or his intent and to provide guidance to the compiler, runtime system, operating system, and even the underlying hardware. This will require significant research and that

research needs to start now for solutions to be ready in the 2030 time frame.

Related to locality is the fact that the developer community needs to change their thinking away from a focus on floating point operations. In the 2030 time frame, FLOPS might be considered “free,” and data movement, synchronization, and all levels of parallelization will become the driving forces for performance. We already see this to some extent with current accelerators like the GPUs from AMD and NVIDIA. We need to start looking at the quality of algorithms from the point of view of arithmetic intensity, that is work per memory access, rather than just looking at floating point operations. Prime examples of algorithms that have, in general, relatively low arithmetic intensity are sparse linear algebra methods. Utilizing the processors in the memory subsystem could increase the arithmetic intensity by delivering the right data to the scalar and streaming processors in a contiguous manner. Of course, as we see today, there will be codes covering the full range from highly optimized codes that run on a single architecture to codes that are highly portable, but not as high performing.

One concept to determine a “sweet-spot” at exascale is to develop more composable programming models. The low-level components will be highly optimized for a given architecture, probably even by the vendor itself, and the higher level applications that build on these low-level components are significantly more portable. Examples of this are Intel’s MKL, or PETSc (Portable, Extensible Toolkit for Scientific Computation<sup>6</sup>) from Argonne National Lab. While achieving high levels of performance will never be a 100% automated process, such a composable programming model should allow the development of transportable software, that is software that can be ported easily from one platform to the next, while still requiring optimizations to achieve full performance.

Another concept that will become important for software will be specialization within applications. As pointed out earlier, it might be necessary to have dedicated processes dealing with I/O in parallel to the computation. Other processes might analyze or process the data generated by the main algorithm on the fly, and only the processed data is actually stored. For example, visualizations of results and calculations of derived properties might be done in parallel with the main calculations rather than after the main simulation finishes. On a lower level, separate processes might be used to gather data for upcoming calculations, and scatter the results of calculations as mentioned above. This will be especially important considering the extreme levels of parallelism we forecast the hardware will provide in 2030.

With the increased complexity comes the need for improved programming tools like profilers, compilers, and debuggers. These need to be (relatively) easy to use and allow the developer a deep understanding of the behavior of their codes and the barriers to good performance on a given system. Having

the ability to inform the developer of the inhibitors in order to move software to the next generation of HPC systems and of the changes to make that will allow good performance on both current and future systems will significantly increase the productivity of the developers and utilization of future HPC systems.

This leads to the need for a well-trained developer workforce. Even application developers utilizing libraries or advanced programming models need to understand the basic principles of parallelism and the need to utilize and express locality and the other demands on software by the hardware in 2030. We also need developers that can build and optimize the lower level components of the software architectures. These developers must have a deep understanding of the hardware architectures, as well as work closely with the application developers to provide the high-level components they need.

### *Alternative Computer Architectures*

Up to this point, our analysis is based on the evolution of current technology. Such evolution has provided an exponential increase in performance over several decades; while there are many challenges in continuing the same rate of increase, the assumptions in this report represent a likely path for computer architecture. However, other device technologies could give rise to computers with very different capabilities. A few that were discussed include:

1. **Quantum Computers.** There is steady progress on fabricating practical quantum computers, and such systems may be available in 2030. However, while a quantum computer can be used for some linear algebra calculations (after all, the Schrodinger equation involves linear operators), a quantum computer is not necessarily a faster computer for CFD calculations.
2. **Superconducting logic.** For example, Rapid Single Flux Quantum (RSFQ) logic gates were demonstrated at over 770 GHz, and 100 GHz gates are available now. A drawback of this device technology (as currently implemented) is significantly lower density; as an immature technology, cost is also an issue.
3. **Low-power memory.** Many novel memory designs are being developed that use something other than charge to store data. Some have much higher latencies but provide much lower power use and higher densities of storage.
4. **Massively parallel molecular computing.** This is a very different paradigm, and uses far higher levels of parallelism (typically  $10^{23}$ ) but also gives up determinism. It is not clear how to cast CFD calculations into a form suitable for molecular computing.

Many of these revolutionary architectures will also require revolutionary changes to the full software ecosystem, especially quantum computers and molecular computing. Considering the long development timeframes for software, early examples of these technologies need to be available to a larger developer community in the 2020-2023 time frame to en-

sure that these new architectures will have broad impact on more than a very small subset of the HPC user community.

Moreover, while we can foresee significant progress in pushing HPC technology to the next level using approaches that are more evolutionary until the 2030 timeframe, we are much more skeptical for the time after 2030. As we pointed out earlier in the evolutionary approach, the semiconductor industry predicts feature sizes of 4 nm. This means that a feature will consist of small numbers of atoms, and significant quantum effects will play a role. An end of the ability to further shrink feature size is clearly in sight at that time. Even if the above listed revolutionary changes are not necessary to reach goals for 2030, they are certainly important for allowing us to move beyond 2030. Some technologies might not seem attractive now (e.g., too expensive, too slow, too hard to program) but we need to invest in them to overcome those faults to be able to take advantage of their benefits.

### Research Suggestions

We conclude with a list of research that needs to be started now and in the coming years to enable our predictions of HPC in 2030 to be realized. While not complete, this list is a good starting point for the community. There is no order of importance implied in this list. We need to develop and implement all the items in this list and then demonstrate them on important use cases.

- Alternate Hardware Technologies
  - Quantum Computers
  - Superconducting logic
  - Low-power memory
  - Massively parallel molecular computing
  - Next generations of “traditional” processor technologies
  - On-chip optics
  - Advanced memory technologies (e.g., 3D memory)
- Advanced Algorithms
  - Data movement aware (not FLOPS oriented) algorithms
  - Power aware algorithms
- Advanced Programming Models and Systems
  - Locality aware, abstract programming models
  - Composable programming models
  - Transportable, extremely parallel programming models
  - Transportable, extremely parallel HPC software
  - Highly scalable and manageable data management systems
  - Compiler interfaces that allow better expressions of developer intent
  - Improved programming tools like compilers, profilers and debuggers

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<sup>1</sup> Anderson, W. K., Gropp, W. D., Kaushik, D. K., Keyes, D. E., and Smith, B. F., “Achieving High Sustained Performance in an Unstructured Mesh CFD Application”, *Proceedings of the ACM/IEEE SC99 Conference on High Performance Networking and Computing*, 1999, IEEE Computer Society.

<sup>2</sup> The exact dates for these achievements depend on your definition of peak and sustained performance.

<sup>3</sup> Wikipedia article on PERCS:

<http://en.wikipedia.org/wiki/PERCS>

<sup>4</sup> See: S. Hirata, *J. Phys. Chem.* **2003**, *107* (46), 9887-9897.

<sup>5</sup> Esmailzadeh, H., et al., “Power challenges may end the multicore era”, *Commun. ACM*, 2013. **56**(2): p. 93-102.

<sup>6</sup> PETSc (Portable, Extensible Toolkit for Scientific Computation) homepage, <http://www.mcs.anl.gov/petsc/>