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Simulation of Turbulent Flow on Emerging HPC – An Aerospace Perspective

DOE ASCR Workshop on Turbulent Flow Simulation at the Exascale: Opportunities and Challenges
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"I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic."

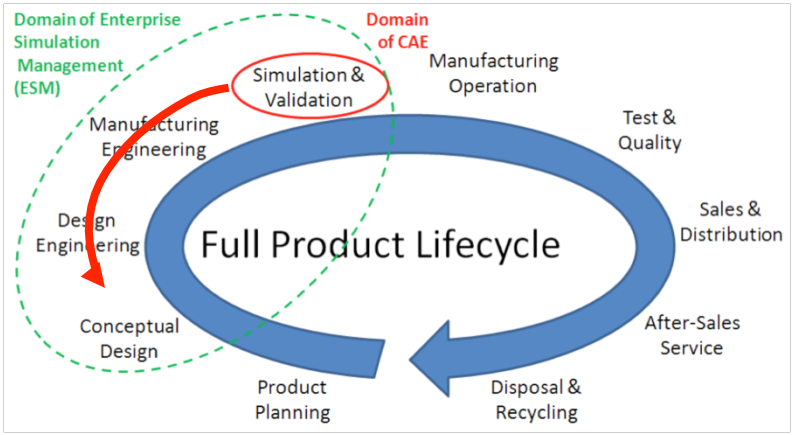
— *Sir Horace Lamb*

Outline

- Background – Turbulence Simulation in Aerospace
- Vision 2030 CFD Study
- Open Issues
- Emerging HPC
- Turbulence Modeling on Exascale – Challenges
- Research Thrusts
- Outlook
- Opportunities

Aerospace CFD Today: Success Driving Opportunity

- **Physics-based numerical simulation continues to expand into all development phases of the aerospace vehicle/system lifecycle.**
  - Drive to reduce non-recurring product development costs and risk
  - Drive to create products that are environmentally cleaner, more fuel efficient, etc.
  - Drive to attain designs close to the optimum

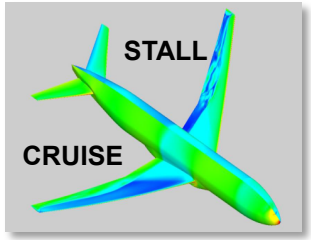


Hanna, K. and Parra, J "BACK TO THE FUTURE: TRENDS IN COMMERCIAL CFD" www.mentor.com

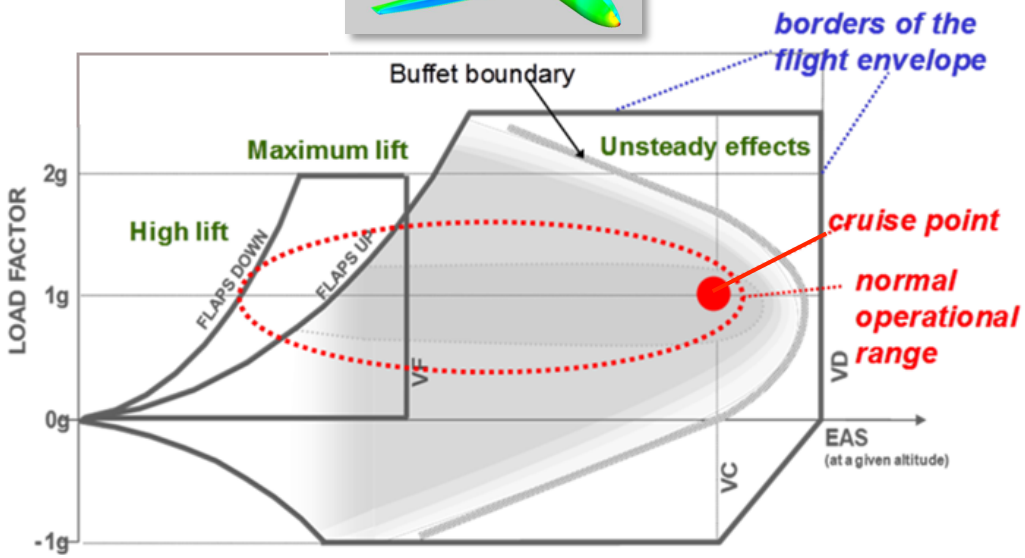
- **Obtaining reasonably accurate simulations with full configuration geometry and complex flow physics is now commonplace:**
  - Enabled by ever evolving **High Performance Computing (HPC)** to solve on larger and larger models within an acceptable amount of time
  - Providing **deeper physical insight** into more realistic flow physics
  - Creating full simulation **databases** to support product design and development
  - Pushing into aerodynamic optimization

The accurate simulation of turbulence is critically important in determining aerodynamic characteristics and performance

Opportunity: Commercial Aviation



- **High-fidelity CFD tools and methods are enabling:**
  - Significant **reductions in non-recurring product development costs** (e.g., experimental loads and performance testing)
  - Increasing **expansion of CFD prediction** at the **edges of the flight envelope** (e.g., high-lift, S&C)
  - **GOAL: Certification and/or Qualification by Analysis**

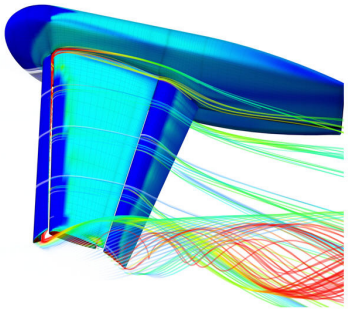


Source: O. Brodersen, C.-C. Rossow, N. Kroll, "Digital-X: Towards Virtual Aircraft Design and Testing Based on High-Fidelity Methods - Recent Developments at DLR," DLR Institute of Aerodynamics and Flow Technology, Prof. A. Jameson 80th Symposium on Mathematics, Computing & Design – Where Analysis and Creativity Combine, 20-21 Nov. 2014, Stanford, USA

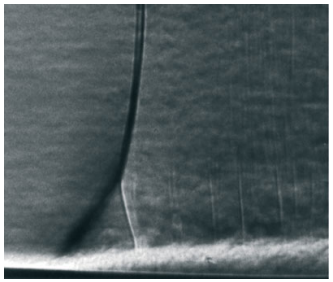
- **Challenges:**
  - Flow physics (with multiple **sources of error**)
  - **Large database** coverage required (with **extremely large grid models**)
  - Requires rigorous documentation, best practices, and data management
  - Need for **well defined and consistent processes**

Flow Turbulence in Aerospace Applications

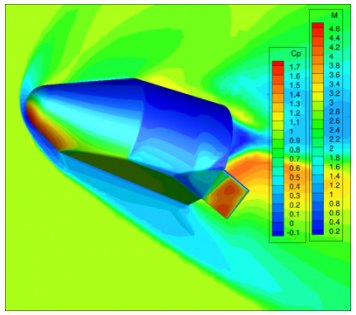
- **Viscous Flow Physics**
  - adversely affects the aerodynamic performance of aerospace vehicles primarily through **flow separation.**
- **Multiple Types of Separation:**
  - **Smooth body (incipient) –** separation driven by adverse pressure gradients on curved surfaces
  - **Shock-induced –** separation from shock interactions with the wall boundary layer
  - **Bluff body –** separation due to rapid change in curvature on shapes that have a blunt base in the flow direction



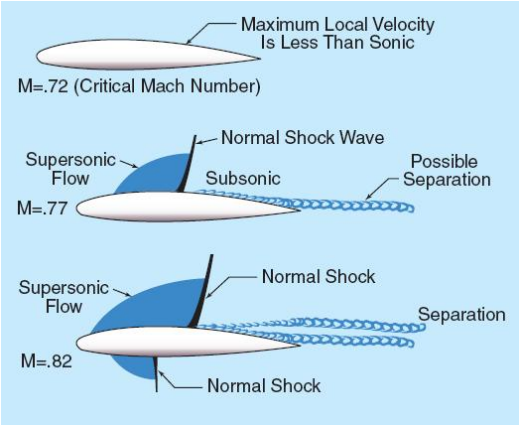
Credit: Ansys



Credit: FAST Project, European Union



Credit: Blue Origin

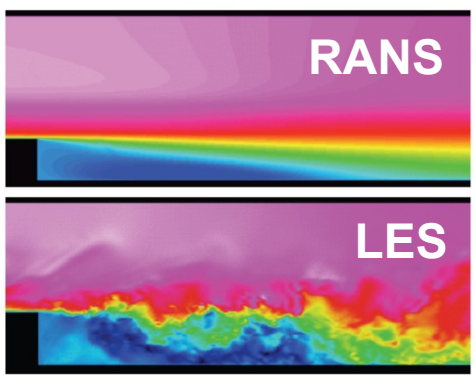


Source: U.S. Federal Aviation Administration - Airplane Flying Handbook. U.S. Government Printing Office, Washington D.C.: U.S. Federal Aviation Administration, p. 15-7. FAA-8083-3A

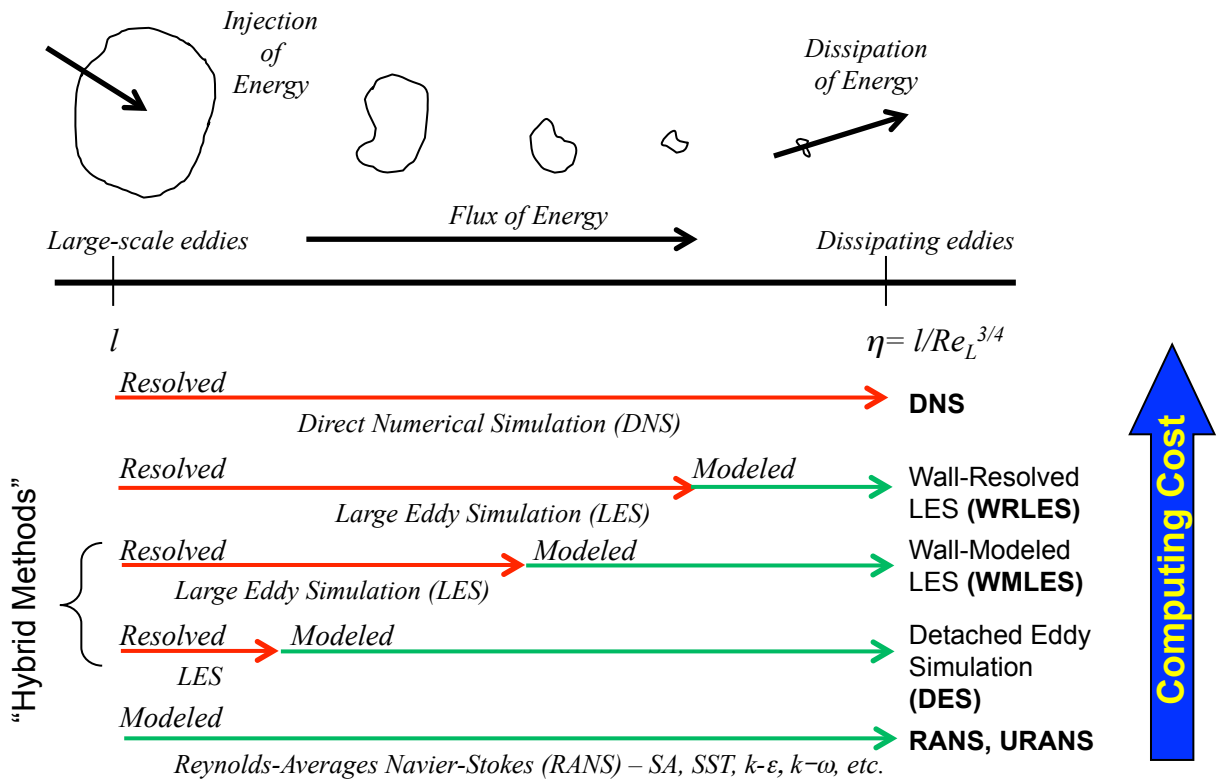
Credit: Ensign John Gay, USS Constellation, US Navy

Numerical Simulation of Turbulence

- **In a CFD simulation, turbulence is either solved directly from the flow equations ("resolved") or approximated ("modeled"). These approaches may (and often) co-exist.**
- **With emerging HPC, simulations that resolve more of the flow turbulence will become more achievable.**



Source: Remy Fransen, 3rd INCA colloquium, ONERA, 2011



Source: Based on the original chart by Andre Bakker

Vision 2030 CFD Study

- **In September 2012, NASA commissioned a one-year contract to develop a comprehensive and enduring vision of future CFD technology and capabilities *specifically for aerospace applications*:**
  - "…provide a **knowledge-based forecast** of the future computational capabilities required for **turbulent, transitional, and reacting flow simulations…**"
  - "…and to lay the foundation for the **development of a future framework/environment** where physics-based, accurate predictions of complex turbulent flows, including flow separation, can be accomplished routinely and efficiently in cooperation with **other physics-based simulations to enable multi-physics analysis and design.**"

NASA Technical Monitor – **Mujeeb Malik**

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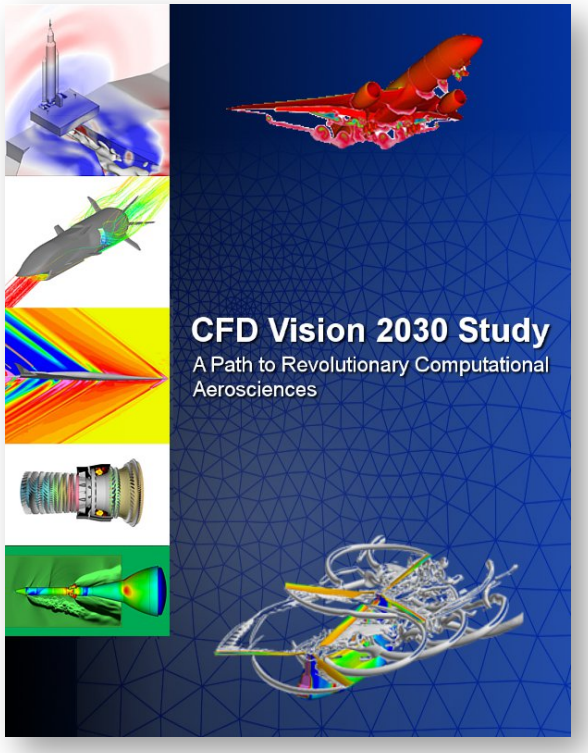
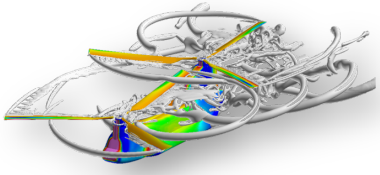
Vision 2030 CFD Study

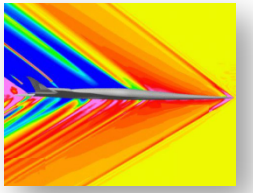


- **Elements of the study effort:**
  - Define and develop **CFD requirements**
  - Identify the most critical **gaps and impediments**
  - Create the **vision**
  - Develop a long-term, actionable **research plan** and detailed **technology development roadmap**
- **Executed user survey and technical workshop**
- **Comprehensive final report – NASA CR 2014-218178**
  - Provides a detailed CFD vision and technology outlook, including assessment of High Performance Computing (HPC)
  - **Guides future CFD technology development** at NASA and within the broader CFD community
  - Being used as an **advocacy document** to drive the implementation of the CFD vision

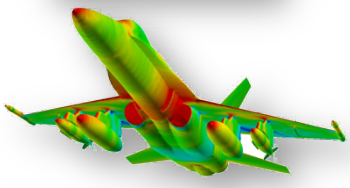
The CFD 2030 Vision



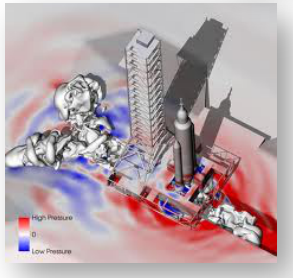
- **Emphasis on physics-based, predictive modeling**
  Transition, turbulence, separation, chemically-reacting flows, radiation, heat transfer, and constitutive models, among others.



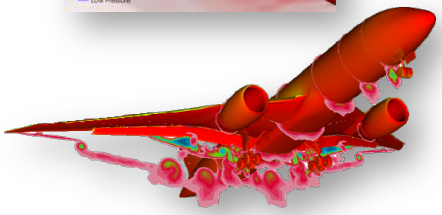
- **Management of errors and uncertainties**
  From physical modeling, mesh and discretization inadequacies, natural variability (aleatory), lack of knowledge in the parameters of a particular fluid flow problem (epistemic), etc.



- **A much higher degree of automation in all steps of the analysis process** Geometry creation, meshing, 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.



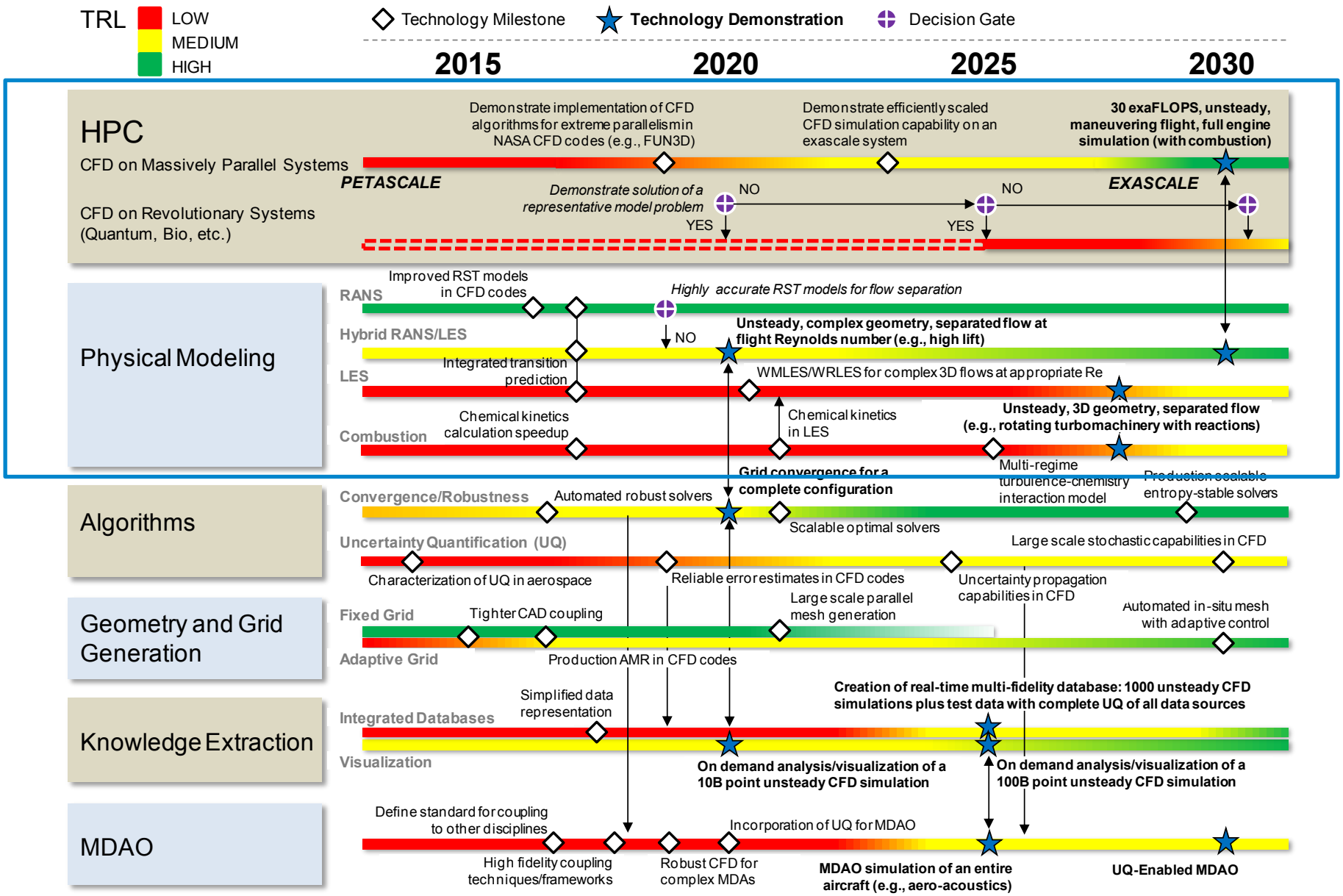
- **Flexible use of HPC systems**
  Capability- and capacity-computing tasks in both industrial and research environments.

- **Seamless integration with multi-disciplinary analyses**
  High fidelity CFD tools, interfaces, coupling approaches, etc.

Vision 2030 CFD Study - Findings

1. **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.
2. **HPC hardware is progressing rapidly** and technologies that will prevail are difficult to predict.
3. The **accuracy of CFD** in aerospace design is severely limited by the **inability to reliably predict turbulent flows** with regions of **separation.**
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.
5. **Revolutionary algorithmic improvements** will be required to enable future advances in simulation capability.
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.
7. Significant advances are required to enable increasingly **multidisciplinary simulations** – for both **analysis and design optimization purposes.**

Vision 2030 CFD Roadmap



Turbulence Simulation – Open Issues from Vision Report

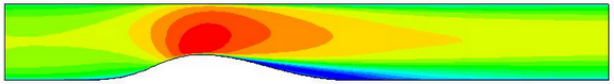
1. **Hybrid RANS-LES capability for engineering applications is:**
   - Cost-prohibitive
   - Not yet able to resolve pre-separation flow physics (provided by RANS) to the required level of accuracy.
   - No robust and effective switch between RANS and LES.
2. **Lack of availability and convergence of complex RANS models in practical codes:**
   - Models with **second moment closures (Reynolds Stress Models)** have not been proven to be more effective than 1-equation models
3. **Effect of grid resolution and solution scheme on assessing models, particularly for complex geometries, is not well understood.**
4. **Lack of foundational experiments to guide turbulence model development (both building-block and "real world")**
5. **Lack of a robust transition prediction capability**
6. **Lack of access to large HPC resources for code development:**
   - Needed to devise and test new techniques on industrial applications
   - Needed to develop highly-scalable software for use with large HPC resources

Turbulence Model Resource

- **Website that serves as a central repository where Reynolds-averaged Navier-Stokes (RANS) turbulence models are documented.**
- ***http://turbmodels.larc.nasa.gov***
- **Effort is guided by the Turbulence Model Benchmarking Working Group (TMBWG), a working group of the Fluid Dynamics Technical Committee of the American Institute of Aeronautics and Astronautics (AIAA).**

Langley Research Center

Turbulence Modeling Resource



Turbulence Models

- One-Equation Models:
  - Spalart-Allmaras
  - Nut-92
- Two-Equation Models:
  - Menter k-omega SST
  - Menter k-omega BSL
  - Wilcox k-omega
  - Chien k-epsilon
  - K-kL
  - Explicit Algebraic Stress k-omega
- Three-Equation Models:
  - K-e-Rt
- Seven-Equation Omega-Based Full Reynolds Stress Models:
  - Wilcox Stress-omega
  - SSG/LRR
- Seven-Equation Epsilon-Based Full Reynolds Stress Models:
  - GLVY Stress-epsilon

Turbulence Model Validation Cases and Grids

- **Basic Cases:**
  - **2DZP:** 2D Zero pressure gradient flat plate
  - **2DML:** 2D Mixing Layer
  - **2DANW:** 2D Airfoil near-wake
  - **2DN00:** 2D NACA 0012 airfoil
  - **ASJ:** Axisymmetric Subsonic jet
  - **AHSJ:** Axisymmetric Hot subsonic jet
  - **ANSJ:** Axisymmetric Near-sonic jet
  - **ASBL:** Axisymmetric Separated boundary layer
  - **ATB:** Axisymmetric Transonic Bump
- **Extended Cases:**
  - **2DZPH:** 2D Zero pressure gradient high Mach number flat plate
  - **2DBFS:** 2D Backward facing step
  - **2DN44:** 2D NACA 4412 airfoil trailing edge separation
  - **2DCC:** 2D Convex curvature boundary layer
  - **2DWMH:** 2D NASA wall-mounted hump separated flow
  - **ASWBLI:** Axisymmetric Shock Wave Boundary Layer Interaction near M=7 <- under construction
  - **3DSSD:** 3D Supersonic square duct

LES Cost Estimate and Outlook for 2030

- **Full LES for engineering use will not be available by 2030.**
- **Estimate for Wall-Modeled LES (WMLES), where the anisotropic near-wall is modeled by some other means:**
  - **Estimates based on "cubes of volume", δ^3 (where δ is the boundary layer thickness) for a NACA 0012 airfoil of unit chord where the flow is computed with an integral BL method and transition estimated using an e^N method:**

Re_c	N^{lam}_{Cubes}	N^{turb}_{Cubes}	N_{cubes} (total)
1e6	1.1e6	1.3e4	1.1e6
1e7	1.1e7	1.5e5	1.1e7
1e8	9.1e7	3.1e6	9.4e7

  - **Estimate of WMLES on HPC in 2030 for Mach=0.2 flow around a unit aspect-ratio wing. Assume current grid/solution scheme, and 1250 flops/iteration/point. PFLOP/s is time to get a converged solution in 24 clock hours**

Re_c	N_{DOF}	FLOP	PFLOP/s
1e6	9.0e9	5.2e20	6
1e7	8.5e10	1.6e22	180
1e8	7.5e11	4.3e23	5000

By 2030, **WMLES** will likely be possible for an airfoil test case on exascale systems, but **will not be possible for configurations of engineering interest**

Emerging HPC

'Going to the exascale' will mean a radical change in computing architecture – basically, **vastly increasing the levels of parallelism** to the point of millions of processors working in tandem – which will force radical changes in how hardware is designed (at minimum, driven by **economic limitations on power consumption**), in how we go about solving problems (e.g., the application codes), and in how we marry application codes to the underlying hardware (e.g., the compilers, I/O, middleware, and related software tools).

- "The Opportunities and Challenges of Exascale Computing", Summary Report of the Advanced Scientific Computing Advisory Committee (ASCAC) Subcommittee, Department of Energy, 2010

- **Exascale (10^{18} operations/sec)** will be a fundamentally new computing architecture which will require new computing paradigms for effective and efficient usage.

System Parameter	2011	"2018" Swim Lane 1	"2018" Swim Lane 2	Factor Change
System Peak	2 Pf/s	1 Ef/s		500
Power	6 MW	≤20 MW		3
System Memory	0.3 PB	32–64 PB		100–200
Total Concurrency	225K	1B×10	1B×100	40,000–400,000
Node Performance	125 GF	1 TF	10 TF	8–80
Node Concurrency	12	1,000	10,000	83–830
Network BW	1.5 GB/s	100 GB/s	1000 GB/s	66–660
System Size (nodes)	18700	1,000,000	100,000	50–500
I/O Capacity	15 PB	300–1000 PB		20–67
I/O BW	0.2 TB/s	20–60 TB/s		10–30

5-6 orders

<1 order

- "Scientific Discovery at the Exascale: Report from the DOE ASCR 2011 Workshop on Exascale Data Management, Analysis, and Visualization", 2011

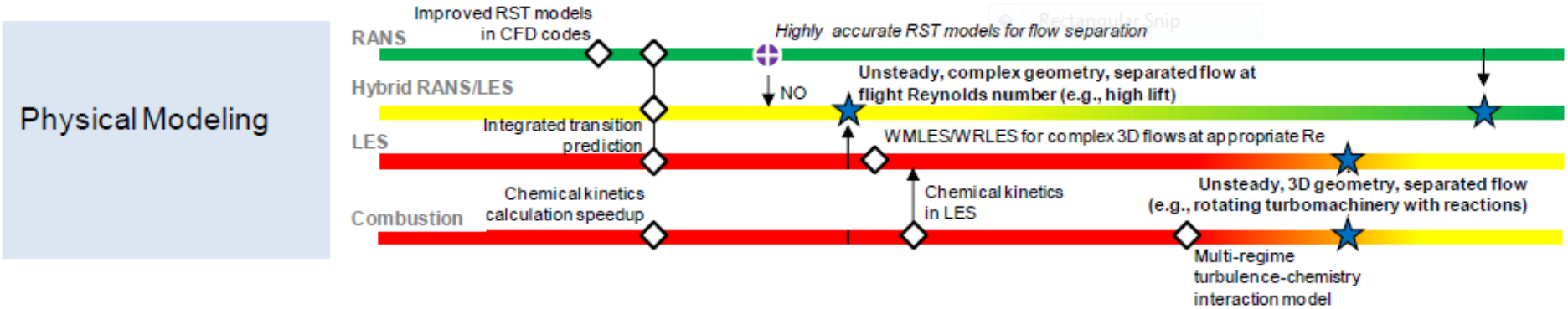
Emerging HPC – Expected Features of Exascale Systems

- **Sample Exascale System**
  - Each node has 16 1-GHz scalar processors
  - Each processor has a 1000-core "streaming" (i.e. distributed memory vector) processor (e.g., Intel Xeon Phi)
  - Each node performs at 128 Tflops; **10,000 nodes performs at 1 exaFlop**
- **Programming**
  - **Integrated, optimized language(s) will likely not be available** → expect special-purpose software that allows programming at a higher, abstracted level (likely a combination of C++/Fortran with MPI/OpenMP combined with Co-Array Fortran and/or CUDA + special tools for accelerators and/or co-processors).
- **Issues**
  - **I/O** → current data movement paradigms will not be effective.
  - **Power** → slower processor speeds, complex elements, lower memory/processor, increased data locality
  - **Fault tolerance** → likely to be higher, mainly due to power compromises
  - **Latency** → will be large, for both local and remote memory references

Turbulence Modeling on Exascale – Challenges

- **Largely dependent on the effectiveness of numerical algorithms on exascale architectures:**
  - Use of standard, currently-formulated implicit solution schemes to solve the non-linear, time-dependent NS and RANS model equations (using a matrix and/or iterative solve) is both memory bandwidth and communication intensive.
  - Explicit methods require significantly smaller times steps (and consequently large compute resources) to be stable, particularly as the grid resolution increases ($\Delta t \rightarrow 1/\Delta x^2$)
    - Might make sense to use for pure LES simulations where the temporal and spatial scales are more similar.

Recommended Research Thrusts in Physical Modeling



- **Multiple tracks:** **2020** **2025**
  1. **RANS Models**
     - Systematic assessment of Reynolds Stress Models.
  2. **Hybrid RANS/LES**
     - Improved RANS (for turbulence initiated in the boundary layer)
     - Seamless, automated RANS-to-LES switch to enhance robustness
  3. **LES**
     - More effective discretizations and solvers tuned for emerging HPC
     - Improved reliability for Wall-Modeled LES (WMLES)
  4. **Combustion**
     - Improved, validated, predictive tool for turbulent reactive flows.
     - Robust switch between combustion regimes (premixed, non-premixed, etc.)
  5. **Transition Modeling**
     - Fully automatic prediction of transition of all types (T-S, cross-flow, etc.)

Outlook

- The DOE clearly understands the need for improved physical modeling in large-scale numerical simulations, and is **actively investing in foundational research**, particularly in anticipation of exascale**.**
- **Focus is on *science*, not on industrial aerospace applications** → "hero" applications, not design exploration (e.g., large heterogeneous databases, etc.)

> *"Today, the advocacy for high performance computing (HPC) is **largely driven by the science community**, with the argument that increased investments in HPC will **lead to greater scientific discoveries**, using simulation as a third pillar in the scientific process, along with theory and experiment [3, 4, 5]. Unfortunately, this **argument does not hold for engineering applications**, since **engineering is not discovery driven**. Engineering problems can differ substantially from science applications, and generally focus on their own set of design-driven objectives, which incur a different set of barriers to effective use of HPC architectures.*

Mavriplis, D. J.,"High Performance Computational Engineering: Putting the 'E' Back in 'CSE' " for Proceedings of the 21st International Conference on Parallel Computational Fluid Dynamics (ParCFD 2009).

- Expect significant progress, but additional effort will be required to **"productionize"**, particularly for engineering applications.

Opportunities

- **Vision 2030 recommendation:** "*NASA should develop, foster, and leverage* ***improved collaborations*** *with* ***key research partners and industrial stakeholders*** *across disciplines within the* ***broader scientific and engineering communities***".
- **DOE does acknowledge the need for collaboration in advancing the state-of-the-art in in-situ processing:** *"It should be a collective effort beyond the DOE community to include the* ***National Aeronautics and Space Administration****, the National Science Foundation, the* ***Department of Defense****, and international partners".*

"Scientific Discovery at the Exascale: Report from the DOE ASCR Workshop on Exascale Data Management, Analysis, and Visualization", February 2011.

Opportunity: Upcoming NASA-sponsored workshop on "Implementation of the 2030 CFD Vision"