Exascale Opportunities for Aerospace Engineering

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University of Wyoming
and
the Vision CFD2030 Team

Background

- **Aerospace engineering historically has been a strong driver in advancing computational science and engineering**
  - NASA-led computational fluid dynamics for aeronautics
    - Many /most current algorithms developed with NASA funding
- **Lately, perception that CFD has matured**
  - Commoditized applications using 0(1000) cores (not 1M)
  - Important but limited impact in product design cycle
  - Lack of investment in new fundamental developments
  - Poorly positioned to exploit coming exascale revolution in HPC
- **NASA commissioned study**
  - Identify barriers to progress
  - Provide knowledge-based forecast of future computational capabilities
  - Develop a long-term actionable research plan with a system-level view of technology required for 2030 time frame

Engineering, Operations & Technology
Boeing Research & Technology

NASA Vision 2030 CFD Code

Final Technical Review

Contract # **NNL08AA16B** (Order # NNL12AD05T)
Deliverable # 6

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NASA Langley Research Center

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Technical Approach

Today → 2030

NASA

Requirements developed for N+2/N+3 systems, including noise, emissions, fuel consumption targets, etc.

Academics
Gov't Labs
Industry Labs

Identify current CFD technology **gaps** and **shortcomings**

Industry

Define anticipated aerodynamic and performance **requirements** for competitive aerospace vehicle and systems

HPC

Establish expected **computing performance** and **likely outlook for CFD technology application**

DoD

Community Input

Survey

Workshop

Define barriers and impediments

Detailed Research Plan and Technology Roadmap

Petaflops Opportunities for the NASA Fundamental Aeronautics Program

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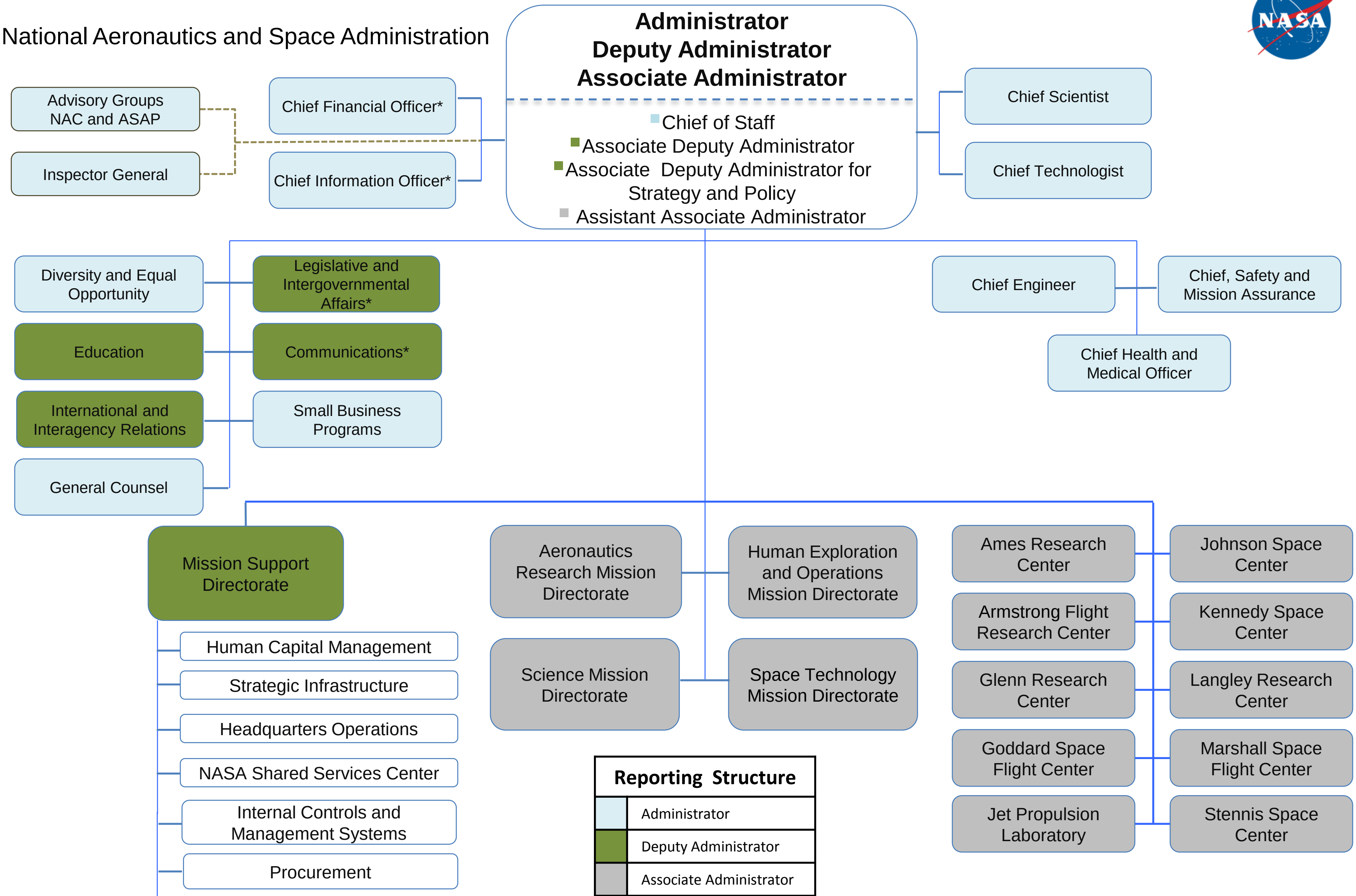
David Darmofal (MIT)
David Keyes (Columbia University)
Mark Turner (University of Cincinnati)

AIAA 2007-4048

National Aeronautics and Space Administration



Note:
* Center functional office directors report to Agency functional AA. Deputy and below report to Center leadership.

March 2014

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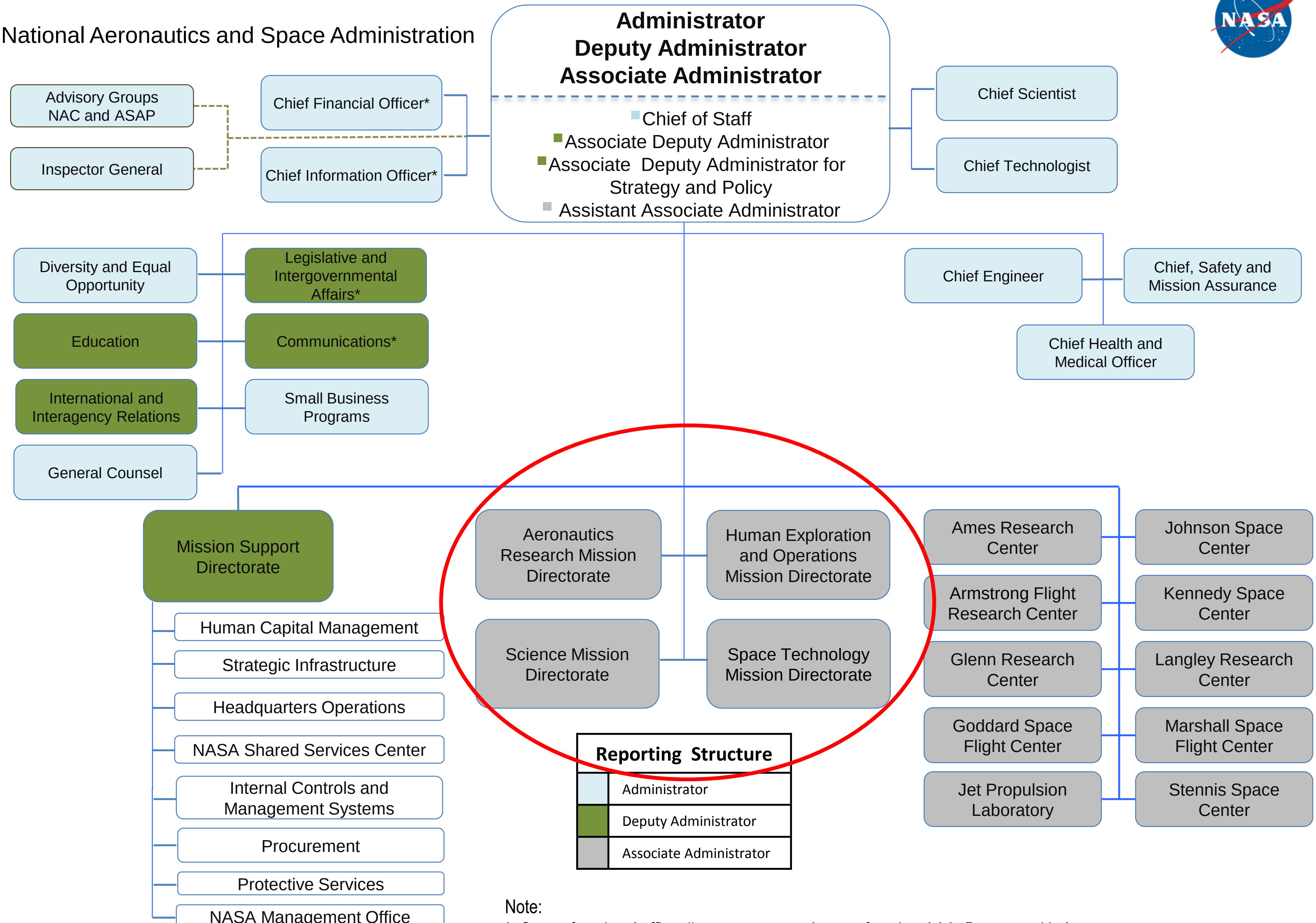
National Aeronautics and Space Administration



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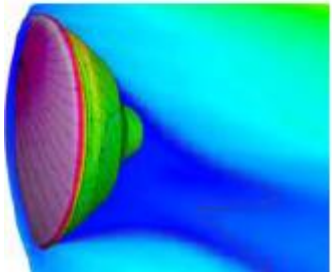
Computational Methods within NASA Mission Directorates



- Science Mission Directorate (SMD):
  - Climate, weather, environment
  - Planetary entry systems (MSL/Curiosity)
- Human Exploration and Operations (HEO):
  - Development of Space Launch System, Orion
- Aeronautics Research (ARMD):
  - Subsonic and supersonic civil aircraft and rotorcraft technology development
  - **Basic computational tool development**
    - **ARC3D, CFL3D, Overflow, LAURA,**
    - **FUN3D, CART3D…**

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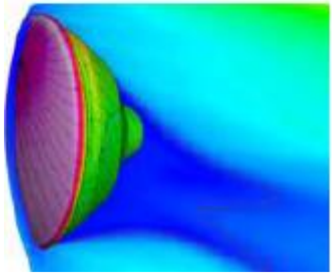

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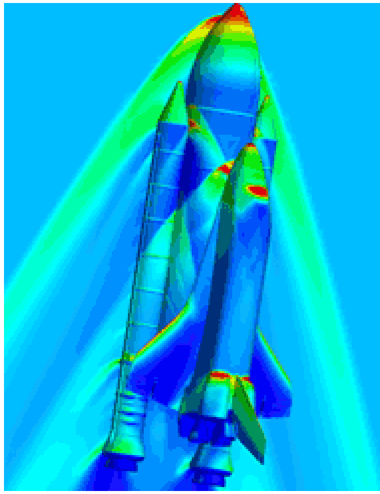

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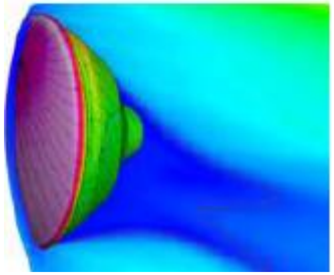

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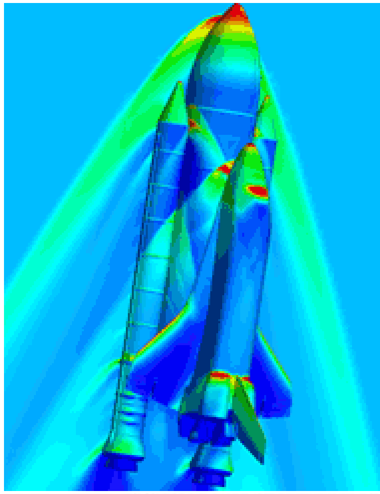
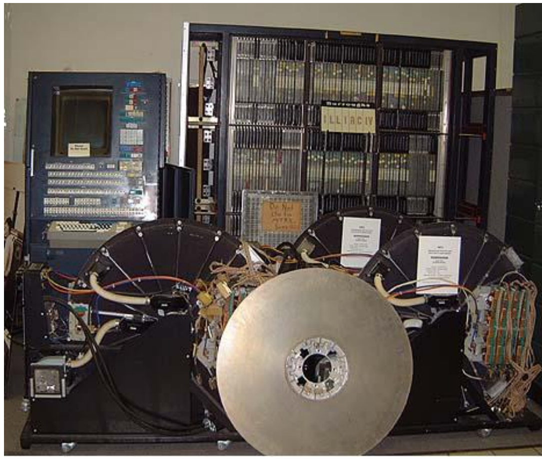


ARMD's Historic HPC Leadership (Code R)



- ILLIAC IV (1976)
- National Aerodynamic Simulator (1980's)
- 1992 HPCCP Budget:
  - $596M (Total)
    - $93M Department of Energy (DOE)
    - $71M NASA
      - Earth and Space Sciences (ESS)
      - Computational Aerosciences (CAS)

- Computational Aerosciences (CAS) Objectives (1992):
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  - *"… develop algorithm and architectural testbeds … scalable to sustained teraflops performance"*

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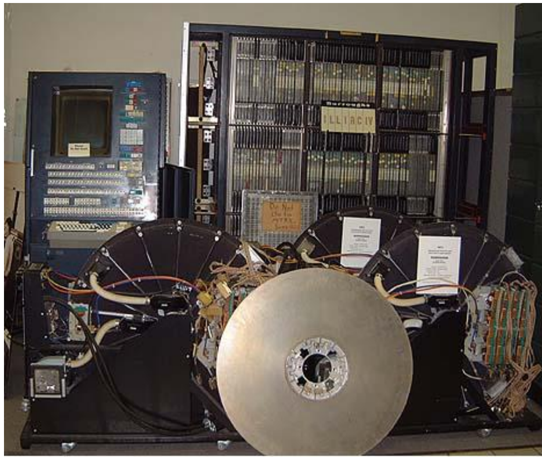

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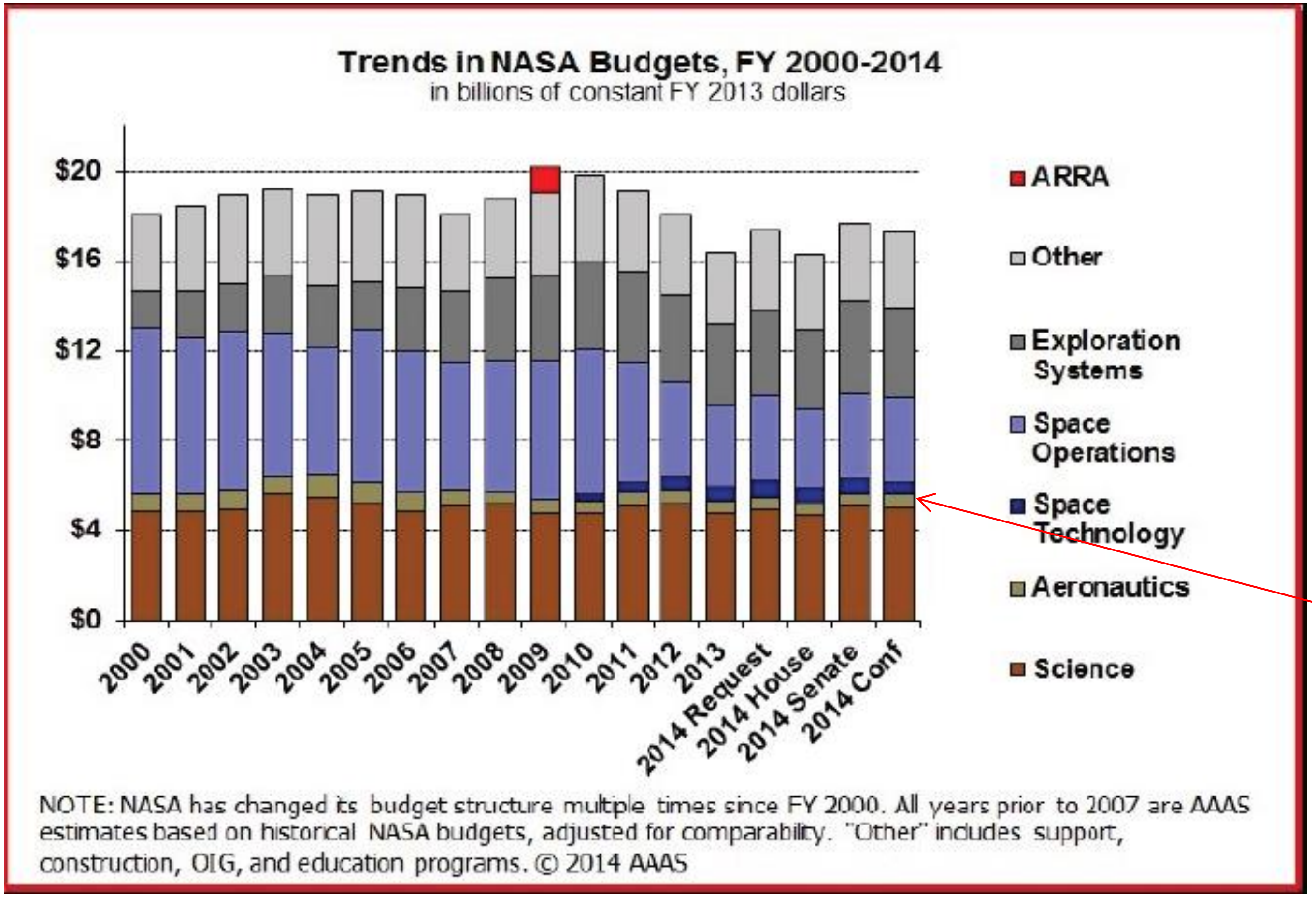
exascale

Recent NASA Funding Trends



ARMD=$500M 3% NASA budget

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.**
   - Physics-based simulation is a cross-cutting technology that impacts all of NASA aeronautics missions and vehicle classes – *NAE Decadal Survey*
   - R&D in computational methods and resulting tools have impact far beyond NASA's aeronautics mission (Science, Space, other engineering fields)
   - Advances in simulation capabilities are often driven by the requirement of short-term impact, or in response to simulation failure on a program → *results in incremental improvements to CFD software*
   - NASA's Revolutionary Computational Aerosciences (RCA) project is a step in the right direction *and should be maintained and expanded*

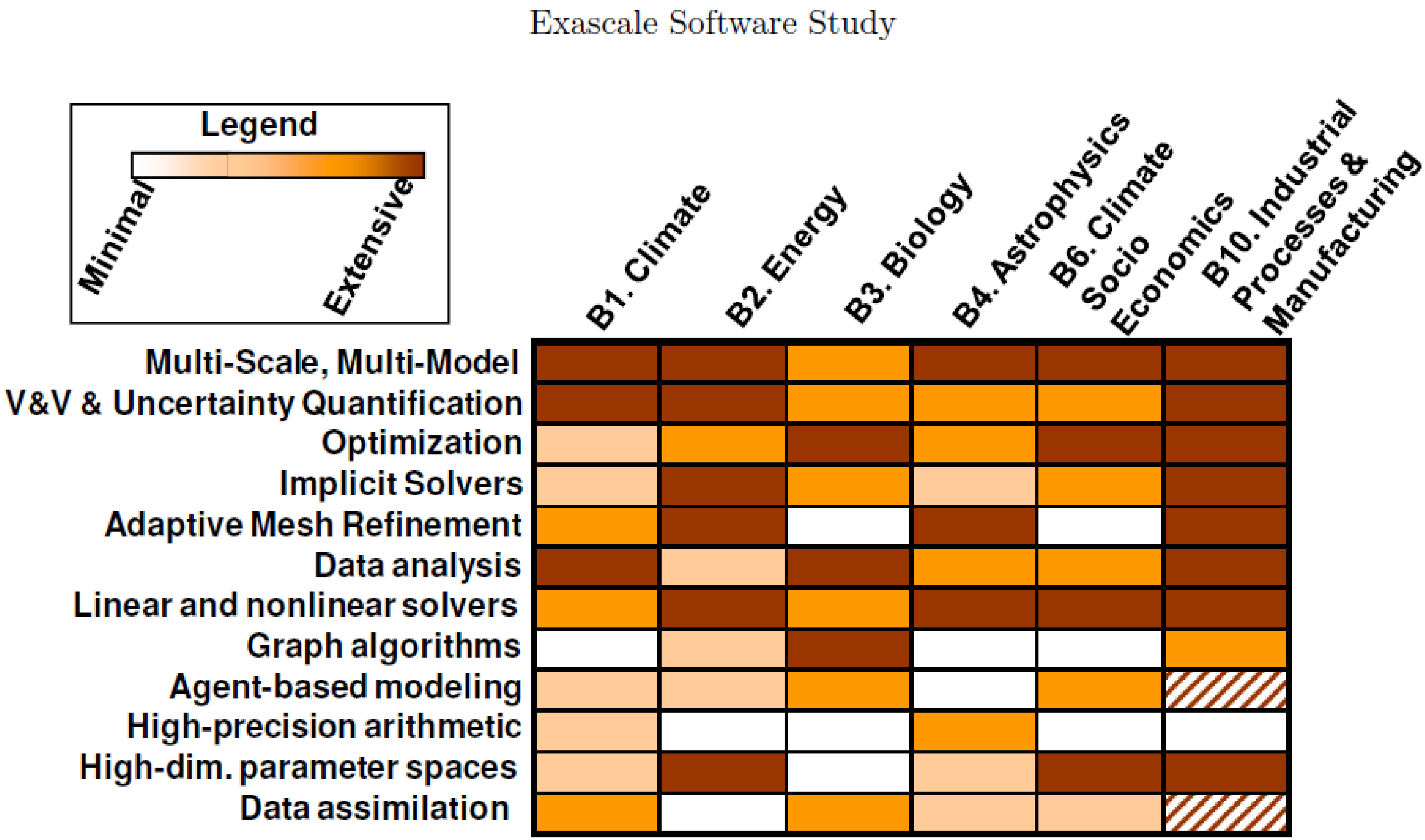
Findings CONTINUED

2. HPC hardware is progressing rapidly and technologies that will prevail are difficult to predict.

- Current predictions of exascale hardware architecture involve scalar processors with 1000’s of “streaming” processor cores, highly parallel memory interfaces, and advanced interconnects → *focus is on power consumption and failure recovery*
- Advanced software programming environments with higher levels of software abstraction will be required
- Many current CFD tools and processes do not scale well on today’s Petaflops systems, poorly prepared for exaflop revolution
  - *Mature (outdated ?) algorithms*
  - *Failure to provide consistent access to leading edge HPC for development/testing*
  - *Stagnation/commoditization of capabilities in government as well as industry*
- *Monitoring and assessment of disruptive technologies*
  - *e.g. quantum computing*

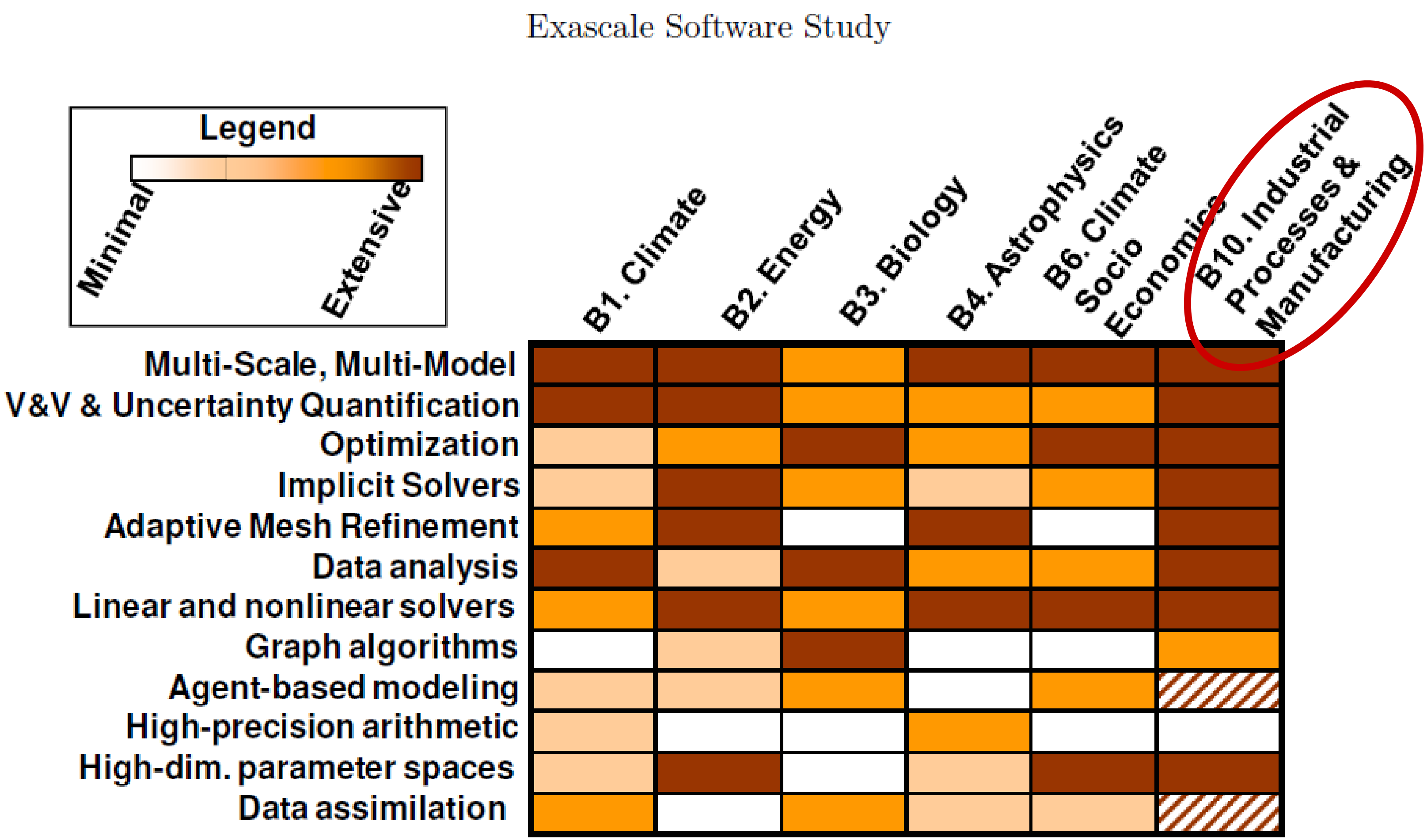
Aeronautics/Aerospace HPC

- Aerospace is **engineering** based discipline
- HPC advocacy increasingly has been taken up by the **science** community
  - Numerical simulation is now the third pillar of scientific discovery on an equal footing alongside theory and experiment
  - Increased investment in HPC will enable new scientific discoveries
- Engineering is not discovery based
  - Arguably more difficult to reach exascale
    - Complex geometries, Multidisciplinary, Uncertainties, Risk/Cost
    - e.g Gradient-based optimization is inherently sequential



- From: DARPA/IPTO/AFRL Exascale Computing Study (2008)

http://users.ece.gatech.edu/~mrichard/ExascaleComputingStudyReports/ECS_reports.htm



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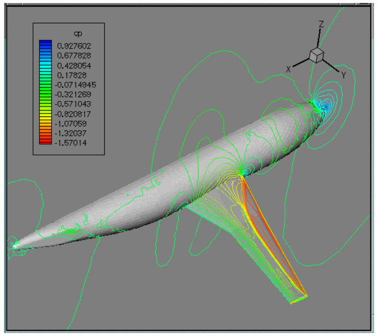
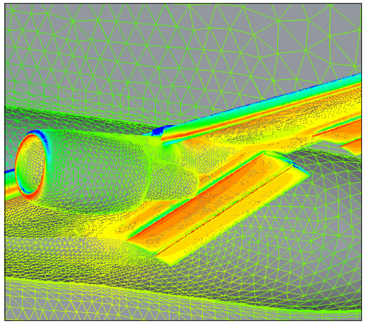
Findings CONTINUED

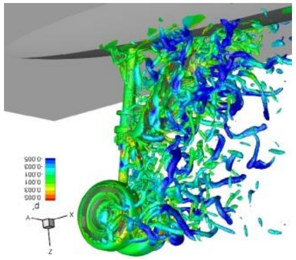
3. The accuracy of CFD in the aerospace design process is severely limited by the inability to reliably predict turbulent flows with significant regions of separation



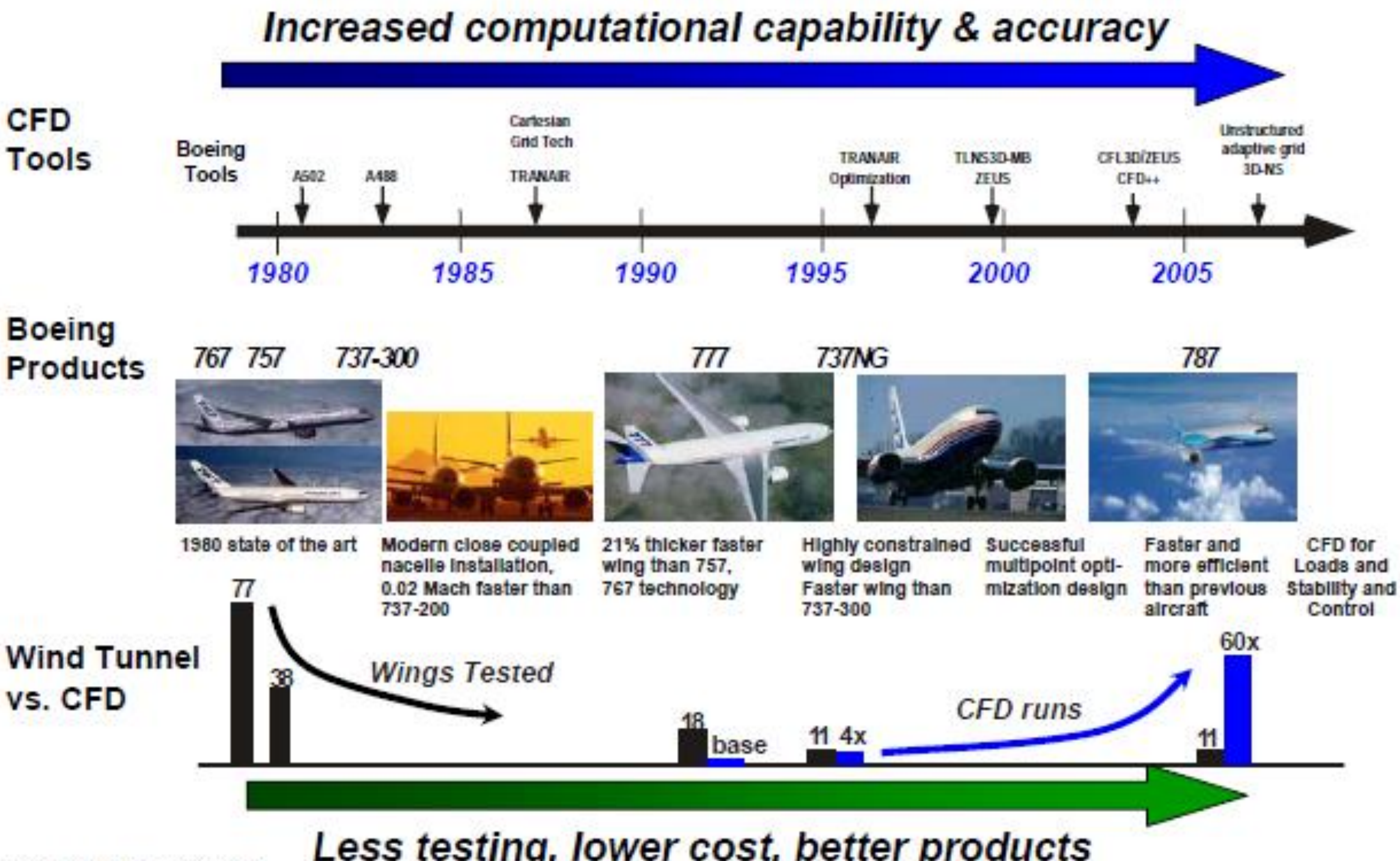
- Steady progression in physical fidelity
  - Panel methods (incompressible, inviscid) : 1960s
  - Linearized compressible flow methods : 1970s
  - Non-linear potential flow methods: 1980s
  - Reynolds averaged Navier-Stokes methods: 1990s to today !!
    - Increase in accuracy driven by finer grids, better HPC
    - **Plateau in physical/modeling fidelity for separated flows**



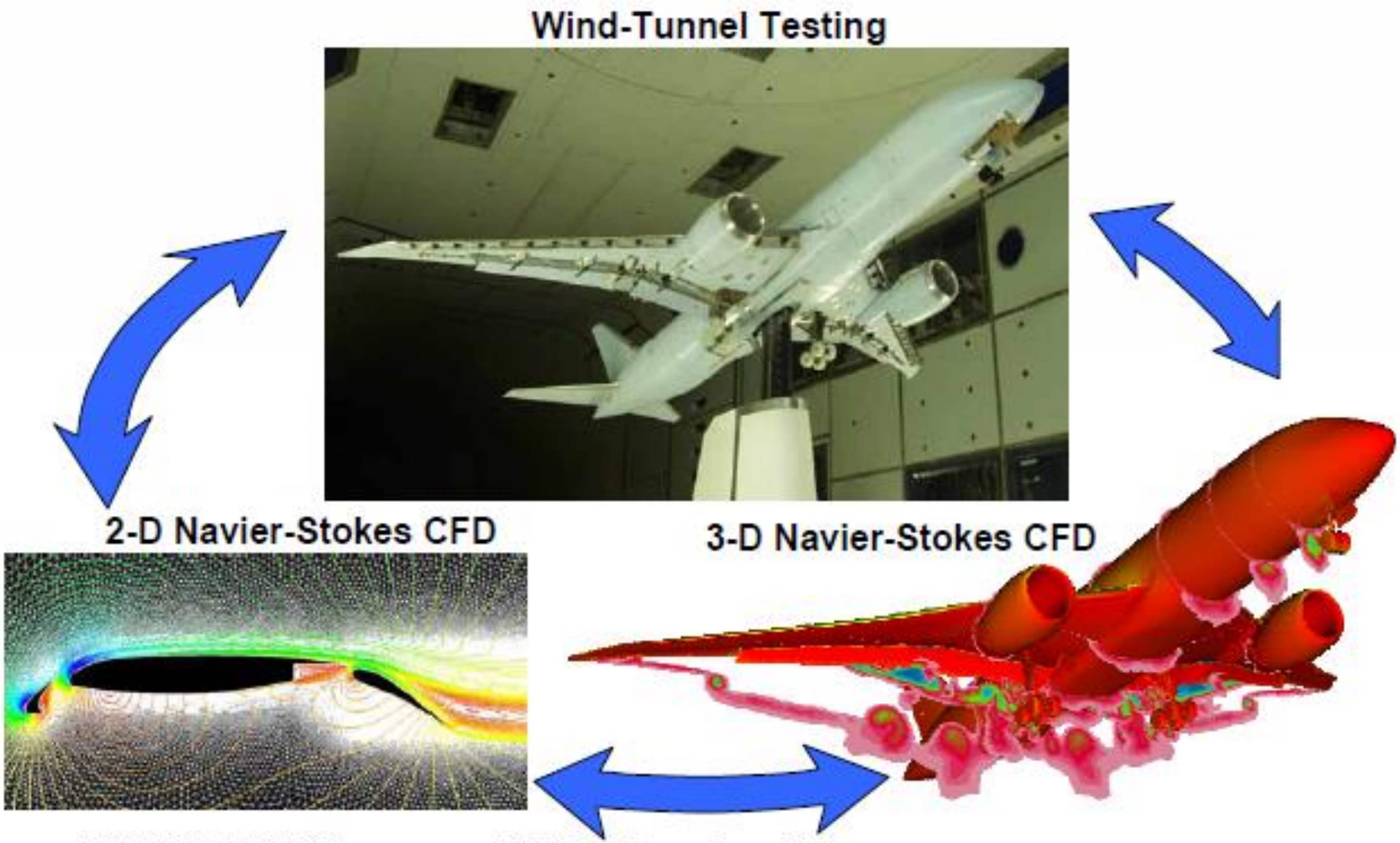
- CFD notably successful in nominal region of design space
  - Cruise condition (aircraft), nominal operating conditions (propulsion)
  - High accuracy requirements
  - Little or no flow separation by design
- LES not feasible for foreseeable future due to range of turbulence scales at flight Reynolds numbers
  - Hybrid RANS-LES, Wall Modeled LES



CFD Has Significantly Improved the Wing Development Process



Complementary Use of CFD and Wind Tunnels for High-Lift Design



Successful in Small/Important Region of Flight Envelope

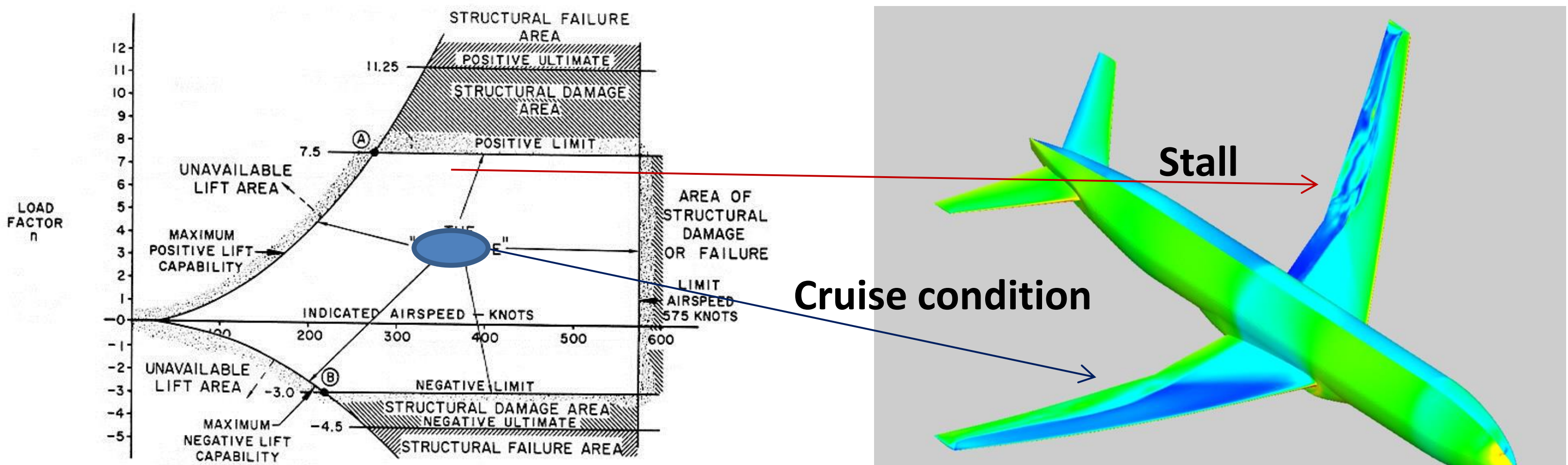
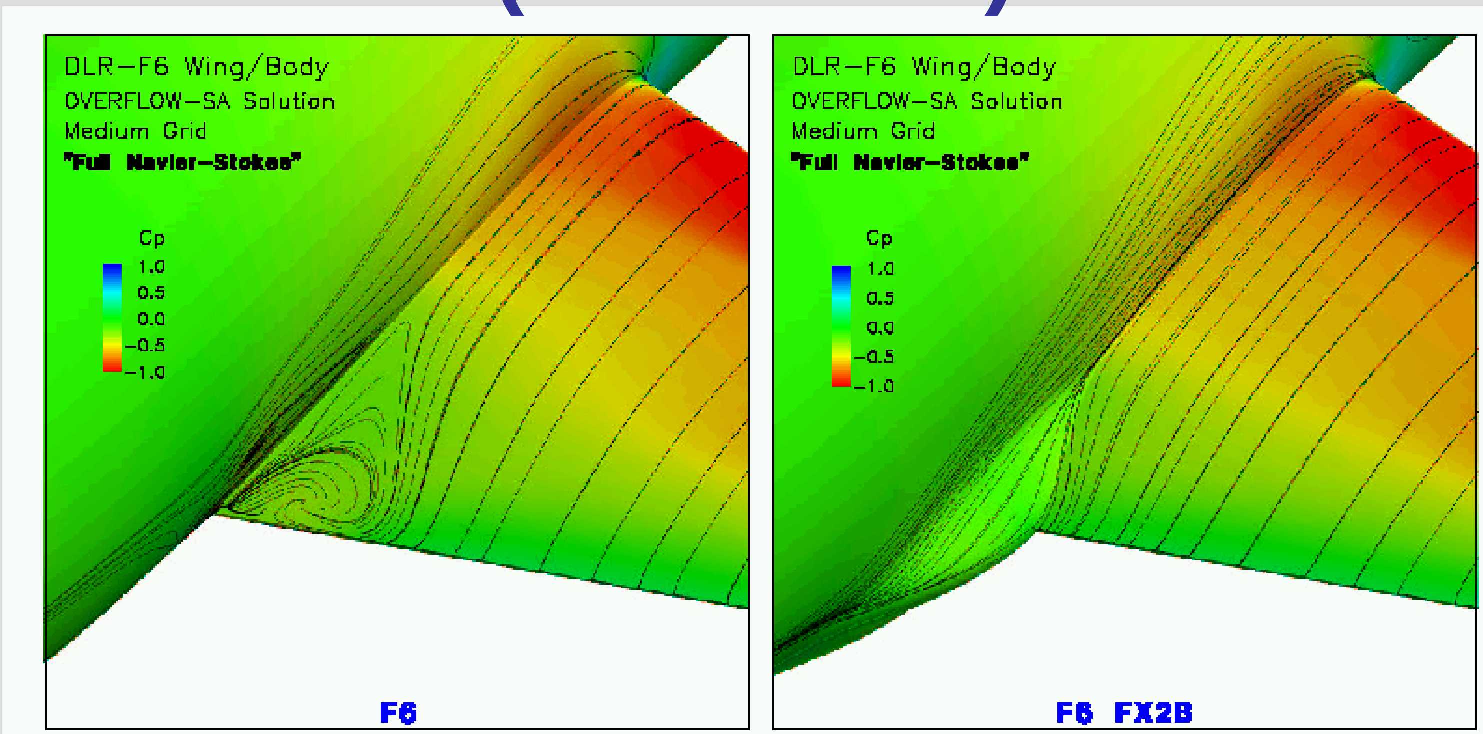


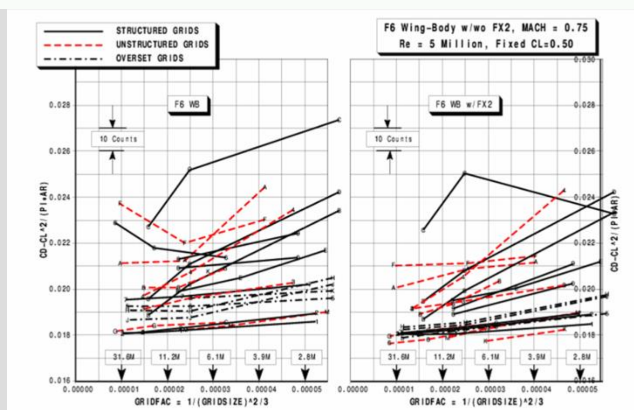
Figure 5.4. Significance of the V–n Diagram

- High accuracy required: 1 count of drag (10^{-4} of C_D)
  - CFD approaching wind tunnel accuracy in this flight regime
  - Necessary to reduce risk: Manufacturer performance guarantees
- Predictive ability lacking in most other regions
- **Edges of flight envelope required for certification/safety**

Drag Prediction Workshop (2001-2012)

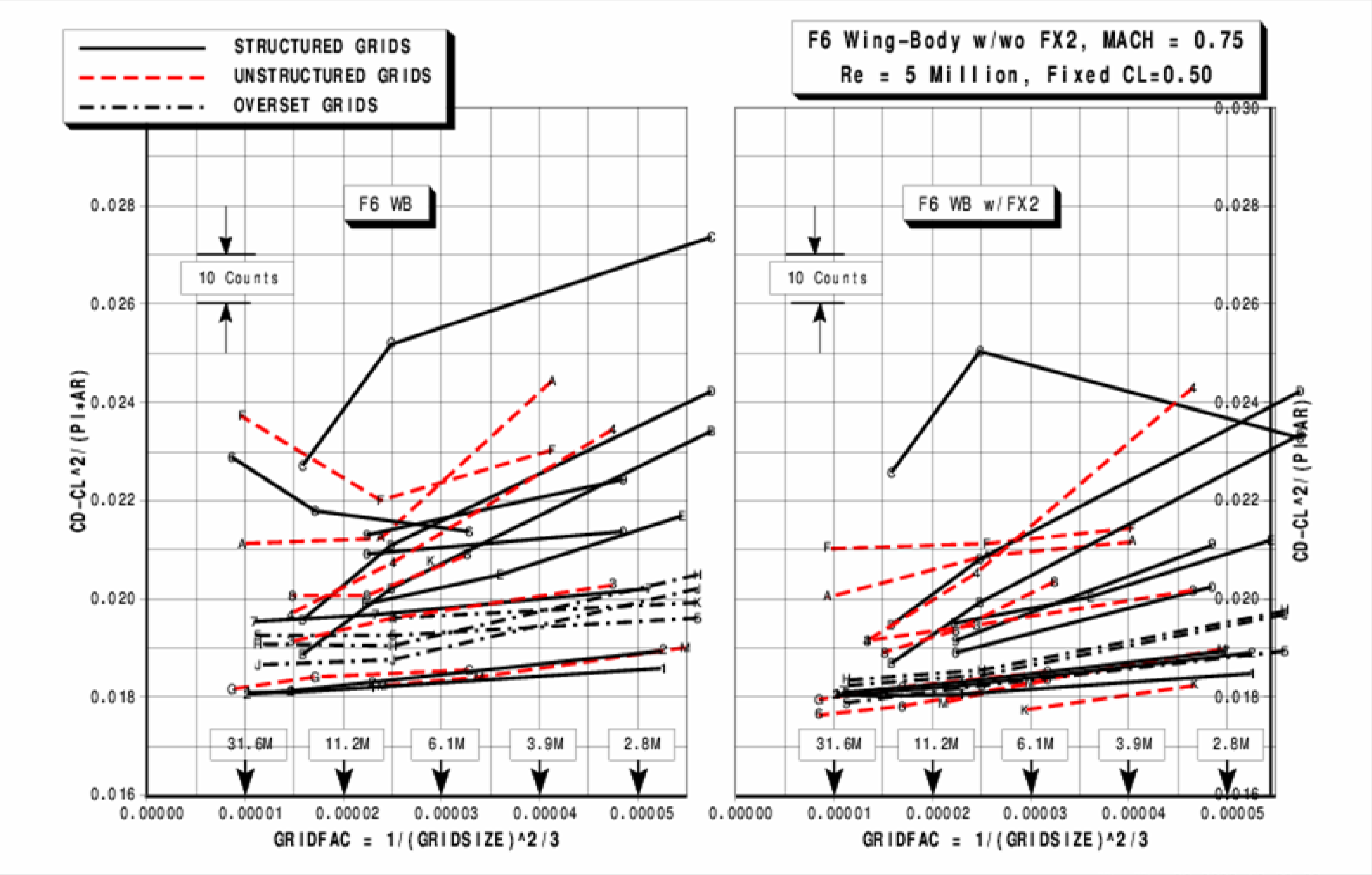


> 20 count scatter as grid is refined



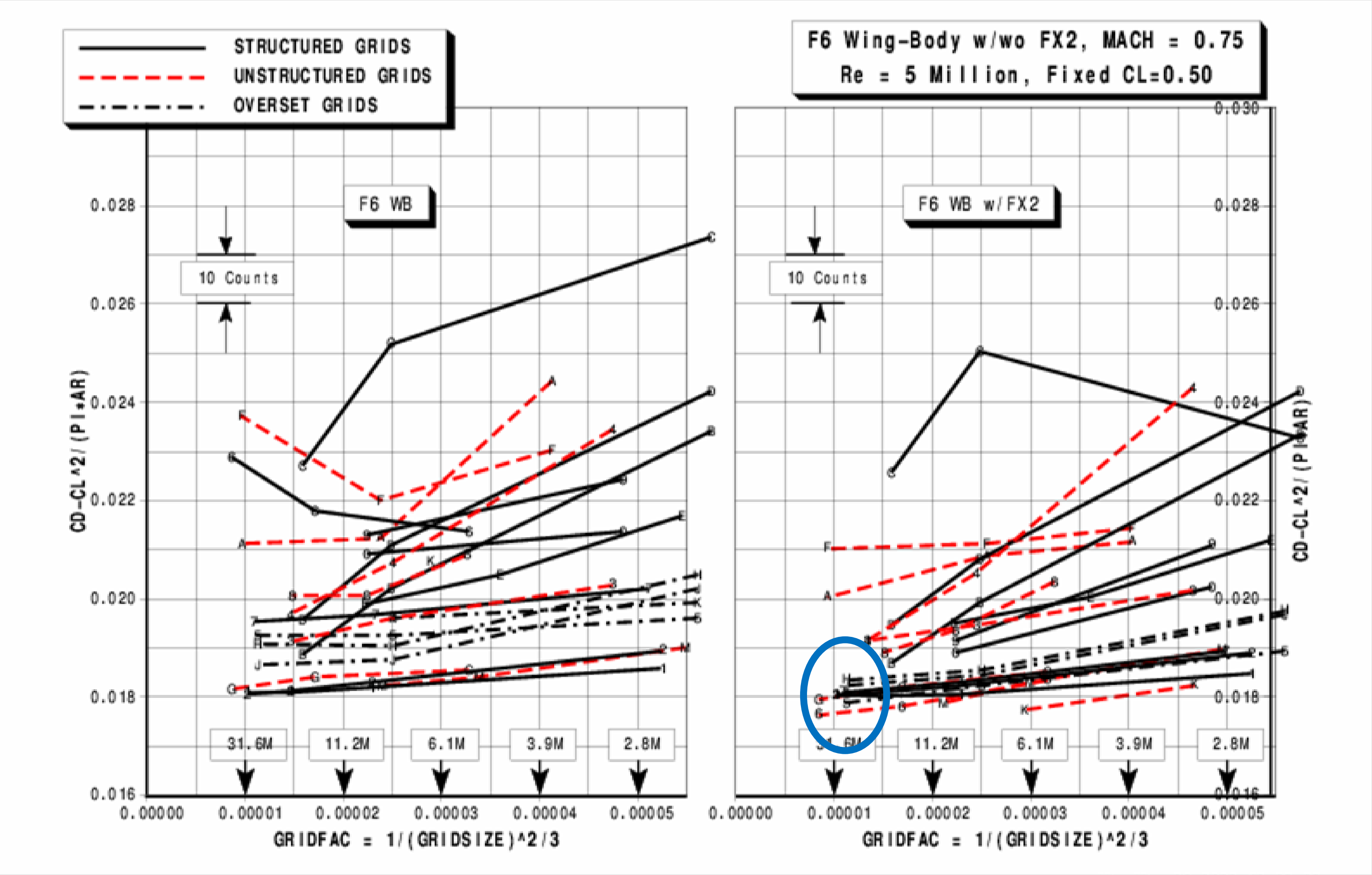
5 count scatter as grid is refined

Collective Workshop Results



- Idealized drag vs grid index factor ($N^{-2/3}$)
  - Wing-body and Wing-body+fairing

Collective Workshop Results



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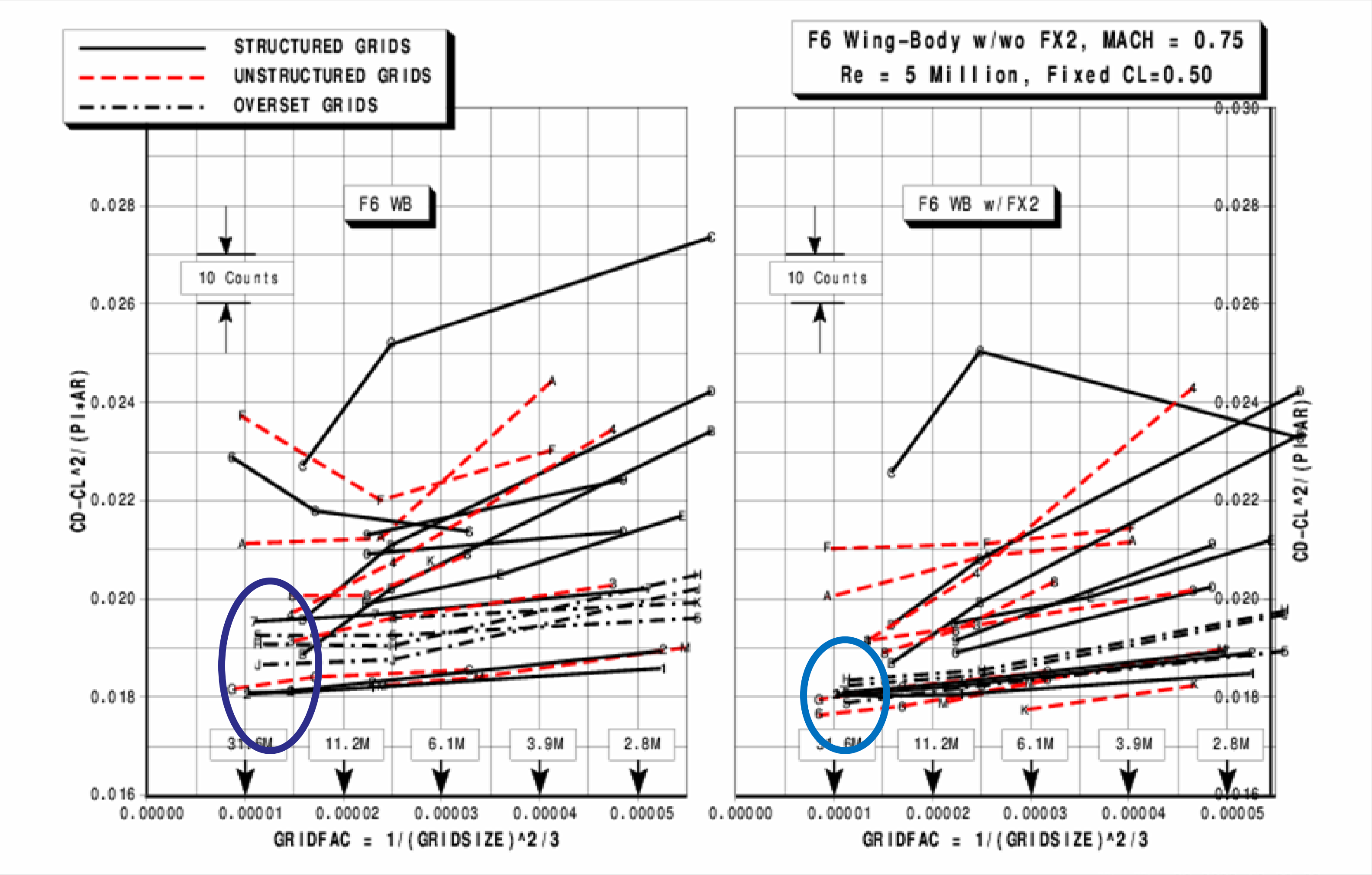

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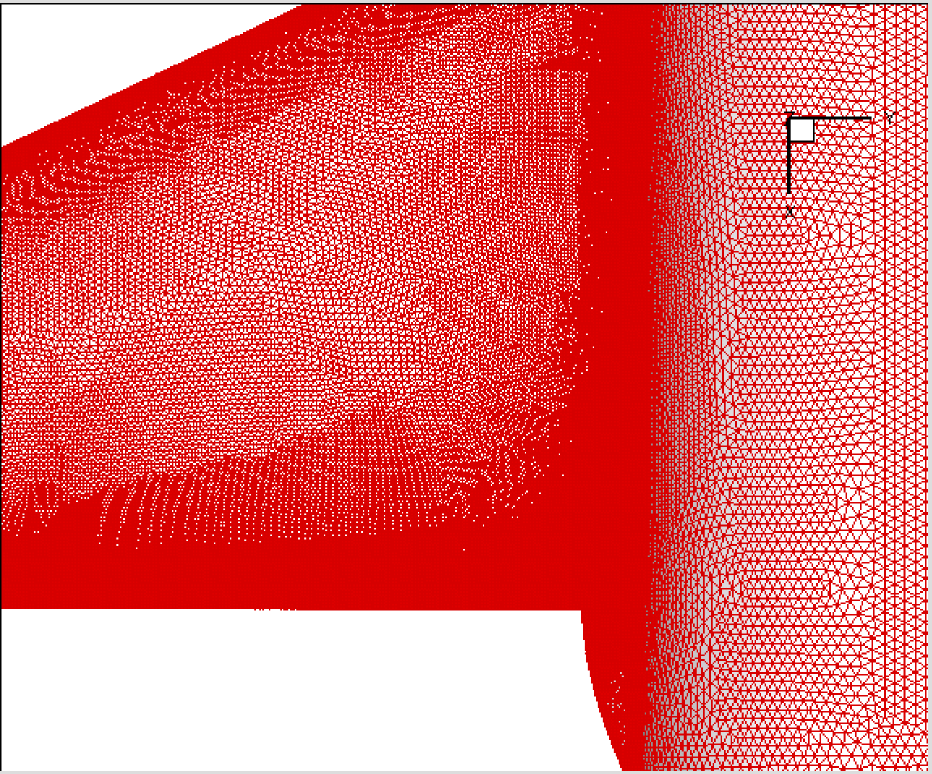
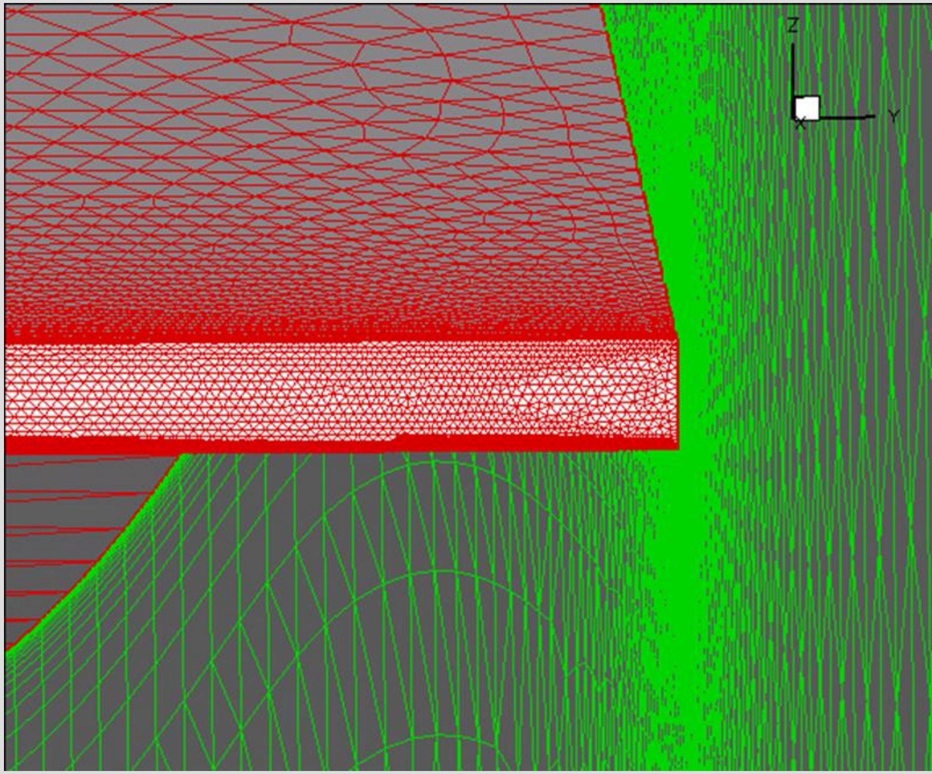
Steady RANS Meshing Requirements

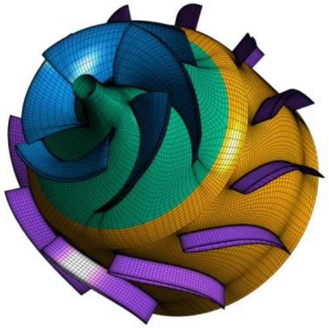


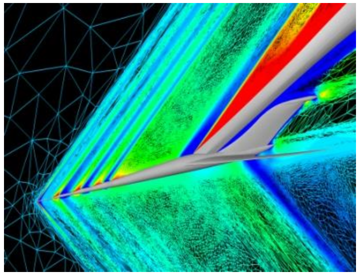


- Range of spatial scales
  - Highly anisotropic cells in boundary layer: Resolve to $y^+=1$, 10^{-6} to 10^{-7} wing chords
  - Far-field located 50 to 100 chords
- Production run meshes currently in range ~100 million points/cells
- **Spatial discretization error still dominant (workshop conclusions)**

Findings CONTINUED

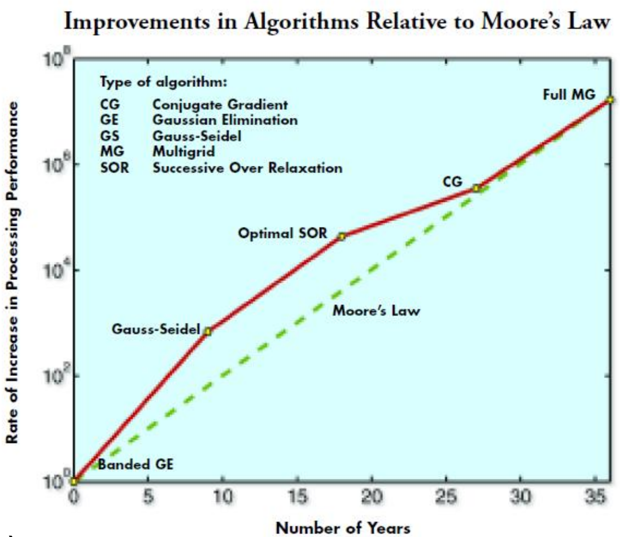
4. **Mesh generation and adaptivity continue to be significant bottlenecks in the CFD workflow, and very little government investment has been targeted in these areas.**
   - Streamlined and robust geometry (e.g., CAD) access, interfaces, and integration into CFD processes is lacking
   - Large-scale, automated, parallel mesh generation is needed as the size and complexity of CFD simulations increases → *goal is to make grid generation invisible to the CFD analysis process*
   - Robust and optimal mesh adaptation methods need to become the norm
   - Curved mesh element generation for higher-order discretizations is needed
   - Consider newer strategies like cut cells, strand grids, "meshless"





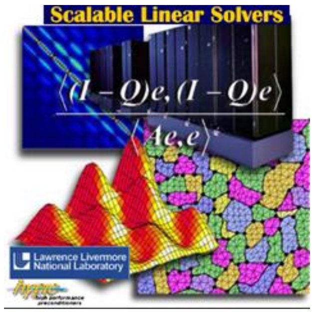
Findings CONTINUED

5. **Revolutionary algorithmic improvements will be required to enable future advances in simulation capability.**
   - Traditionally equivalent advances in simulation capability derived from:
     - *Advances in HPC hardware*
     - *Algorithmic improvements*
       - *(increasingly important for large problems)*
   - NASA investment in solver technology has stalled
     - e.g. Multigrid methods pioneered by NASA (circa 1980's)
     - *Unlikely solvers developed in other applications can be leveraged without substantial investment*
       - *e.g. parallel algebraic multigrid*



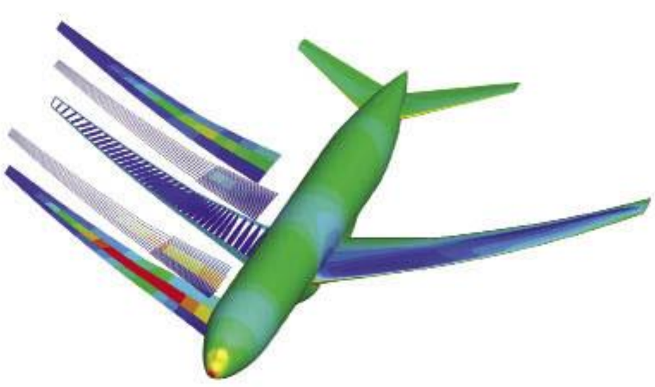
from: SCaLeS 2003, PITAC 2005

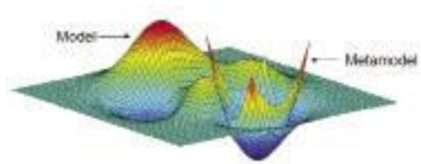
- Algorithmic breakthroughs required for:
  - (Adaptive) error estimation and control
  - Long-time integration problems (limited spatial parallelism)
  - Uncertainty quantification (curse of dimensionality)
  - Optimization

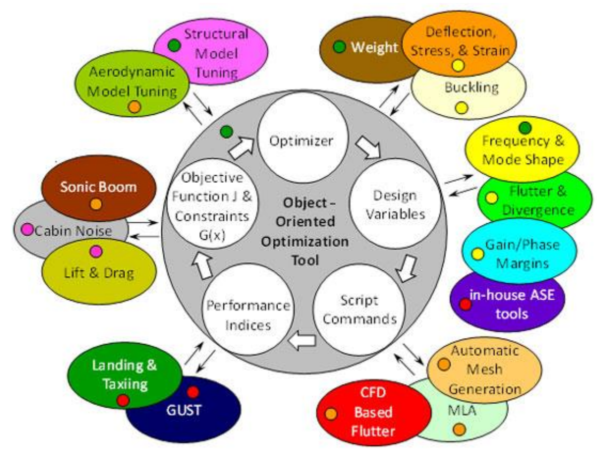


Findings CONTINUED

7. **In order to enable increasingly multidisciplinary simulations, for both analysis and design optimization purposes, several advances are required:**
   - Individual component CFD solver robustness and automation will be required.
   - Development of standards for coupling of CFD to high-fidelity simulations of other disciplines
   - Emphasis on the Science of MDAO and the development of stable, accurate and conservatives techniques for information transfer
   - Techniques for computing sensitivity information and propagating uncertainties in the context of high-fidelity MDAO problems

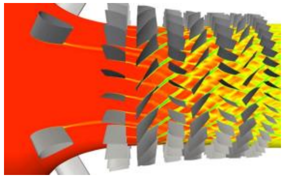
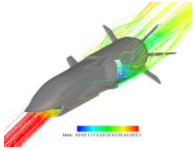
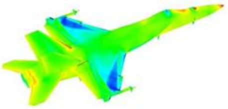
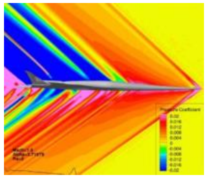
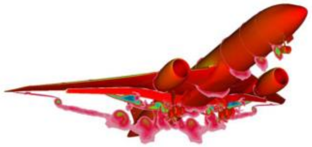
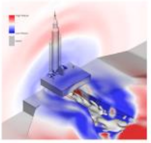
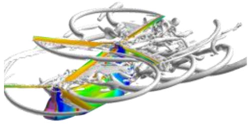






Vision of CFD in 2030

- **Emphasis on physics-based, predictive modeling**
  Transition, turbulence, separation, chemically-reacting flows, radiation, heat transfer, and constitutive models, among others.
- **Management of errors and uncertainties**
  From physical modeling, mesh and discretization inadequacies, natural variability (aleatory), lack of knowledge in the parameters of a particular fluid flow problem (epistemic), etc.
- **A much higher degree of automation in all steps of the analysis process** Geometry creation, mesh generation and adaptation, large databases of simulation results, extraction and understanding of the vast amounts of information generated with minimal user intervention.
- **Ability to effectively utilize massively parallel, heterogeneous, and fault-tolerant HPC architectures that will be available in the 2030 time frame** Multiple memory hierarchies, latencies, bandwidths, etc.
- **Flexible use of HPC systems**
  Capability- and capacity-computing tasks in both industrial and research environments.
- **Seamless integration with multi-disciplinary analyses**
  High fidelity CFD tools, interfaces, coupling approaches, etc.

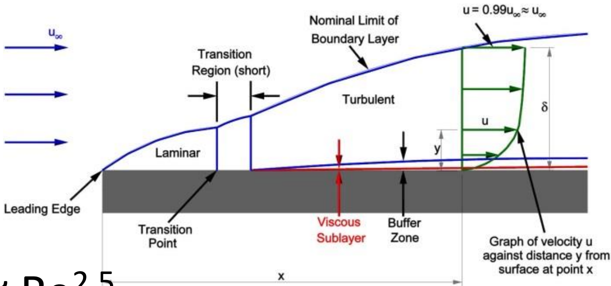








Grand Challenge Problems

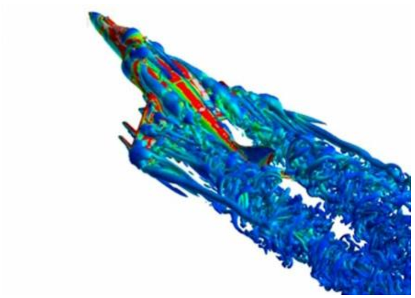
- **Represent critical step changes in engineering design capability**
- **May not be routinely achievable by 2030**
- **Representative of key elements of major NASA missions.**

1. Large Eddy Simulation (LES) of a powered aircraft configuration across the full flight envelope
2. Off-design turbofan engine transient simulation
3. Multi-Disciplinary Analysis and Optimization (MDAO) of a highly-flexible advanced aircraft configuration
4. Probabilistic analysis of a powered space access configuration

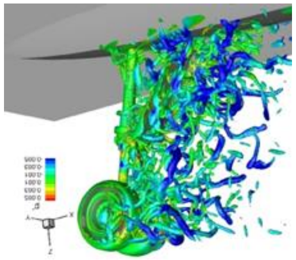
GC1: Estimates for Full Aircraft LES



- **Pure LES intractable due to range of scales in Boundary Layer**
  - Large aircraft flight Reynolds number ~ 50M
  - LES* (explicit in time) : grid resolution ~ $Re^{13/7}$, FLOPS ~ $Re^{2.5}$
    - Resolved to $y^+ = 1$
  - Wall Modeled LES* (explicit): grid res. ~ Re, FLOPS ~ $Re^{1.3}$
    - Resolved to $y^+ = 100$



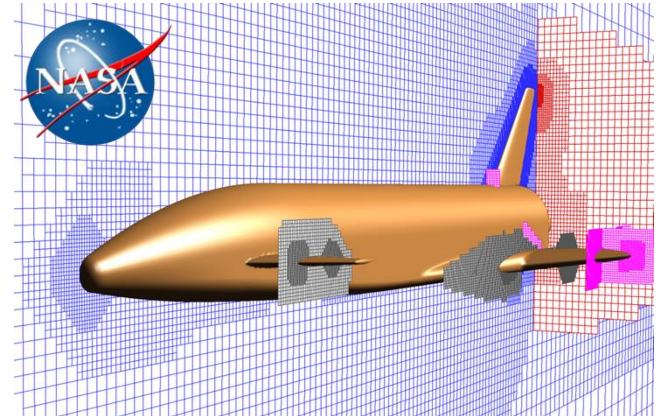
- **Estimates for WMLES for simple wing (AR=10) at flight Re**
  - 10^{11} to 10^{12} grid points, 500 Pflops for 24hr turnaround
  - Simulating transition adds factor of 10 to 100
  - Feasible on Exaflop machine
- **Hybrid RANS-LES (DES) starting to be used today**
  - **Increasing regions of LES (resolved) vs RANS (modeled)**
    - **HPC advances, Algorithmic advances**



[*]Choi and Moin, "Grid point requirements for LES: Chapman's estimates revisited", Phys. Fluids, 24, 011702 (2012)

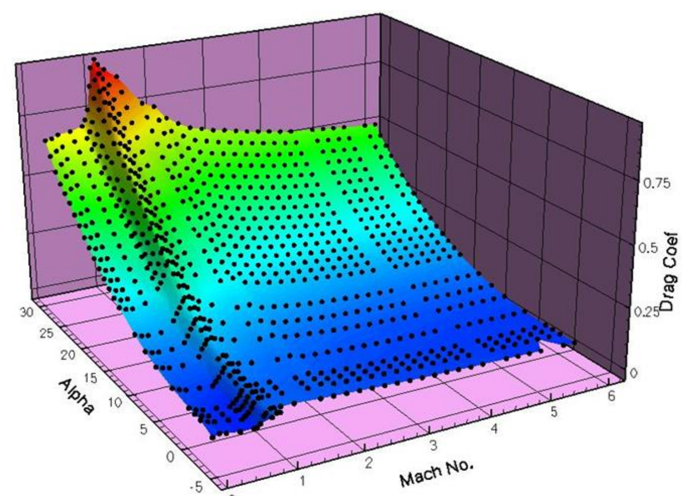
GC1:Filling in the flight envelope

- Simple inviscid flow example with 3 parameters
    - **Wind-Space:**
      M_∞ ={0.2-6.0}, α ={-5°–30°}, β ={0°–30°}
    - ***P* has dimensions (38 x 25 x 5)**
    - **2900 simulations**
- Complete envelope characterization may involve > 10,000 cases



- Liquid glide-back booster
    - Crank delta wing, canards, tail
- Wind-space only

- Alternatively, digital flight simulation with prescribed time dependent maneuvers
    - Aerodynamics (CFD)
    - Structural dynamics
    - Flight control system
    - Full dynamic effects
- Initially require lower fidelity modeling



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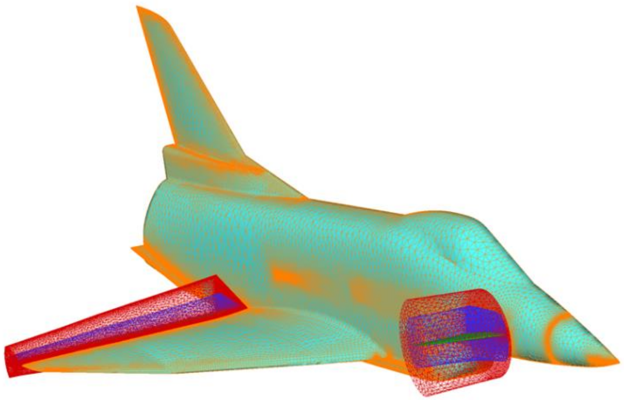

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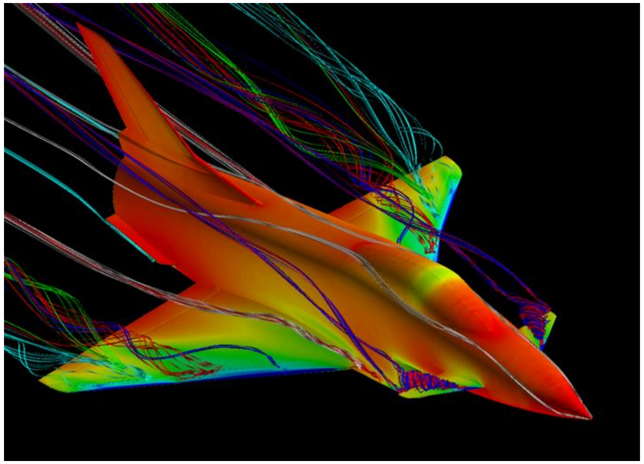

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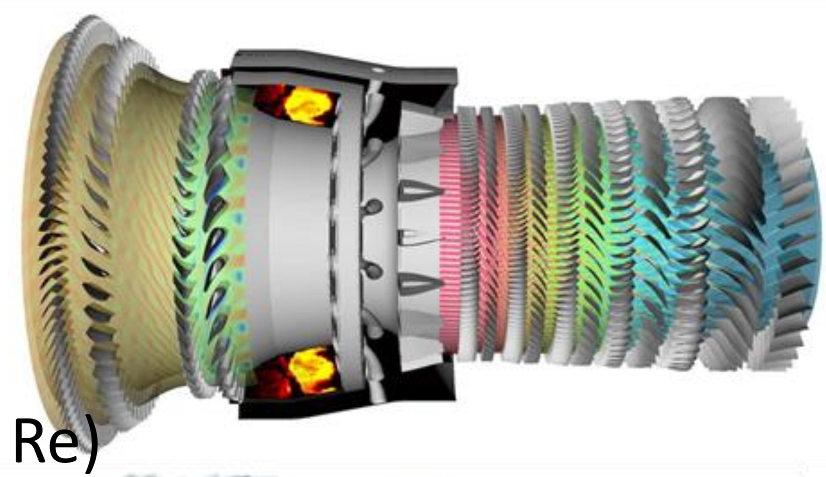
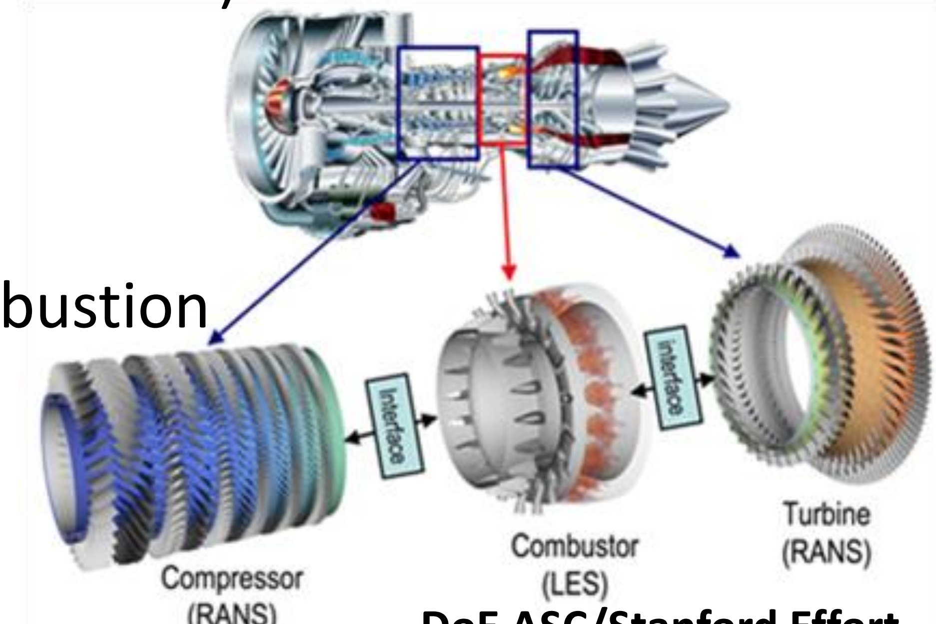
- A. Schutte, G. Einarsson, A. Raichle, B. Schoning, M. Orlt, J. Neumann, J. Arnold, W. Monnich, and T. Forkert. *Numerical simulation of maneuvering aircraft by aerodynamic, flight mechanics and structural mechanics coupling*. **AIAA Paper 2007-1070**

GC2: Transient/Off Design Full Engine Simulation

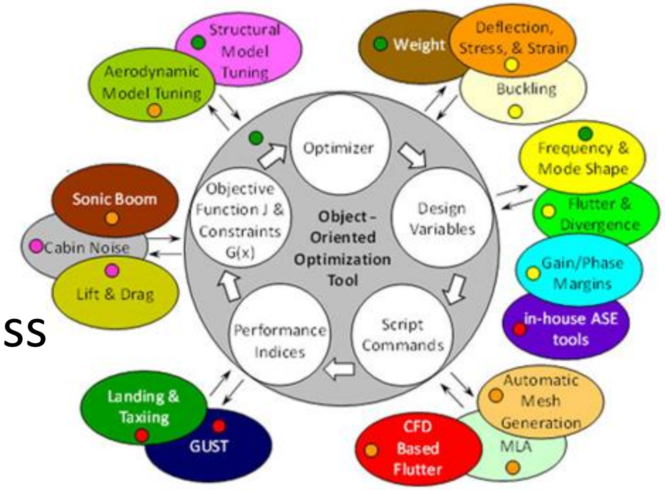


- Complex geometry
- Rotating/static components
- Turbulence and transition
  - Combustor LES feasible (lower Re)
- Conjugate heat transfer
- Combustion
  - NASA computational combustion effort lags DoE, AFOSR

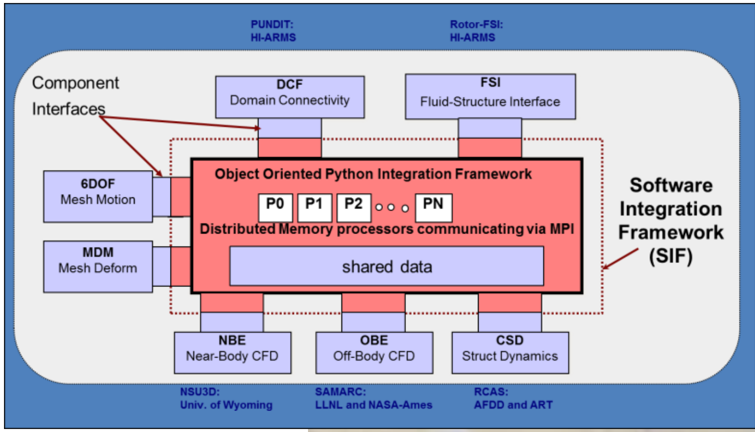


DoE ASC/Stanford Effort

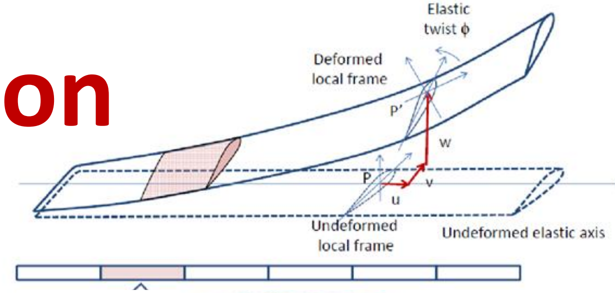
GC3: Multidisciplinary Analysis and Optimization



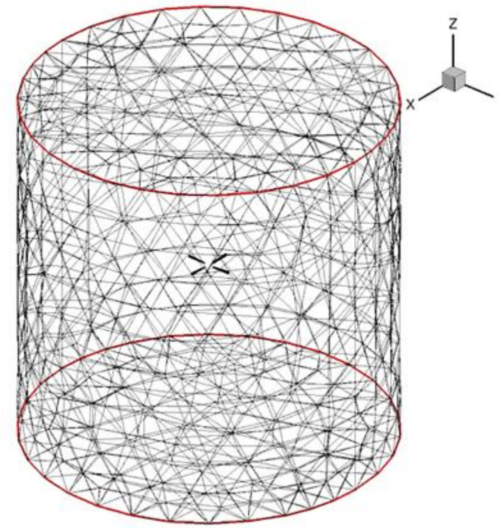
- Large scale coupling of multiple disciplines
  - Aero, structures, thermal, controls, acoustics
  - Improvements in disciplinary solver robustness
  - Science of coupling
  - Interfaces and standards
- Difficulties for effective exascale
  - Multiple disciplinary codes
  - Long time histories
    - Limited spatial parallelism in many cases
      - Good enough mesh resolution
  - Gradient-based optimization
    - Sequential iterative in nature

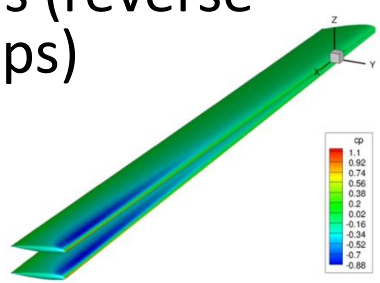


Example: Time Dependent Aeroelastic Rotor Optimization



- Aerodynamics: 3M point mesh
- Structural model: Beam model 80 elements
- 2.0 degree time step
  - Coupled aero-structural Newton-Krylov solver at each time step
- 20 to 80 design cycles
  - Analysis simulation (forward integration 2000 time steps)
  - Adjoint sensitivity analysis (reverse integration 2000 time steps)
  - Optimization





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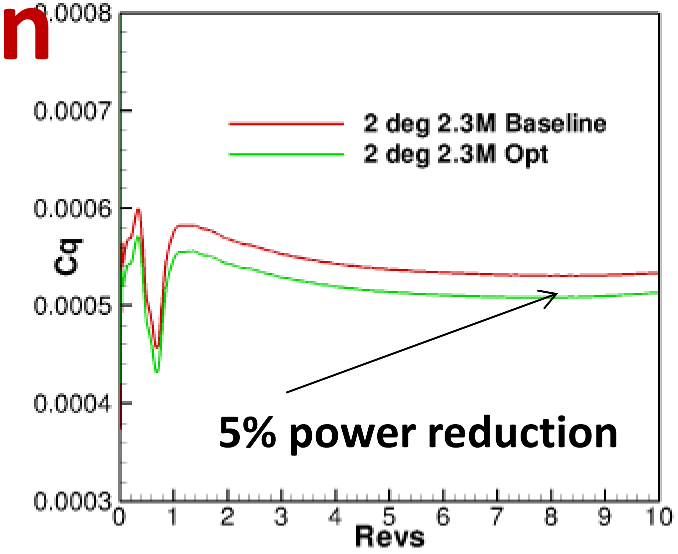
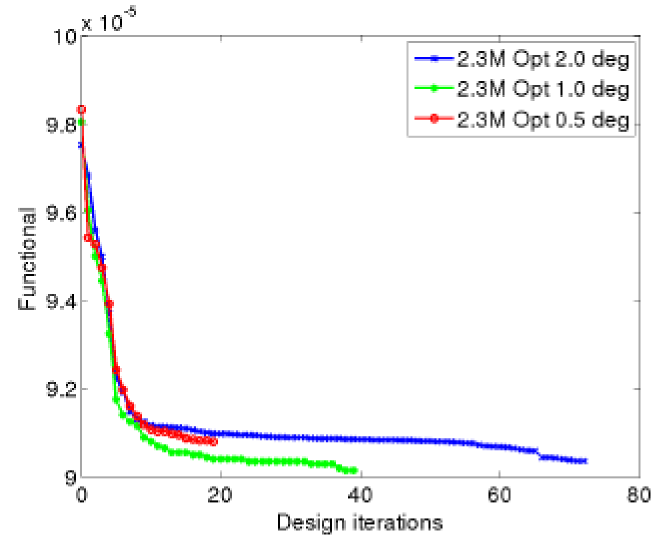
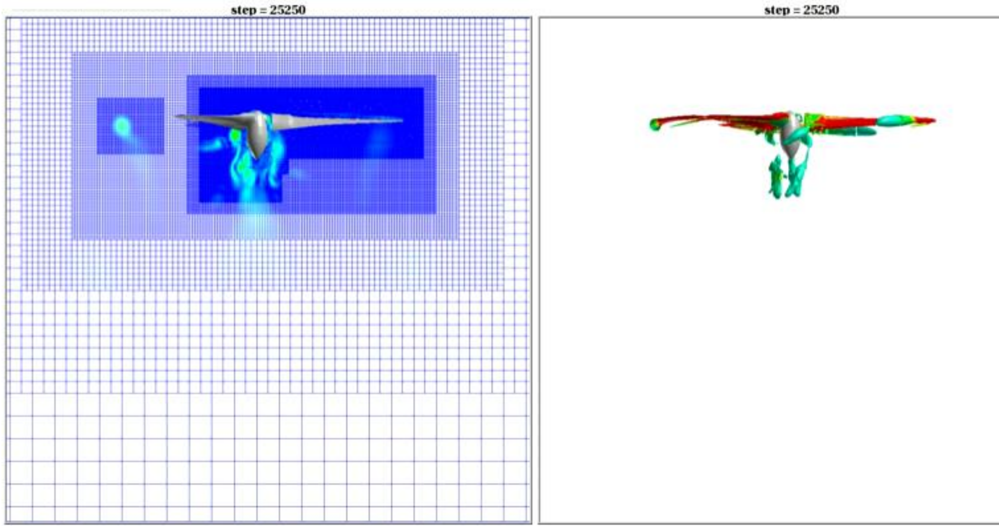
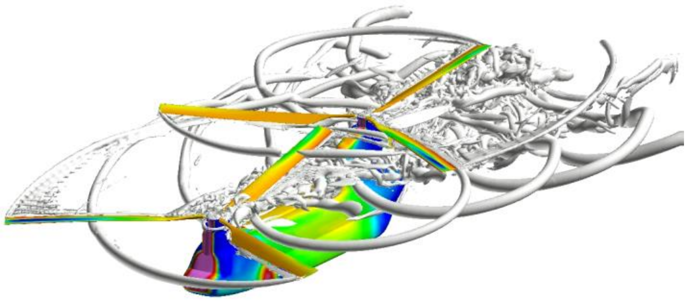




Desired Capabilities

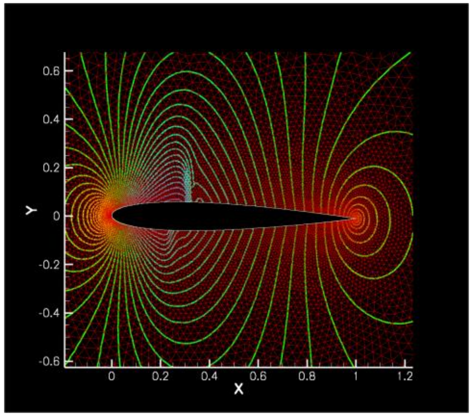


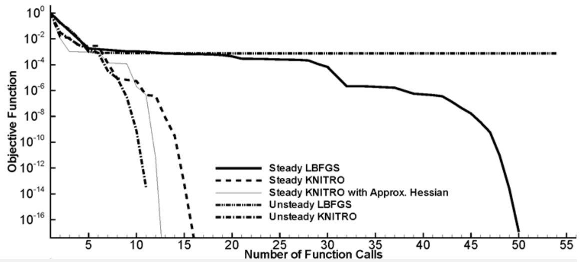
- Full aircraft configuration
  - Overlapping moving mesh system > 100M points
- Smaller time steps, longer time-integration
- Adaptive temporal and spatial error control
- Additional disciplines
  - Aero-thermo-servo-elastic
- Multi-objective, multi-point, multi-constraint optimization
- Optimization under uncertainty
- All assuming RANS is a suitable model



GC3: Algorithmic Opportunities

- Increased accuracy and efficiency
  - High order accurate discretizations (space and time)
- Accelerated solver convergence
  - Scalable solvers
- Reliable (adjoint) error estimation and robust adaptive processes in space and time
- Parallelism in time
  - Space-time methods
  - Time-spectral methods (periodic problems)
- Parallel optimization
  - Parallel Hessian construction for Newton optimization
  - Combined global/local optimization





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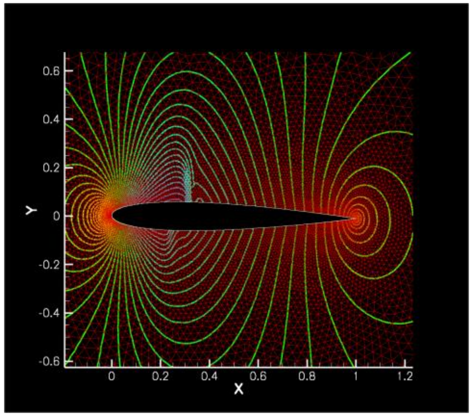
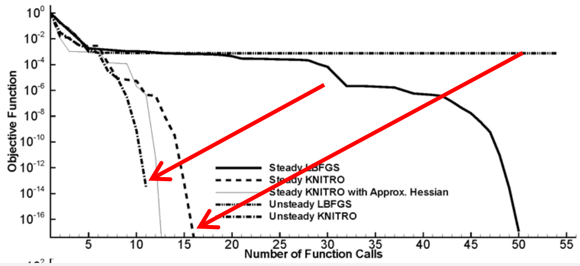
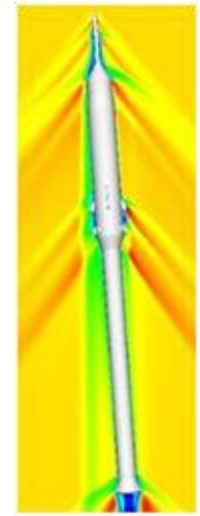
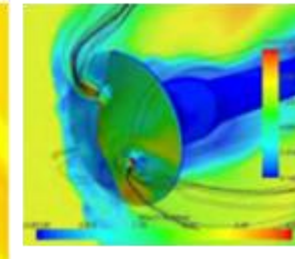
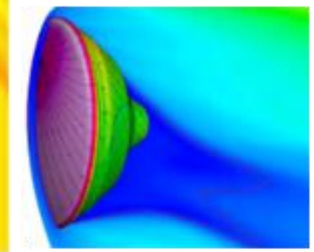




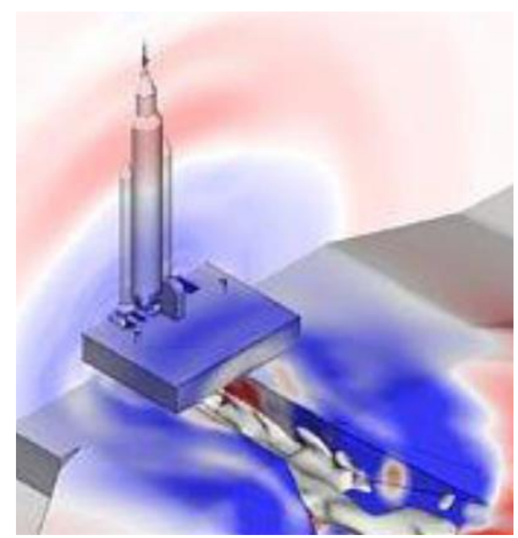
GC 4: Probabilistic Launch Vehicle



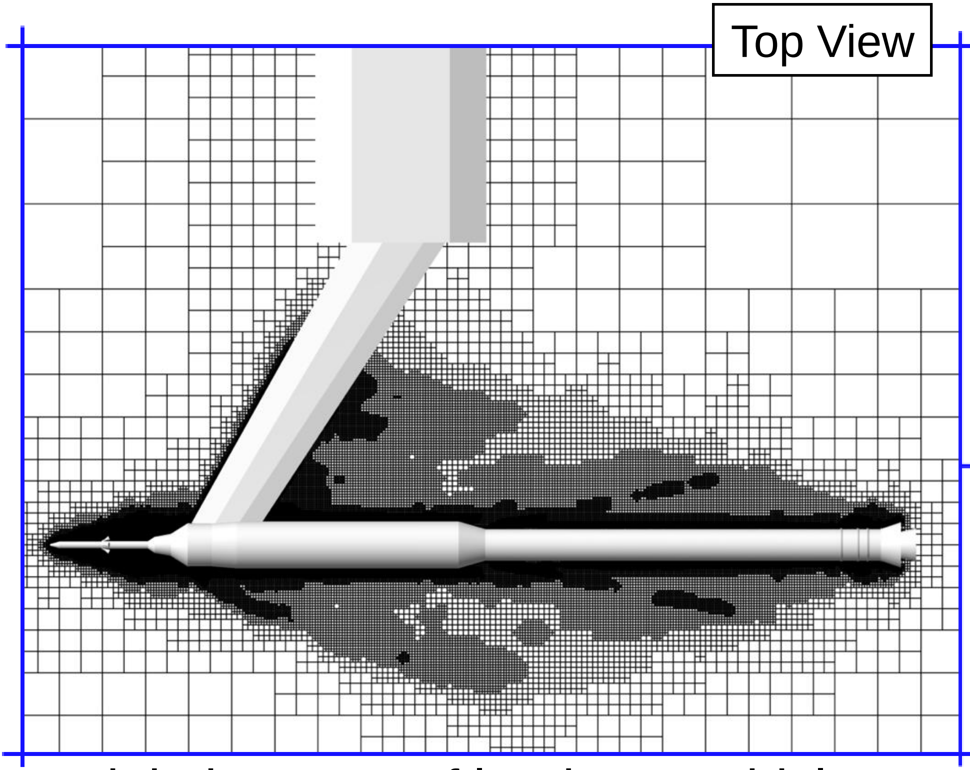


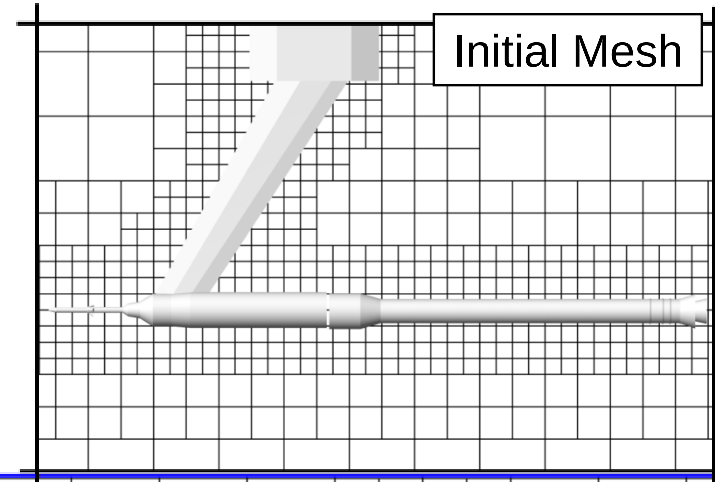


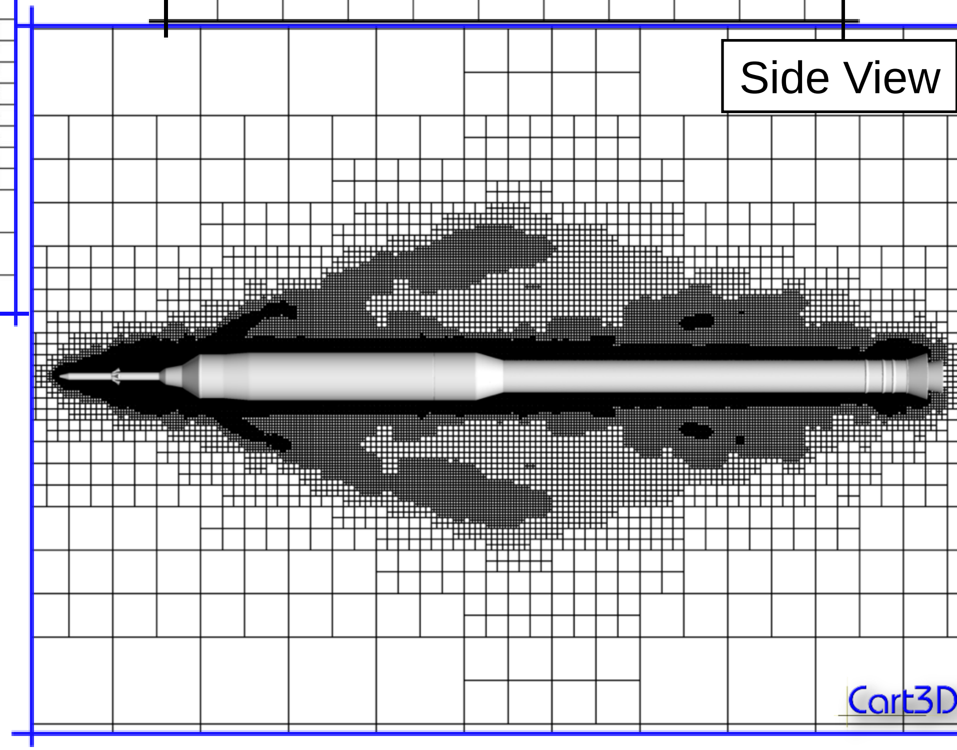
- NASA Space Aerosciences review of capabilities identified principal challenges:
  - Prediction of unsteady separated flows
  - Aero-plume interaction prediction
  - Aerothermal predictions
- Ares I program:
  - Aerocoustic vibrations, buffet
  - Determined CFD more expensive, less reliable than experimental testing (used for unfeasible test conditions)
  - Overly conservative design, reduced payload to orbit
- Mars Science Lab (Curiosity)
  - Data showed overly conservative heat shield design (LAURA)
  - Quantifying uncertainties paramount (1 shot)
- Historically, NASA space programs have used existing computational tools developed within ARMD
  - Columbia Accident Investigation (Overflow, Cart3d)
  - Constellation, SLS, Orion
- Advances will require foundational investments



Adjoint-based Discretization Error Control for Vehicle Stage Separation(CART3D/inviscid)

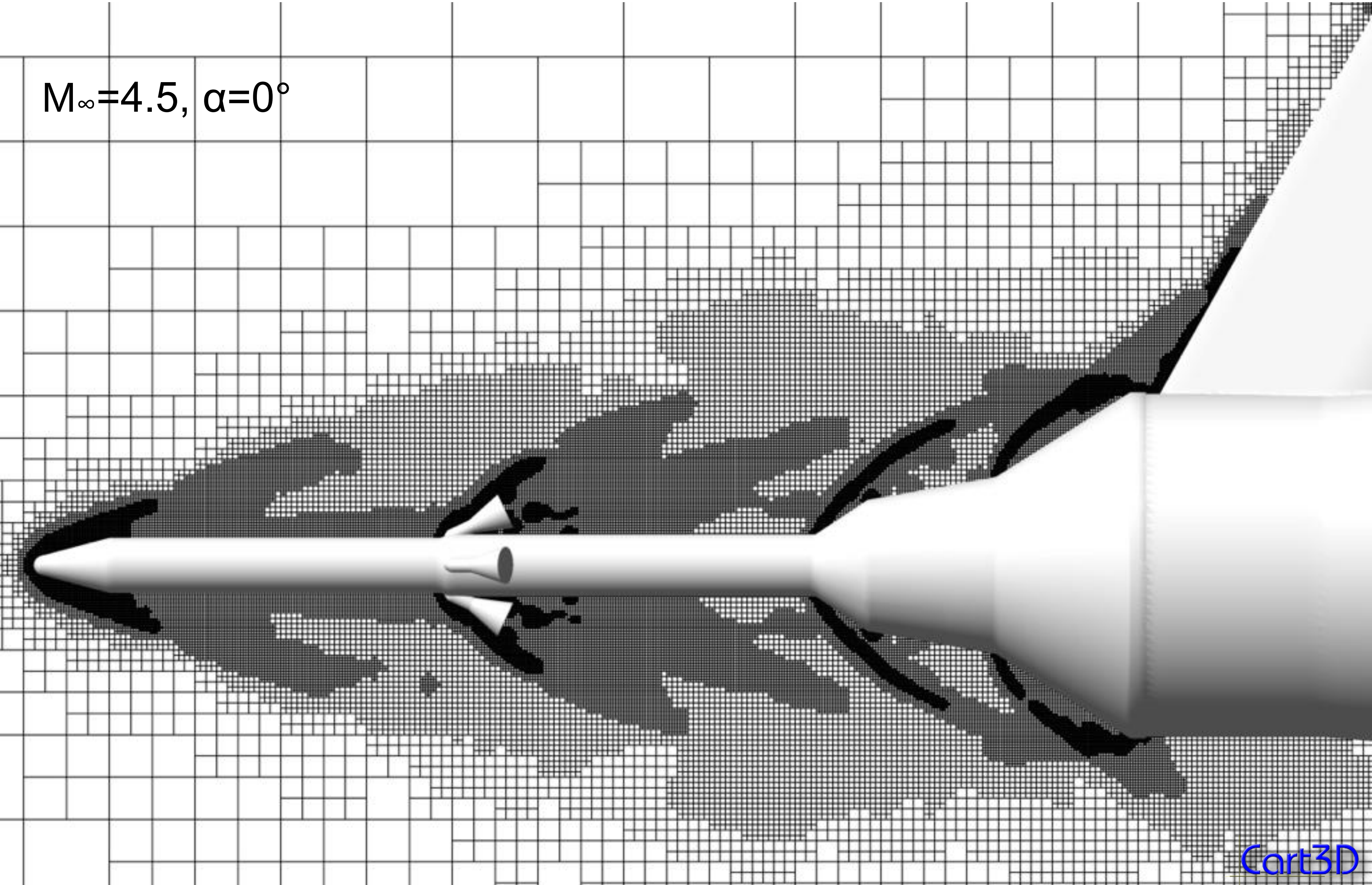


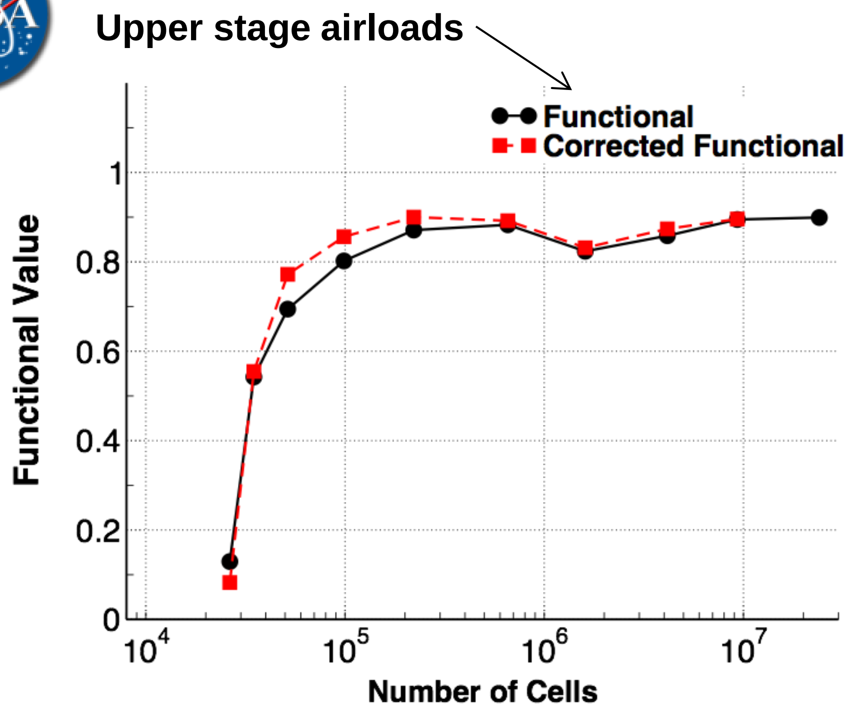


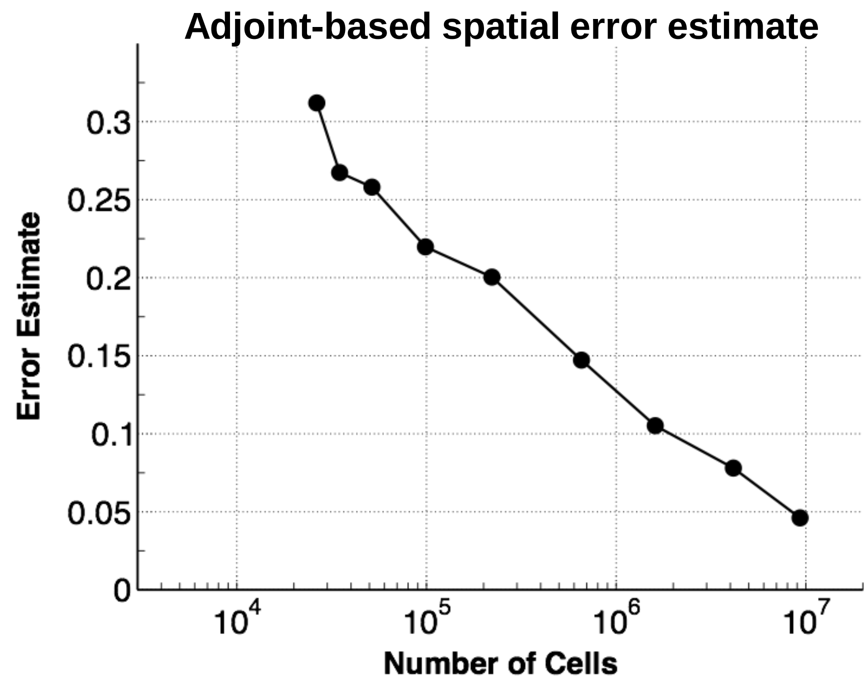


- Minimize error of loads on vehicle upper stage
- Initial mesh contains only 13k cells
- Final meshes contain between 8M to 20M cells

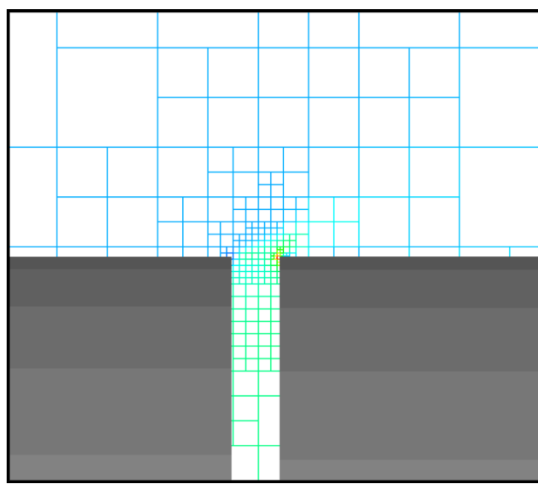
Pressure Contours



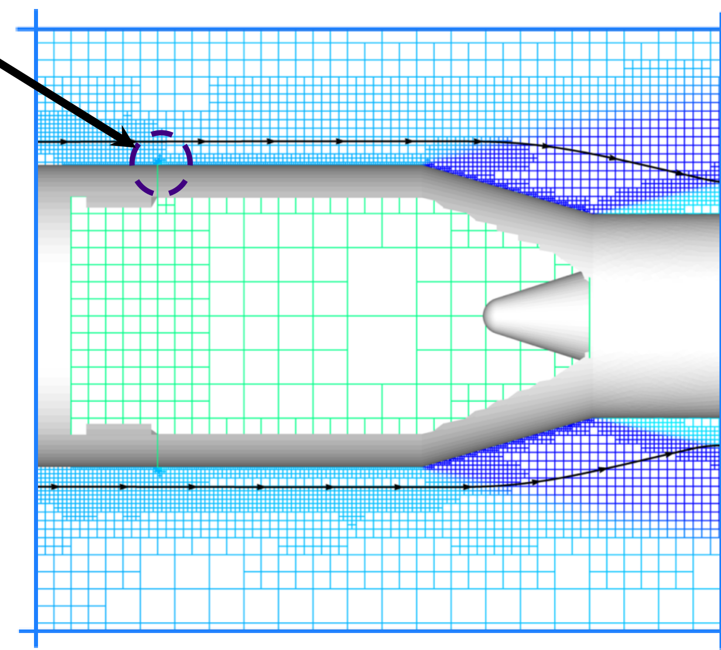




- Minimal refinement of inter-stage region
- Gap is highly refined
- Overall, excellent convergence of functional and error estimate



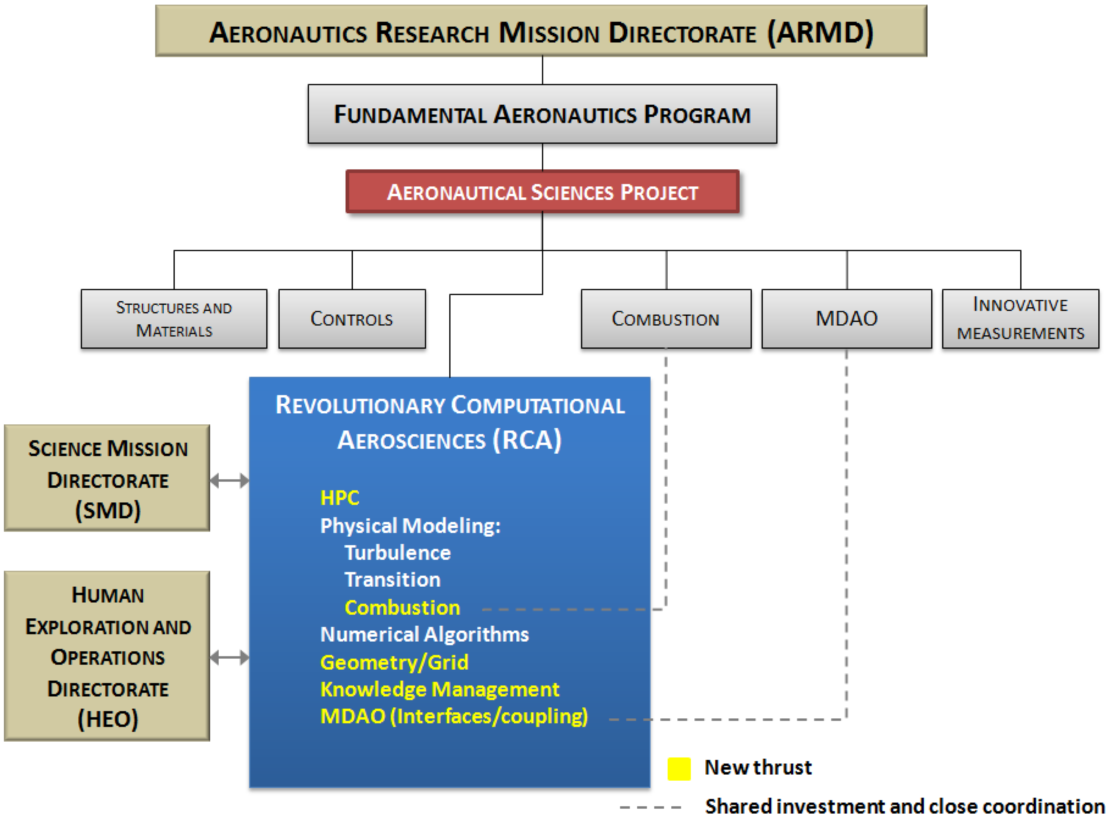
Cutaway view of inter-stage



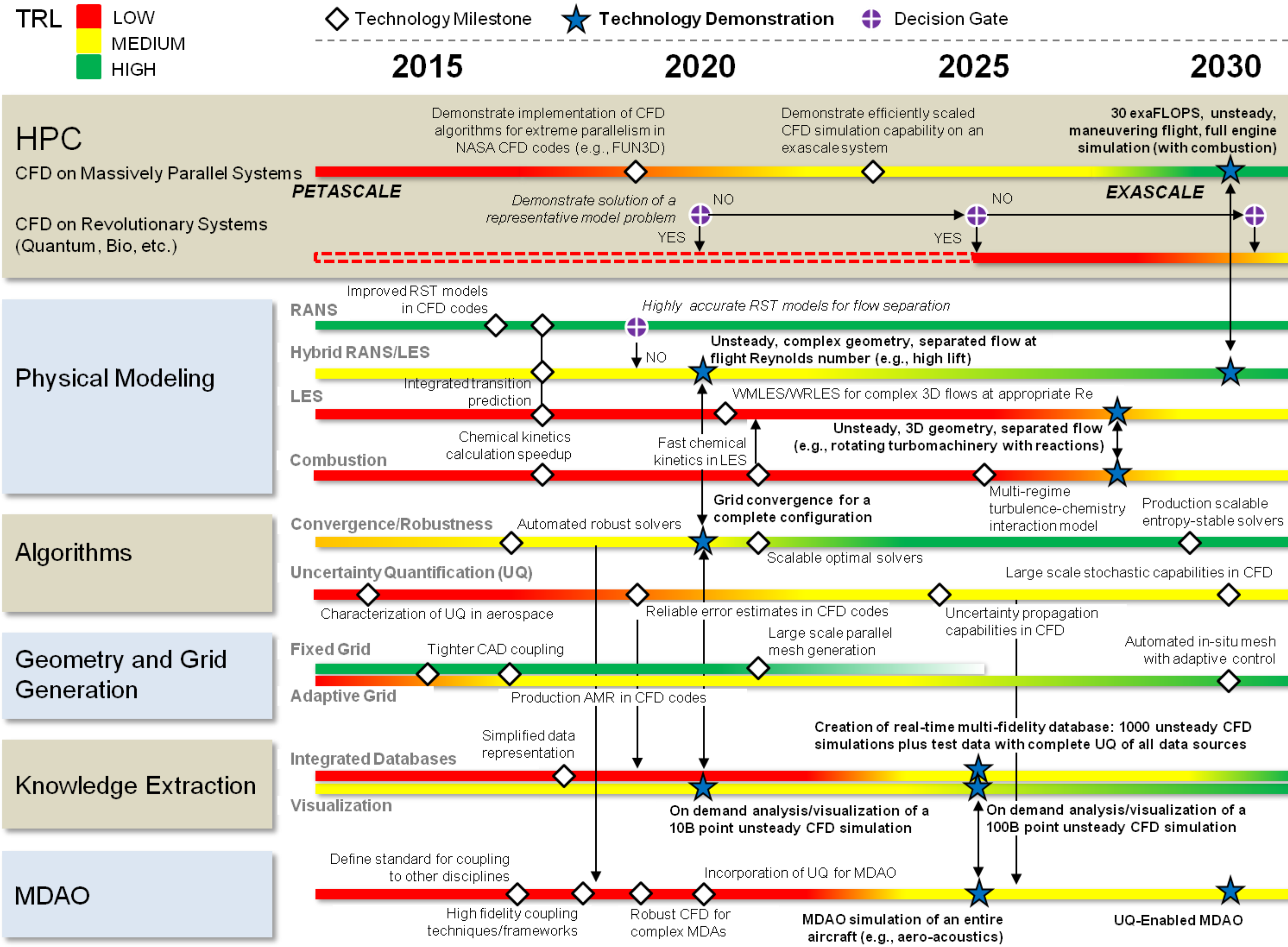
Recommendations

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

   - Required to fulfill technology development plan and address Grand Challenge problems
   - RCA program to coordinate ALL key CFD technologies, including combustion and MDAO → *structured around six technology areas*
   - Success will require collaboration with experts in mathematics, computer science, computational geometry, and other aerospace disciplines



Technology Roadmap



Recommendations CONTINUED

3. Make available and utilize HPC systems for large-scale CFD development and testing.

- Provide access to large-scale computing for both throughput (capacity) to support on-going programs, but also development (capability) to directly support technology demonstrations and progress towards Grand Challenge problems.
- **Survey of NASA Pleiades Supercomputer (October 2013)**
  - 200,000 cores: #19 on Top 500 list
  - 469 jobs, average 457 cores per job
  - Largest job: 5000 cores (only job > 1000 cores)
- **Selected NASA projects using INCITE resources**

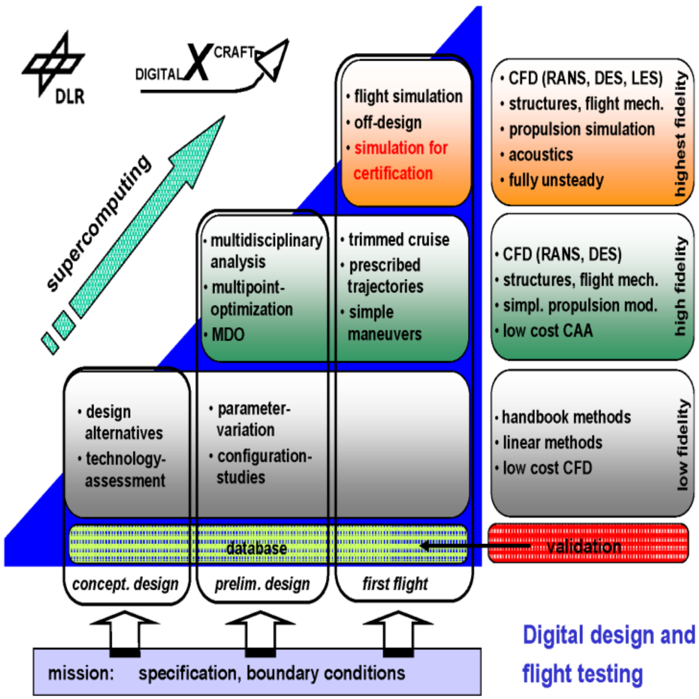
- **Strategic HPC approach required**
  - Make large scale HPC available for software research and development
  - Investigate emerging architectures
  - Shared investment within NASA and across other government agencies

Recommendations CONTINUED

5. **Develop, foster, and leverage improved collaborations with key research partners and industrial stakeholders across disciplines within the broader scientific and engineering communities.**
   - Aerospace engineering arguably has been the leading application in computational engineering
     - Unique interaction between government (NASA, DoD), industry, academia
   - Computational science in aerospace engineering is underfunded and insular
     - National Aerospace R&D Plan (OSTP) focuses on aerospace specific outcomes with no mention of foundational technologies in applied math, computer science, HPC etc.
   - Leverage other government agencies and stakeholders (US and foreign) outside of the aerospace field → *collaborate with DoE, DoD, NSF, NIST, etc.*
   - Re-emphasize basic funding in applied math and computer science → *Advanced developments in CFD will require breakthroughs in numerical algorithms and efficient solution techniques for emerging HPC systems*

Conclusions

- Exascale will enable revolutionary capabilities in aerospace analysis, design, understanding, capabilities
  - **Decadal Survey of Civil Aeronautics (NAE)**:*"…an important benefit of advances in physics-based analysis tools is the new technology and systems frontiers they open"*
- *Improved simulation capabilities bring:*
  - *Superior/more capable designs*
  - *Reduced development cycle time/cost/risk*
  - *Scientific and industrial competitiveness*
- *Holy grail of aerospace product development:* ***Certification by analysis***
- Achieving exascale for aeronautical /aerospace applications will be very challenging
  - Requires sustained foundational investment
  - Strong engagement with national HPC efforts and CSE communities



Digital design and flight testing