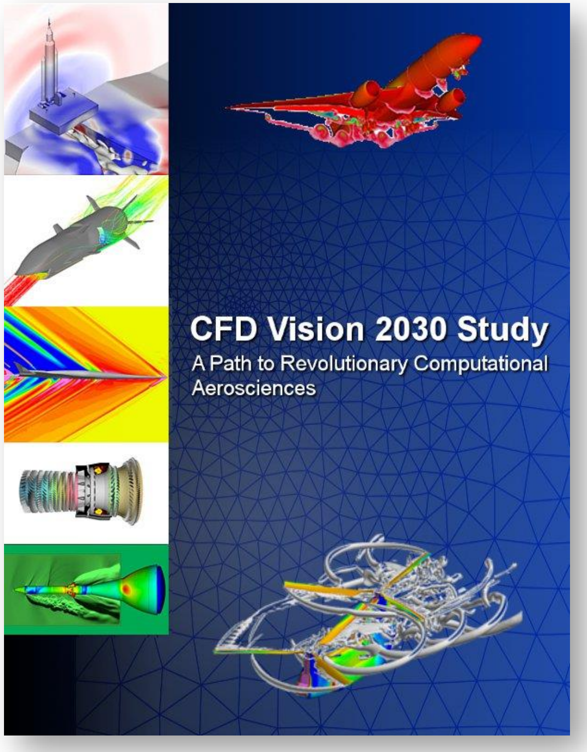
Algorithmic Contributions to the CFD2030 Grand Challenge Problems

Dimitri Mavriplis
University of Wyoming

OVERVIEW

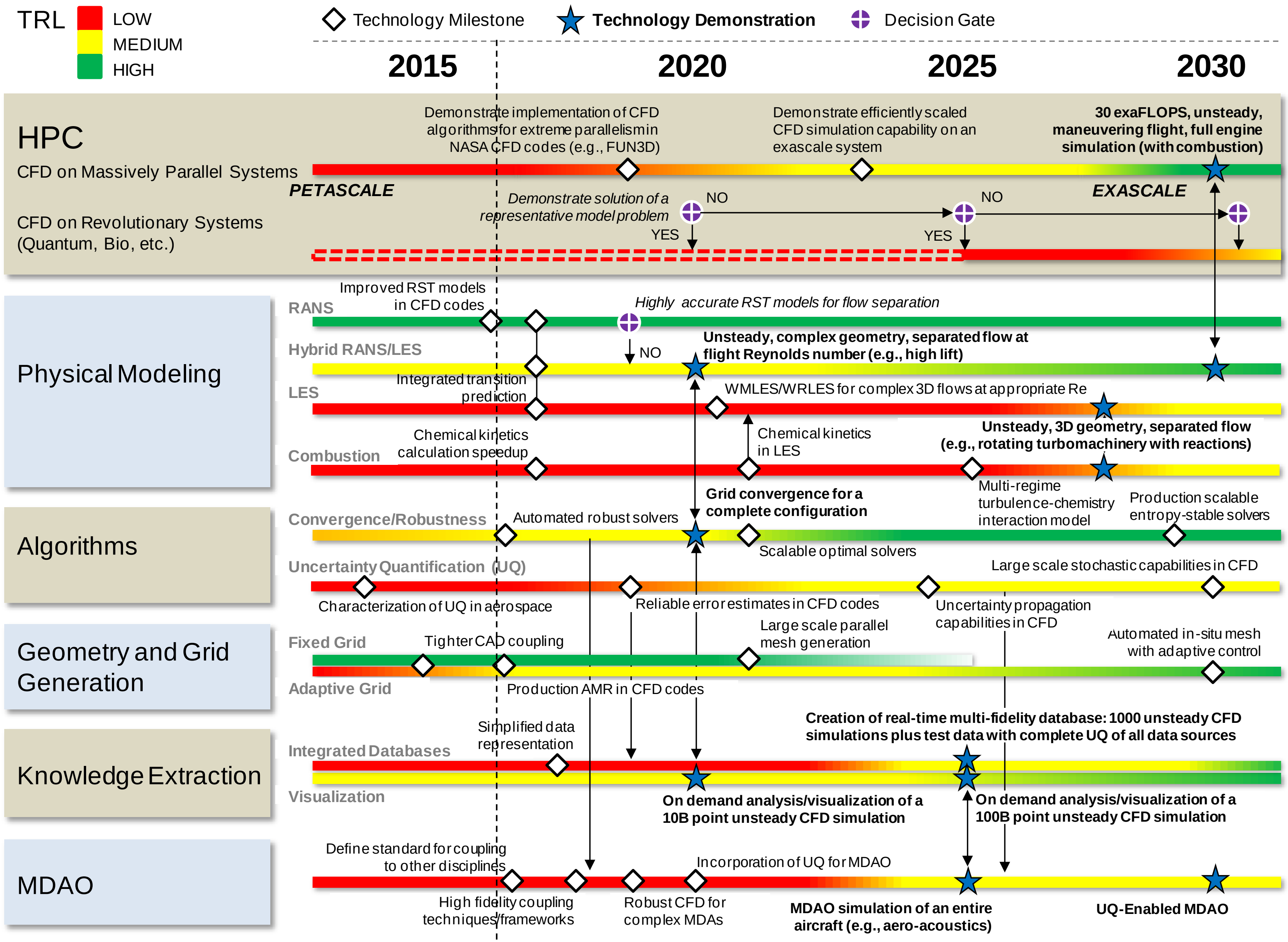
- Introduce Grand Challenge Problems
  - Original notional GCs in CFD2030 report
  - GCs being formulated as part of CFD2030 IC
- Focus on technical challenges to enable GC problems
  - Algorithmic contributions
- Tie back to previous work of A. Jameson
  - Grand Challenges
  - Capabilities enabled by algorithmic contributions of A. Jameson

CFD Vision 2030 Study


CFD Vision 2030 Study
A Path to Revolutionary Computational Aerosciences

- **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

CFD Vision 2030 Roadmap



TRL
🟥 LOW
🟨 MEDIUM
🟩 HIGH

◇ Technology Milestone
★ **Technology Demonstration**
⊕ Decision Gate

2015 2020 2025 2030

HPC

CFD on Massively Parallel Systems

Demonstrate implementation of CFD algorithms for extreme parallelism in NASA CFD codes (e.g., FUN3D)

Demonstrate efficiently scaled CFD simulation capability on an exascale system

30 exaFLOPS, unsteady, maneuvering flight, full engine simulation (with combustion)

PETASCALE

EXASCALE

CFD on Revolutionary Systems (Quantum, Bio, etc.)

Demonstrate solution of a representative model problem

NO
YES
NO
YES

Physical Modeling

RANS
Improved RST models in CFD codes
Highly accurate RST models for flow separation
NO

Hybrid RANS/LES
Unsteady, complex geometry, separated flow at flight Reynolds number (e.g., high lift)

LES
Integrated transition prediction
WMLES/WRLES for complex 3D flows at appropriate Re

Combustion
Chemical kinetics calculation speedup
Chemical kinetics in LES
Unsteady, 3D geometry, separated flow (e.g., rotating turbomachinery with reactions)
Multi-regime turbulence-chemistry interaction model

Algorithms

Convergence/Robustness
Automated robust solvers
Grid convergence for a complete configuration
Scalable optimal solvers
Production scalable entropy-stable solvers

Uncertainty Quantification (UQ)
Characterization of UQ in aerospace
Reliable error estimates in CFD codes
Uncertainty propagation capabilities in CFD
Large scale stochastic capabilities in CFD

Geometry and Grid Generation

Fixed Grid
Tighter CAD coupling
Large scale parallel mesh generation

Adaptive Grid
Production AMR in CFD codes
Automated in-situ mesh with adaptive control

Knowledge Extraction

Integrated Databases
Simplified data representation
Creation of real-time multi-fidelity database: 1000 unsteady CFD simulations plus test data with complete UQ of all data sources

Visualization
On demand analysis/visualization of a 10B point unsteady CFD simulation
On demand analysis/visualization of a 100B point unsteady CFD simulation

MDAO

Define standard for coupling to other disciplines
High fidelity coupling techniques/frameworks
Robust CFD for complex MDAs
Incorporation of UQ for MDAO
MDAO simulation of an entire aircraft (e.g., aero-acoustics)
UQ-Enabled MDAO

Grand Challenge Problems

- Highlight critical **step changes** needed in engineering design capability
- May **not be routinely achievable** by 2030
- Represent 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

Credit: The Boeing Company

Source: Slotnick, et. al, "CFD Vision 2030 Study, A Path to Revolutionary Aerosciences", NASA CR 2014-218178

Proposed GC Problems under CFD2030 IC

  - High Lift Wind up Turn
  - High-Fidelity CFD Based Compressor Performance Map
  - CFD-in-the-Loop Monte Carlo Flight Simulation for Space Vehicle Design
  - Hypersonics Grand Challenge
- Special Session at Aviation 2020

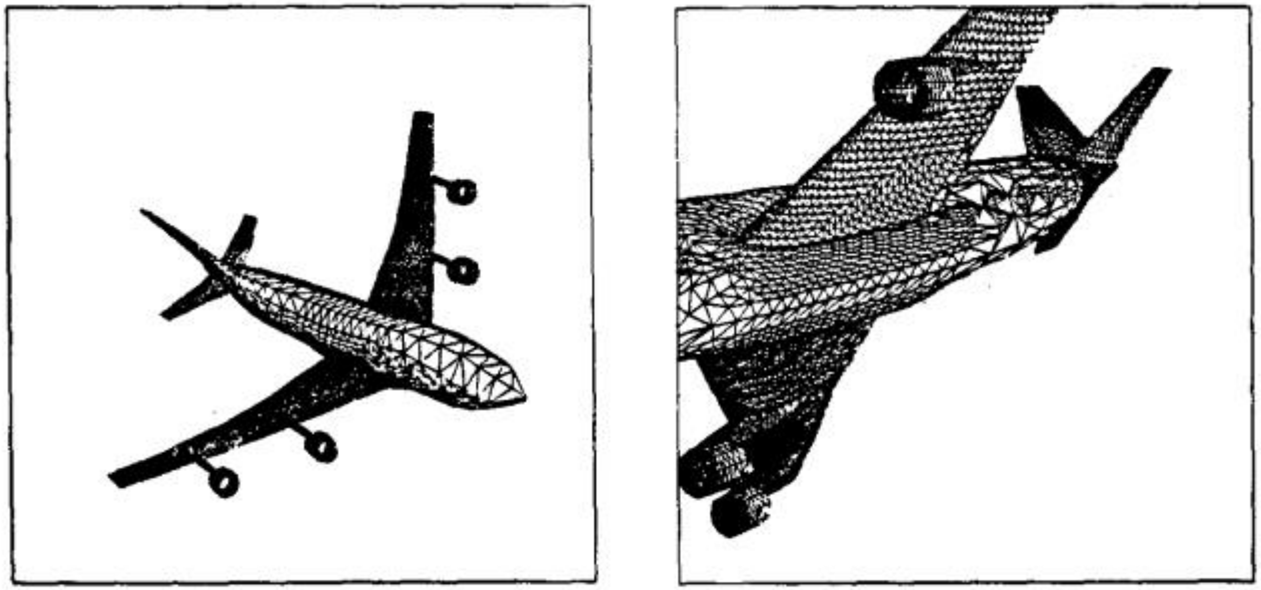
Motivation

- Consideration of Specific GC problem
  - Based on a value proposition: What if ?
  - Identify technical barriers
    - Algorithmic contributions
  - Identify logistical barriers
    - e.g. Computational resources, software engineering
  - Focus resources
  - Promote collaboration towards shared objective
    - CFD technology
    - Meshing technology
    - Disciplinary coupling
    - Uncertainty Quantification
    - Vizualization/Knowledge extraction

Grand Challenge of the 1980's: Full Aircraft CFD Simulation

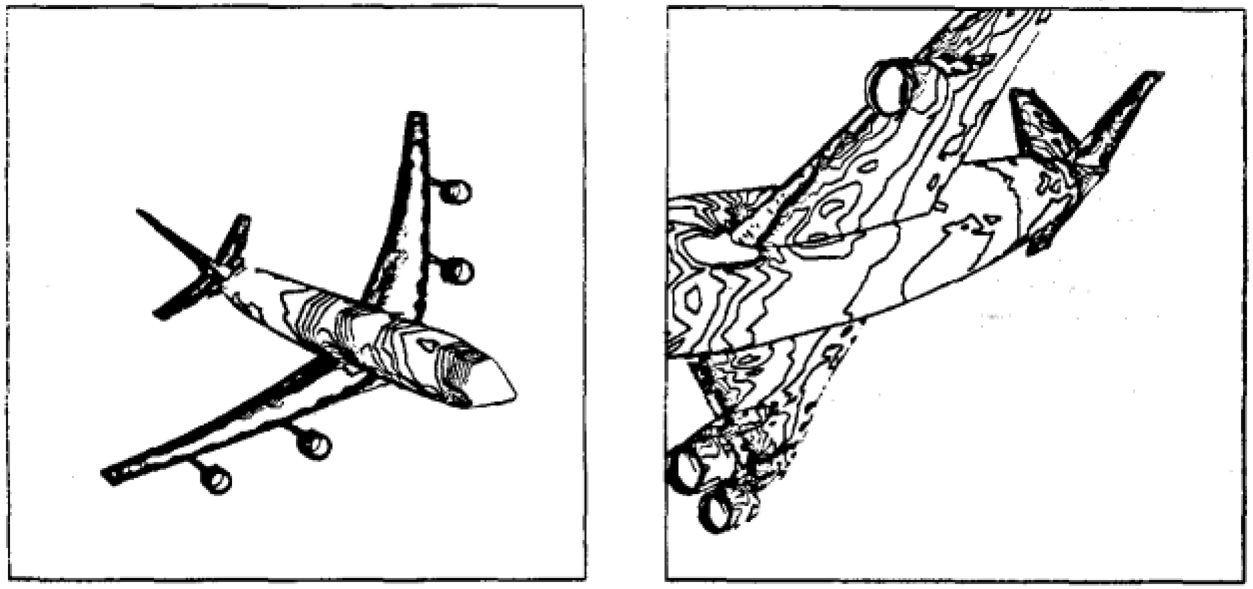
- Wing or wing body configurations SOA
  - Single or multi-block structured meshes
- Extensions to wing-pylon-nacelle difficult
- Extensions to 3D high-lift configurations considered intractable
- Required a rethinking of current approaches
  - Unstructured meshes

1986-87 Jameson Airplane Papers



- Unstructured tetrahedral mesh
  - **35,370 points, 181,959 tetrahedra**
  - Mesh generation: 15 minutes
    - No mention of geometry issues
  - Flow solver : 1 hour on 1 processor of CRAY-XMP
    - Vectorized, later parallelized for CRAY-XMP/YMP

1986-87 Jameson Airplane Papers



- Unstructured tetrahedral mesh
  - **35,370 points, 181,959 tetrahedra**
  - Mesh generation: 15 minutes
    - No mention of geometry issues
  - Flow solver : 1 hour on 1 processor of CRAY-XMP
    - Vectorized, later parallelized for CRAY-XMP/YMP

Jameson Airplane

- Essentially a self-created GC problem
- Largely enabled through algorithmic advances
- Required collaboration and advances on various fronts
  - Mesh generation
    - Delaunay triangulation/Surface recovery
  - Discretization
    - JST scheme on tetrahedral elements/Edge based data structure
  - Parallel computing
    - Cray multitasking

Current Day GC:
High Lift Wind Up Turn

- Aircraft Maneuver at Edge of Flight Envelope
  - Demonstration for design
  - Implications for certification by analysis (CbA)
- Characteristics:
  - Multidisciplinary
    - Aerodynamics, structures, controls
  - Flow physics
    - Stall, buffet, smooth body separation
- Break down into series of challenge problems of increasing difficulty

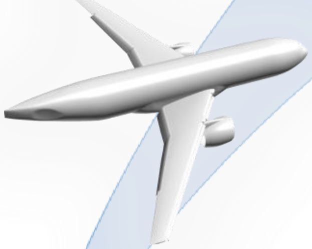
Advancing High Lift Aerodynamic Prediction

Series of Challenge Problems

Improve accuracy and speed of CFD predictions in phased approach

CRM-HL Ecosystem

Sub-Challenge Problem #1
1-3 years



CRM-HL
Landing/TO configuration
Up to flight Re
Flow physics (separation, vortical flow)
Static aeroelastics
Ice effects

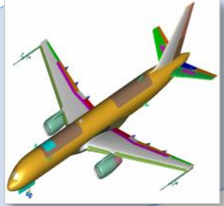
Sub-Challenge Problem #2
3-6 years

CRM-HL + EMPAS
Challenge Problem #1 +
S&C (control surfaces/trim)
Gear effects
Cross-flow
Power effects
Ice prediction

EMPAS = Electric Motor Powered AeroEngine Simulator

Sub-Challenge Problem #3
6-10+ years

LOW-SPEED WIND-UP TURN (or similar)



Sub-Scale Generic Flight Vehicle
Flight Re
Flight geometry
Dynamic, maneuvering flight
Dynamic structural response

*CFD-generated data populates flight simulation database**

Grand Challenge Problem
15+ years

CRITICAL MANEUVER

Full-Scale Generic Flight Vehicle
Flight Re
Flight geometry
Dynamic, maneuvering flight
Dynamic structural response
Environmental effects
Full engine simulation

*CFD-based flight simulation***

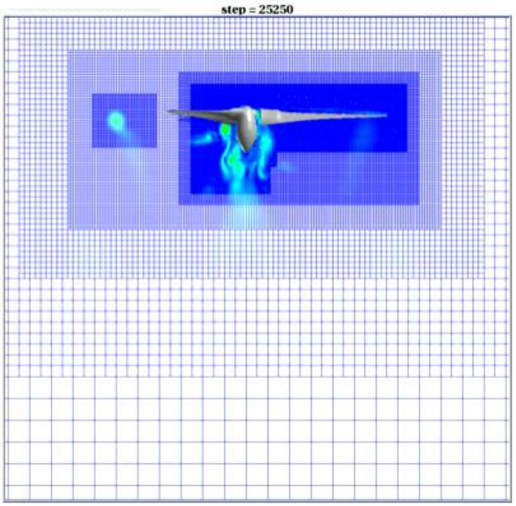
* Accuracy determined by proof-of-match between flight simulation and flight data

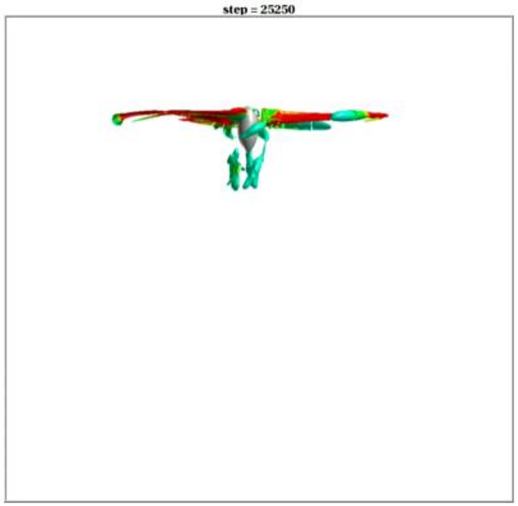
** Flight test used to verify flight simulation

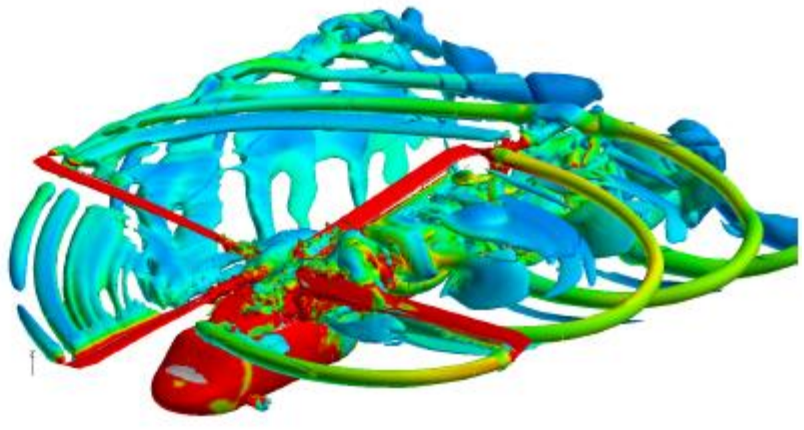
Current Day GC:
High Lift Wind Up Turn

- Logistical Technical Challenges
  - Software coupling of all relevant disciplines
  - Parallel efficiency, emerging hardware trends
  - Software engineering and maintainability
  - Traceable and reproducible (CbA)
- Algorithmic Technical Challenges
  - Very high resolution required
    - Highly detailed water-tight CAD with automatic defeaturing
    - Multi-Billion cell grids/Curved Elements
    - High-order discretizations
    - Efficient implicit solvers
  - Relative geometry motion
    - Dynamic AMR meshes
  - Ability to predict relevant flow physics
    - Scale resolving methods with suitable subgrid scale models
  - Uncertainty Quantification (UQ)
  - In-situ vizualization/Knowledge extraction/ROMs

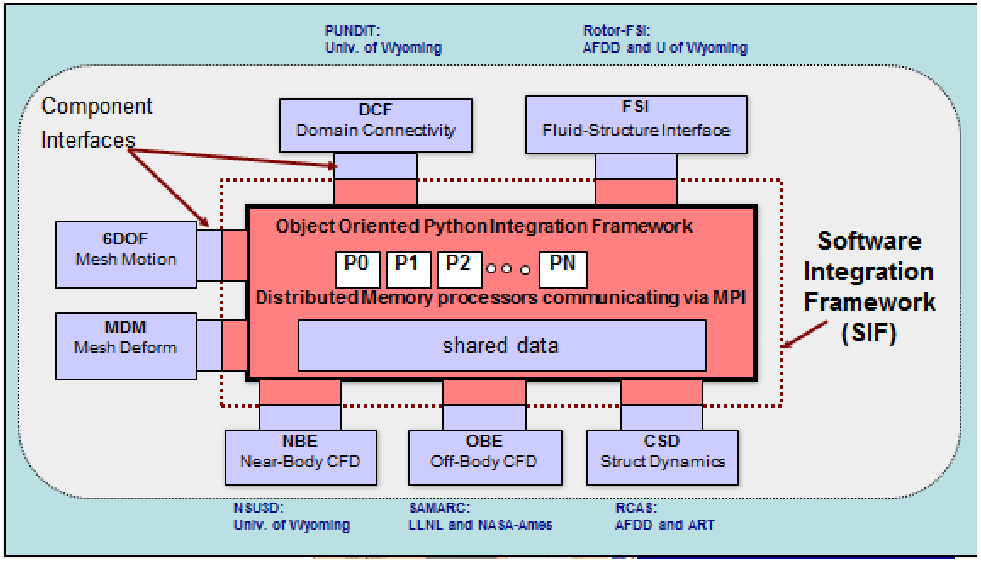
Substantial Advances in Digital Flight
CREATE-AV







- Leveraged dynamic overset, AMR, higher order, multidisciplinary
- Digital fight for rotorcraft even more challenging



PUNDIT:
Univ. of Wyoming

Rotor-FSI:
AFDD and U of Wyoming

Component
Interfaces

DCF
Domain Connectivity

FSI
Fluid-Structure Interface

6DOF
Mesh Motion

MDM
Mesh Deform

Object Oriented Python Integration Framework

P0 P1 P2 ○○○ PN

Distributed Memory processors communicating via MPI

shared data

Software
Integration
Framework
(SIF)

NBE
Near-Body CFD

OBE
Off-Body CFD

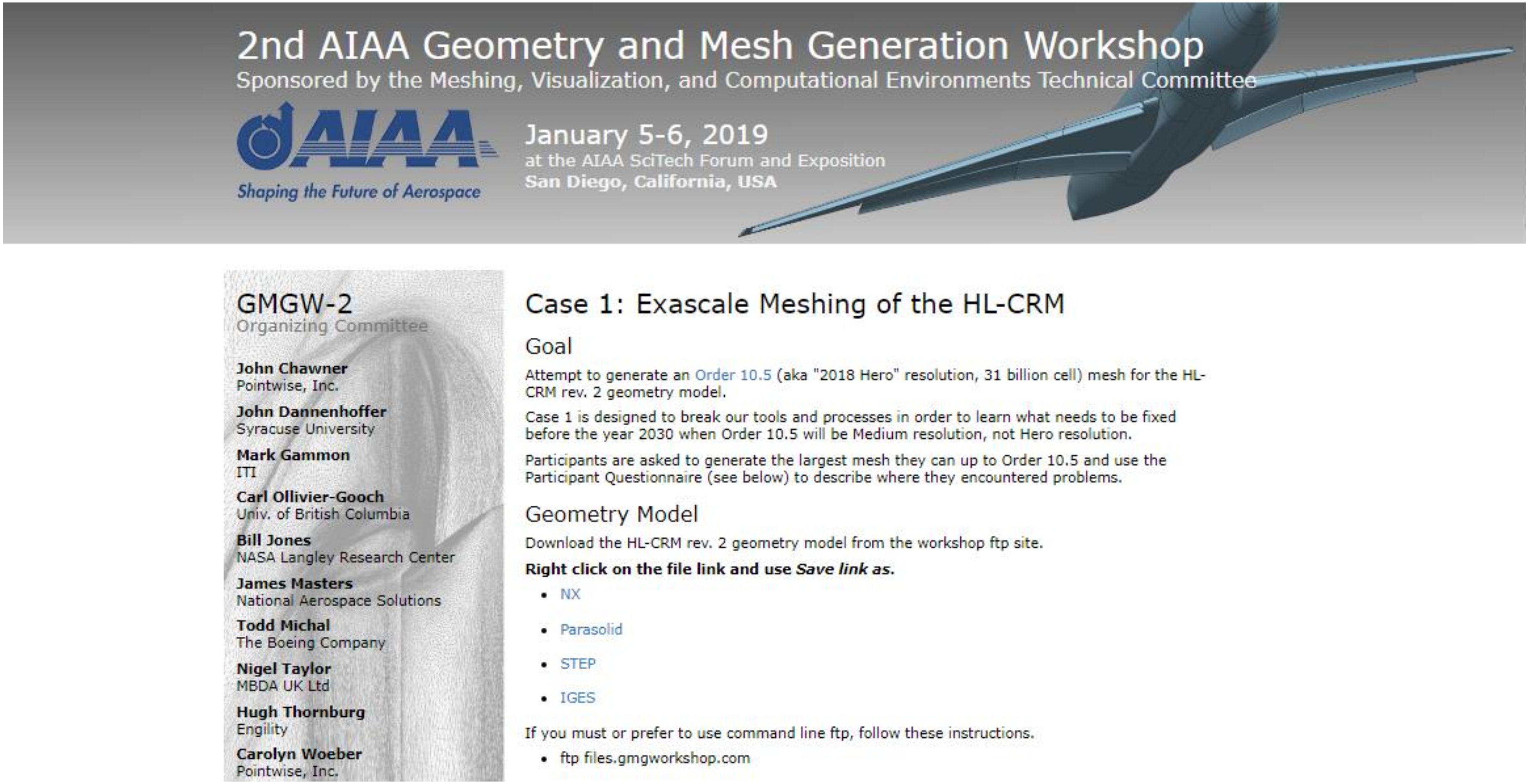
CSD
Struct Dynamics

NSU3D:
Univ. of Wyoming

SAMARC:
LLNL and NASA-Ames

RCAS:
AFDD and ART

GMGW Meshing Challenge



2nd AIAA Geometry and Mesh Generation Workshop

Sponsored by the Meshing, Visualization, and Computational Environments Technical Committee

AIAA

Shaping the Future of Aerospace

January 5-6, 2019

at the AIAA SciTech Forum and Exposition

San Diego, California, USA

GMGW-2

Organizing Committee

John Chawner
Pointwise, Inc.

John Dannenhoffer
Syracuse University

Mark Gammon
ITI

Carl Ollivier-Gooch
Univ. of British Columbia

Bill Jones
NASA Langley Research Center

James Masters
National Aerospace Solutions

Todd Michal
The Boeing Company

Nigel Taylor
MBDA UK Ltd

Hugh Thornburg
Engility

Carolyn Woeber
Pointwise, Inc.

Case 1: Exascale Meshing of the HL-CRM

Goal

Attempt to generate an Order 10.5 (aka "2018 Hero" resolution, 31 billion cell) mesh for the HL-CRM rev. 2 geometry model.

Case 1 is designed to break our tools and processes in order to learn what needs to be fixed before the year 2030 when Order 10.5 will be Medium resolution, not Hero resolution.

Participants are asked to generate the largest mesh they can up to Order 10.5 and use the Participant Questionnaire (see below) to describe where they encountered problems.

Geometry Model

Download the HL-CRM rev. 2 geometry model from the workshop ftp site.

Right click on the file link and use *Save link as*.

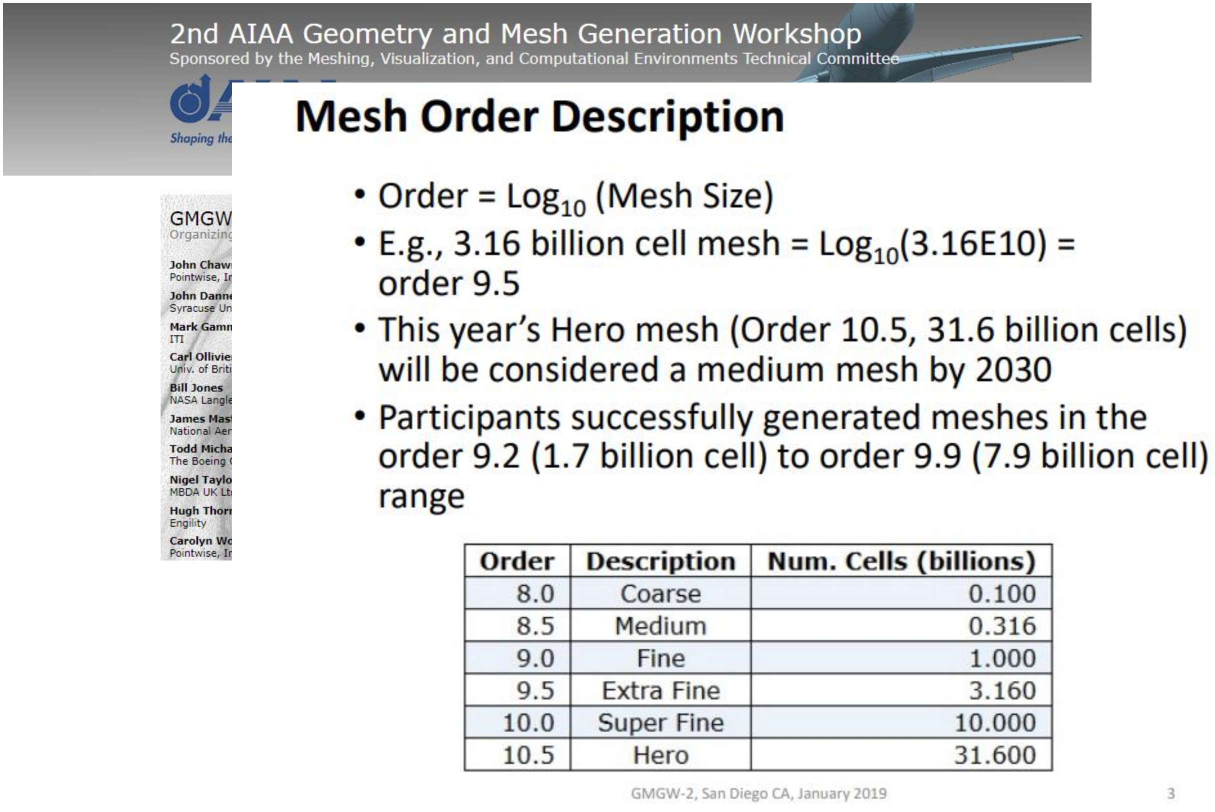
- NX
- Parasolid
- STEP
- IGES

If you must or prefer to use command line ftp, follow these instructions.

- ftp files.gmgworkshop.com

- Billion cell meshes
- Curved element meshes
- CFD2030 driven

GMGW Meshing Challenge



2nd AIAA Geometry and Mesh Generation Workshop

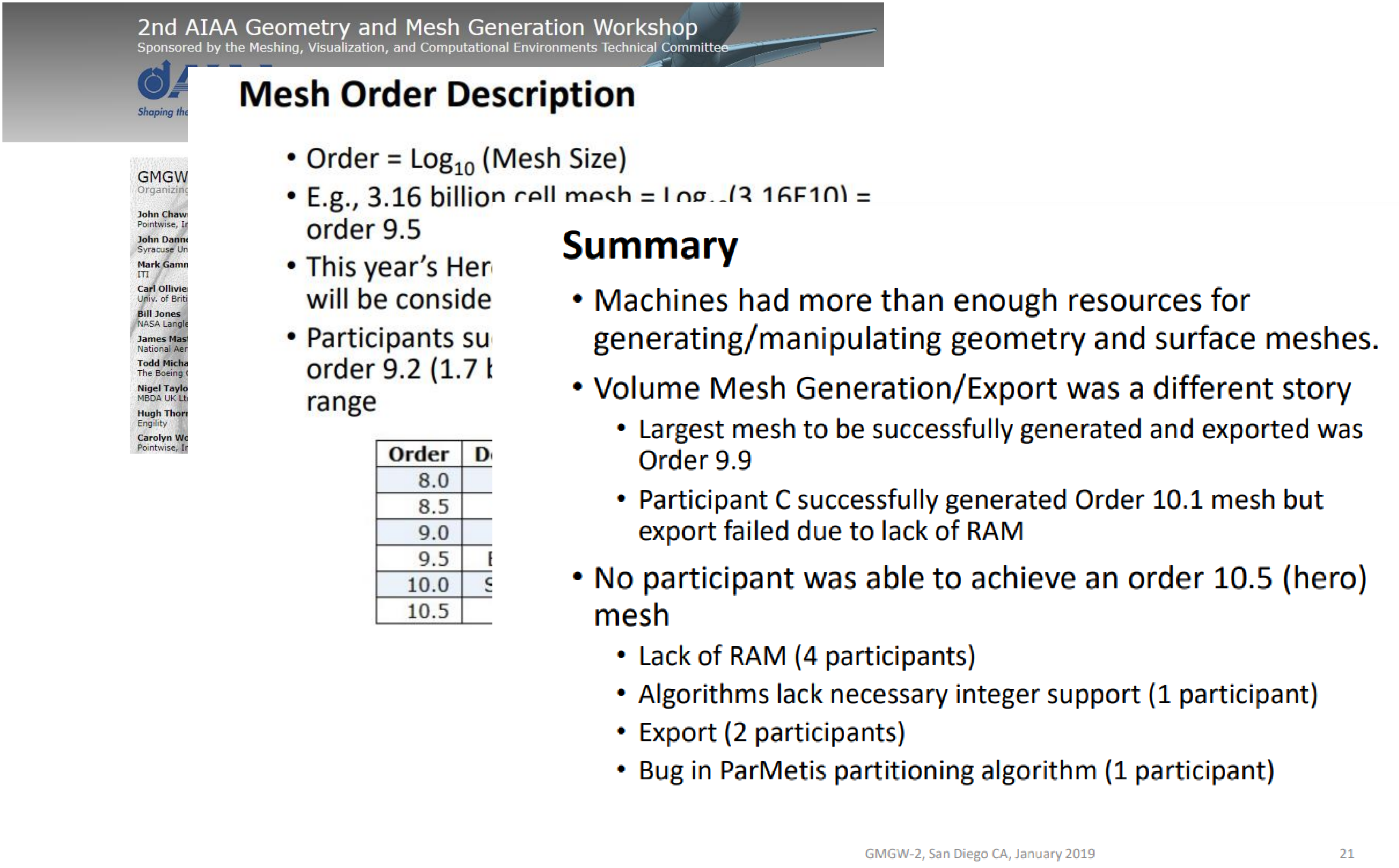
Sponsored by the Meshing, Visualization, and Computational Environments Technical Committee

Mesh Order Description

- Order = Log_{10} (Mesh Size)
- E.g., 3.16 billion cell mesh = Log_{10}(3.16E10) = order 9.5
- This year's Hero mesh (Order 10.5, 31.6 billion cells) will be considered a medium mesh by 2030
- Participants successfully generated meshes in the order 9.2 (1.7 billion cell) to order 9.9 (7.9 billion cell) range

Order	Description	Num. Cells (billions)
8.0	Coarse	0.100
8.5	Medium	0.316
9.0	Fine	1.000
9.5	Extra Fine	3.160
10.0	Super Fine	10.000
10.5	Hero	31.600

GMGW Meshing Challenge



2nd AIAA Geometry and Mesh Generation Workshop
Sponsored by the Meshing, Visualization, and Computational Environments Technical Committee

Shaping the

GMGW
Organizing

John Chaw
Pointwise, Ir
John Danne
Syracuse Un
Mark Gamn
ITI
Carl Ollivie
Univ. of Briti
Bill Jones
NASA Langle
James Mas
National Aer
Todd Micha
The Boeing
Nigel Taylo
MBDA UK Lt
Hugh Thor
Engility
Carolyn W
Pointwise, Ir

Mesh Order Description

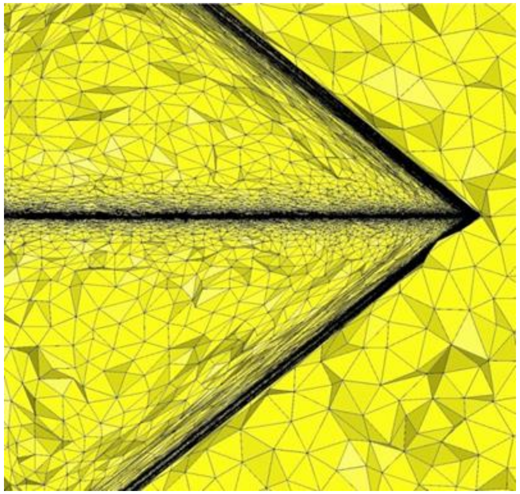
- Order = Log_{10} (Mesh Size)
- E.g., 3.16 billion cell mesh = Log(3.16E10) = order 9.5
- This year's Her will be conside
- Participants su order 9.2 (1.7 range

Order	D
8.0	
8.5	
9.0	
9.5	E
10.0	S
10.5	

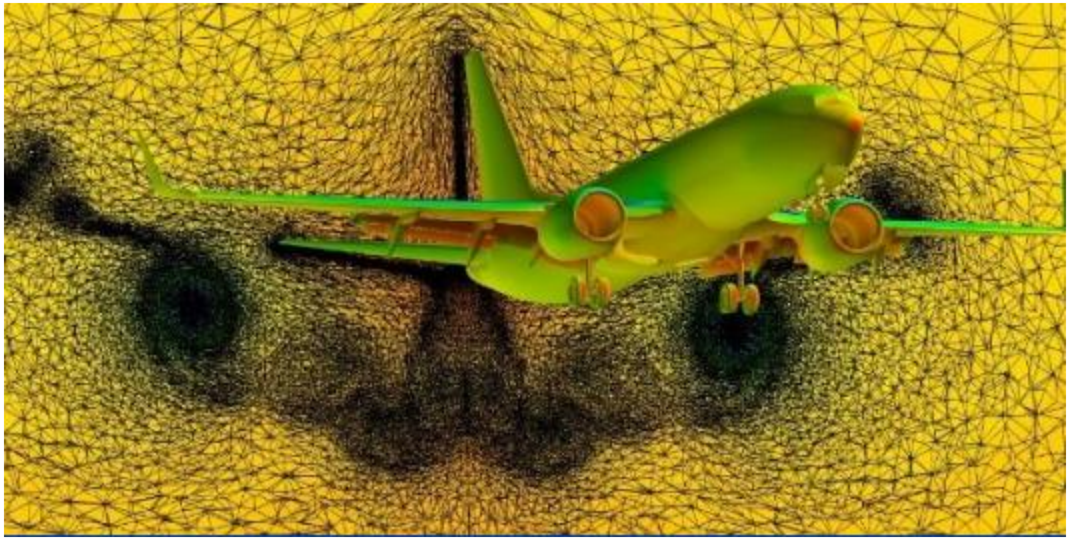
Summary

- Machines had more than enough resources for generating/manipulating geometry and surface meshes.
- Volume Mesh Generation/Export was a different story
  - Largest mesh to be successfully generated and exported was Order 9.9
  - Participant C successfully generated Order 10.1 mesh but export failed due to lack of RAM
- No participant was able to achieve an order 10.5 (hero) mesh
  - Lack of RAM (4 participants)
  - Algorithms lack necessary integer support (1 participant)
  - Export (2 participants)
  - Bug in ParMetis partitioning algorithm (1 participant)

Significant Advances in Adaptive Mesh Refinement (AMR) Capabilities



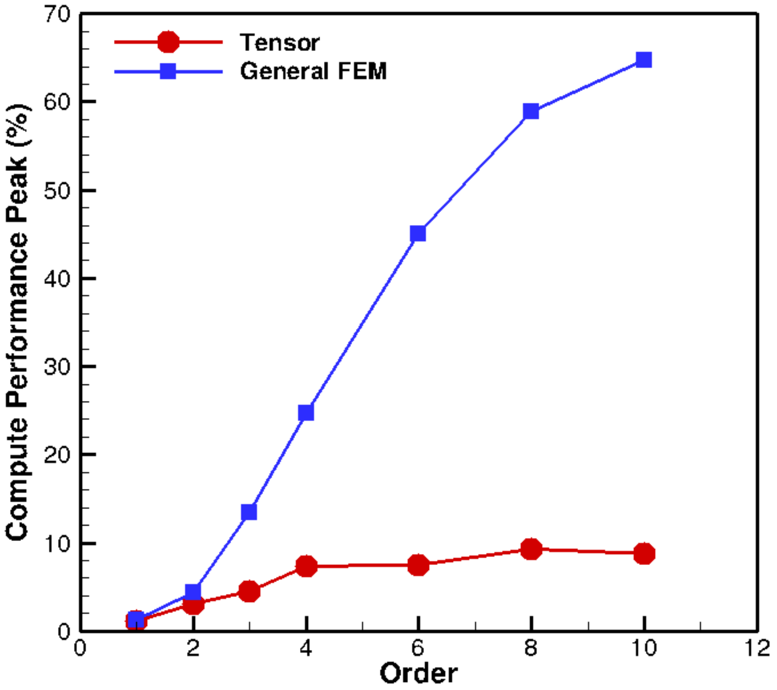
F. Alauzet (INRIA)

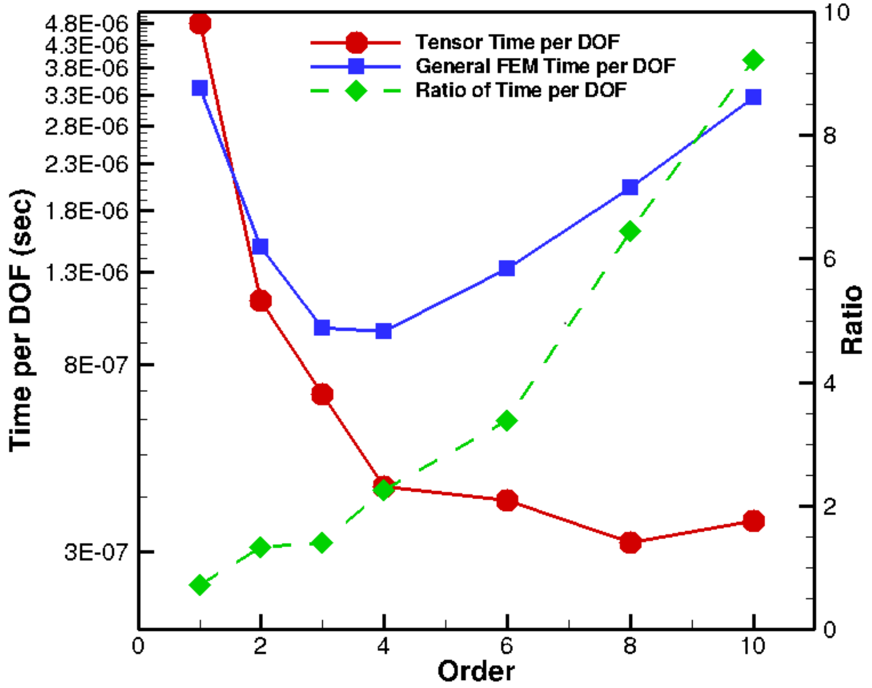


T. Michael (Boeing)

- Enabled though more rigorous algorithms
  - Error estimates (possibly using adjoint methods)
  - Mappings based on continuous spaces
  - Efficient local mesh refinement/improvement operations

Computational Rates for High Order DG Discretizations



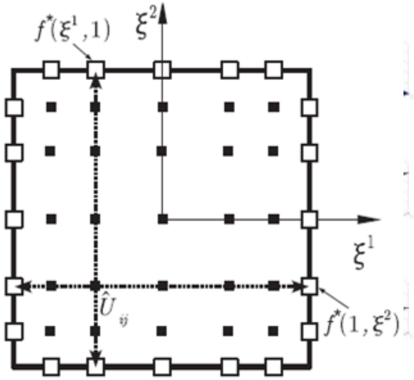


- Less computationally intensive than general formulation
- Overall cost much lower per degree of freedom
  - Cost per d.o.f decreases or flat with larger p
  - Faster than finite-difference

Tensor Product DG

- Abandon flexibility of modal bases for arbitrary element types

$$\psi(\xi,\eta,\zeta)=a+b\xi+c\eta+d\zeta+e\xi^2+f\xi\eta+\dots$$



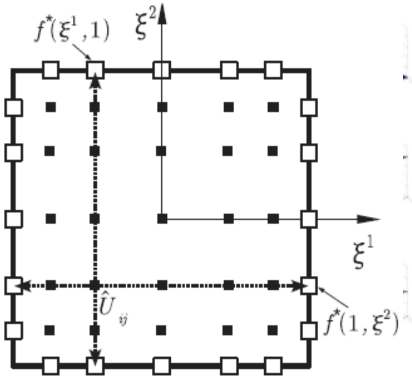
- Tensor product bases:
  - Best suited for hexahedral elements

$$\psi_{ijk}(\xi,\eta,\zeta)=l_i(\xi)l_j(\eta)l_k(\zeta)$$

- l_i, l_j, l_k = 1-D Legendre polynomials:
  - values at quadrature points of integration become solution values
  - Removes requirement of reconstructing solution at quadrature points
  - All integrals reduce to dimension-by-dimension 1-D summations

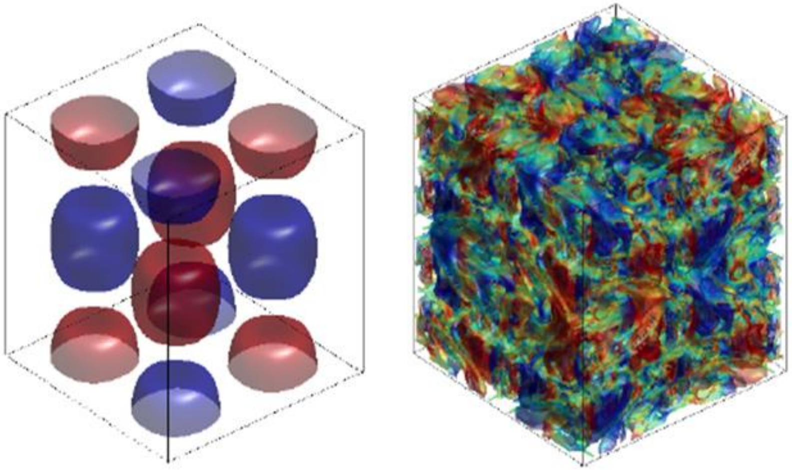
Tensor Product DG

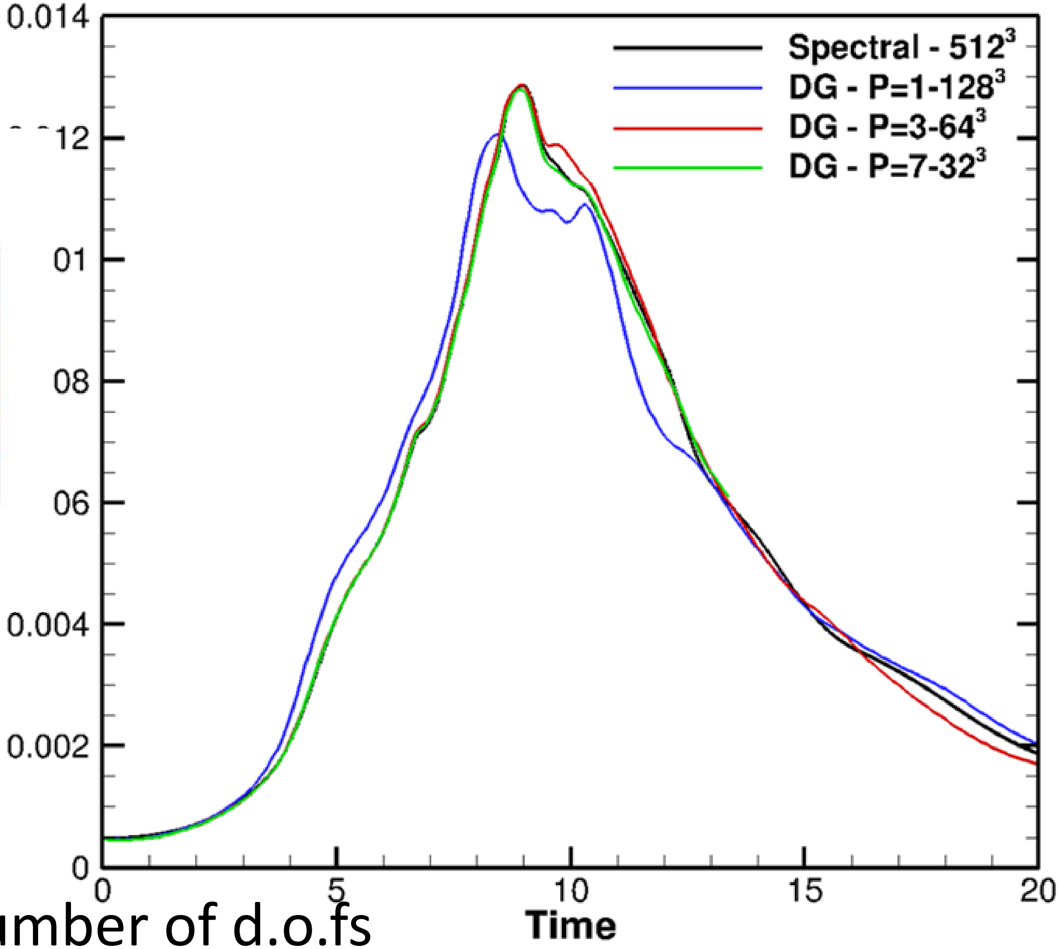
- Abandon flexibility of modal bases for arbitrary element types
  - Cost: O(N^2) or $(p+1)^6$



- Tensor product bases:
  - Cost: O($N^{4/3}$) or $(p+1)^4$
  - N = dof per cell = $(p+1)^3$ in 3D
  - p = basis polynomial degree
  - Order of accuracy = p+1
- Shown to be equivalent in cost to finite differences on cartesian mesh of same order (for residual evaluation)

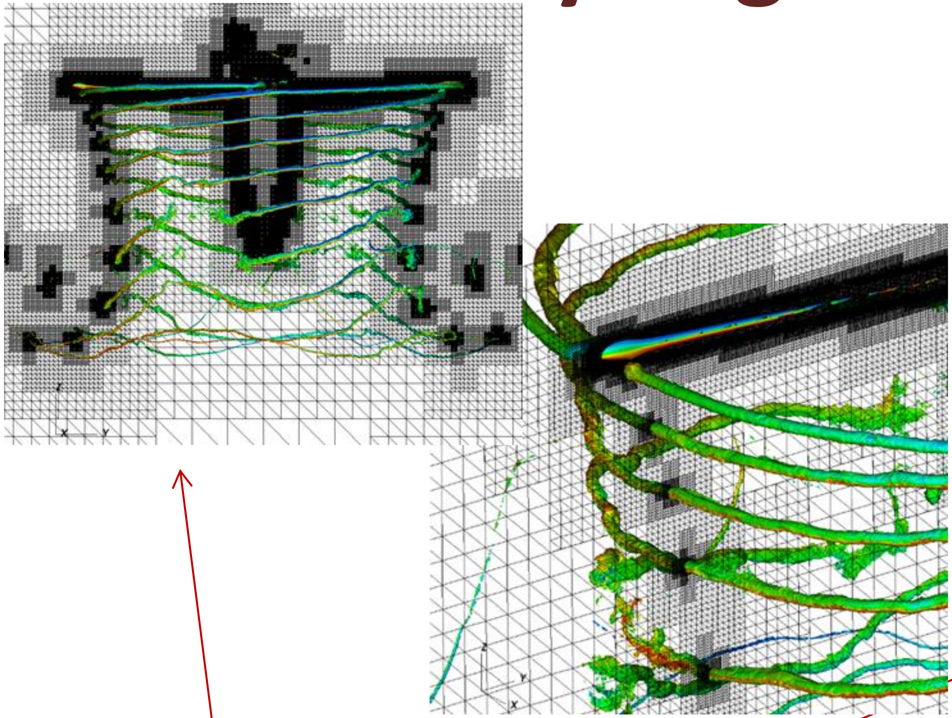
CartDG Solver Validation

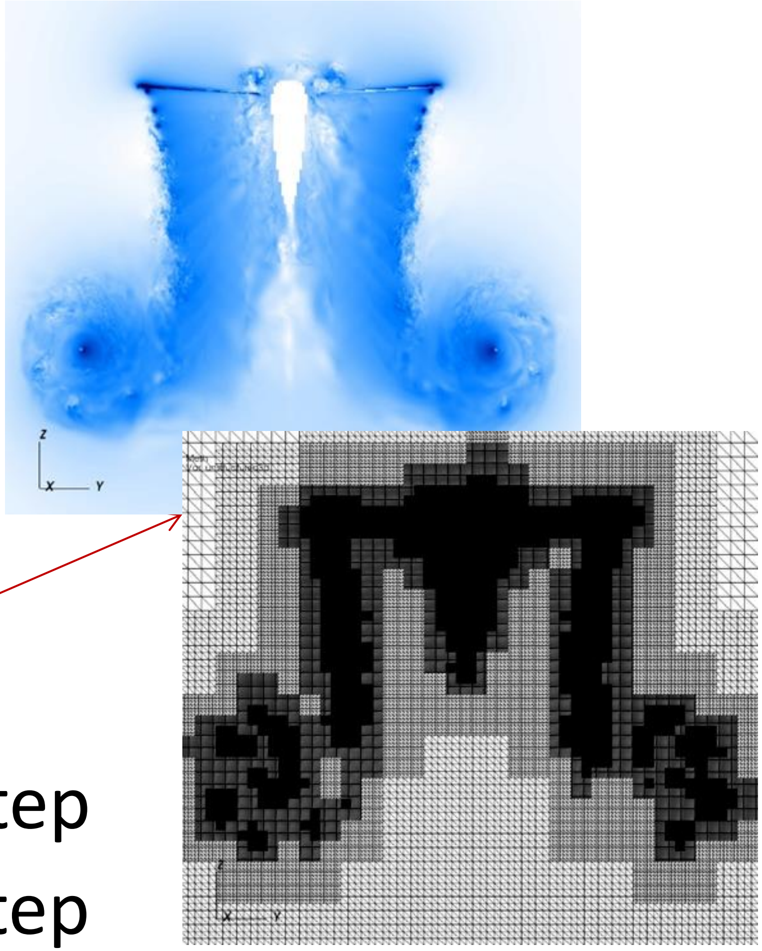




- Increasing p at fixed number of d.o.fs
  - Coarser meshes at higher p
  - Accuracy increases
  - Simulation cost decreases (per time step)

S-76 Rotor using High-order DG in Off-body Region with AMR





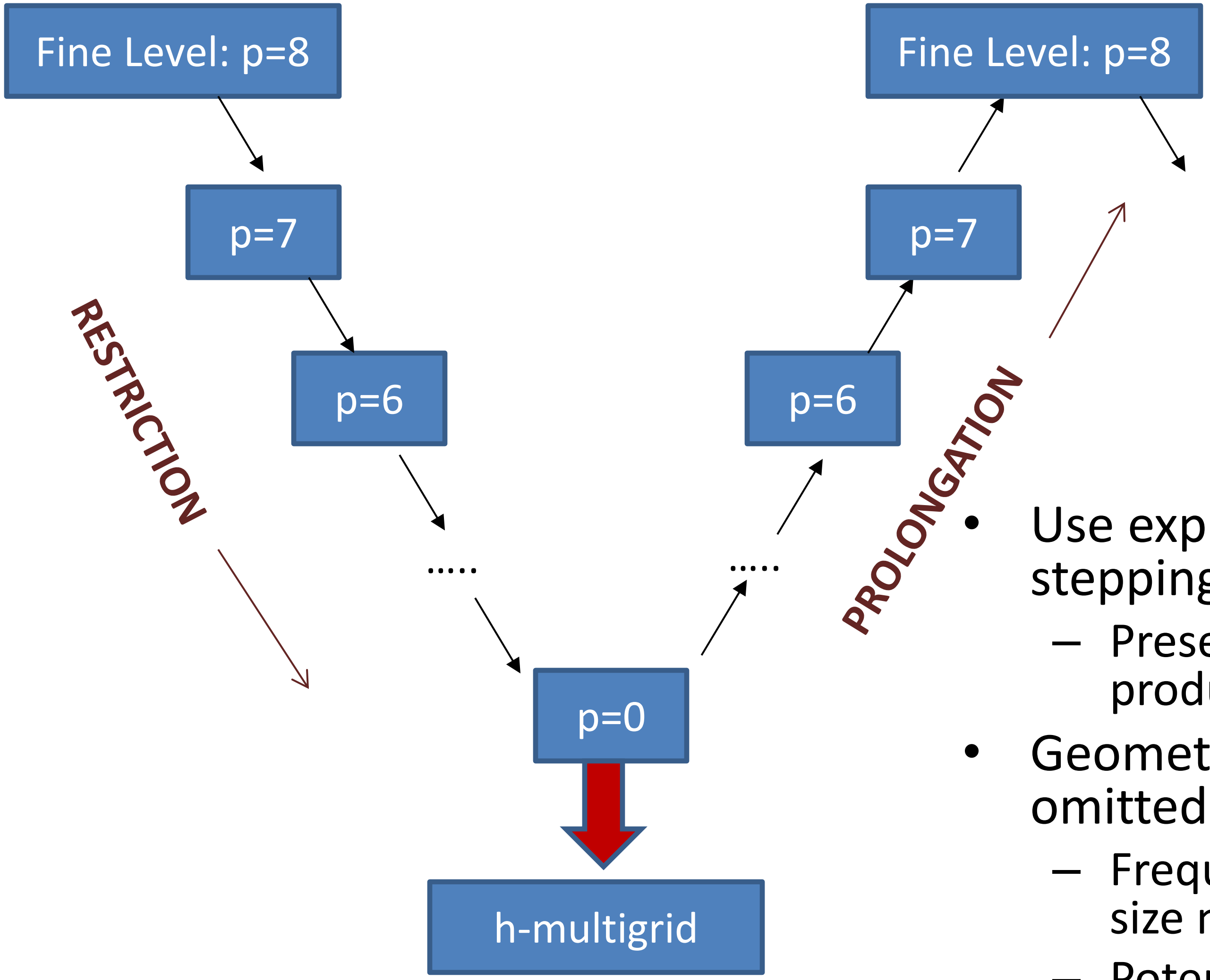
- p_{max}=3 19 secs per time step
- P_{max}=7 12 secs per time step

explicit time step on 5400 cores

Implicit Methods for High p-Order

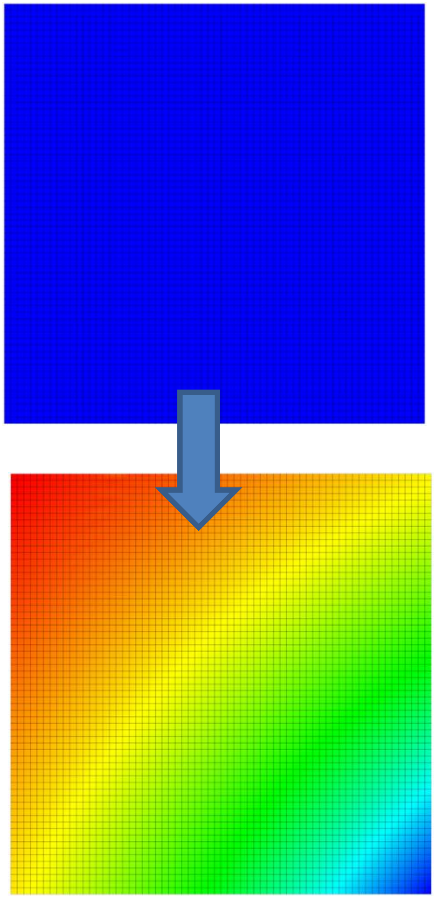
- Tensor product much more efficient for residual evaluation of high p-order discretizations
  - Ideal for explicit methods
- Implicit methods may require forming/inverting Jacobians
  - Prohibitive cost since element matrix is dense
    - Scales as : $O(N^2)$ or $(p+1)^6$ (at a minimum)
- Efficient implicit solver must rely on tensor product operations to be competitive at high p-order
  - Tensor-product preconditioning (Murman et al.: EDDY code)
  - Pseudo-time stepping (Vincent et al.: PyFR code)
  - P-multigrid
    - Use pseudo-time stepping on sequence of meshes or p-levels

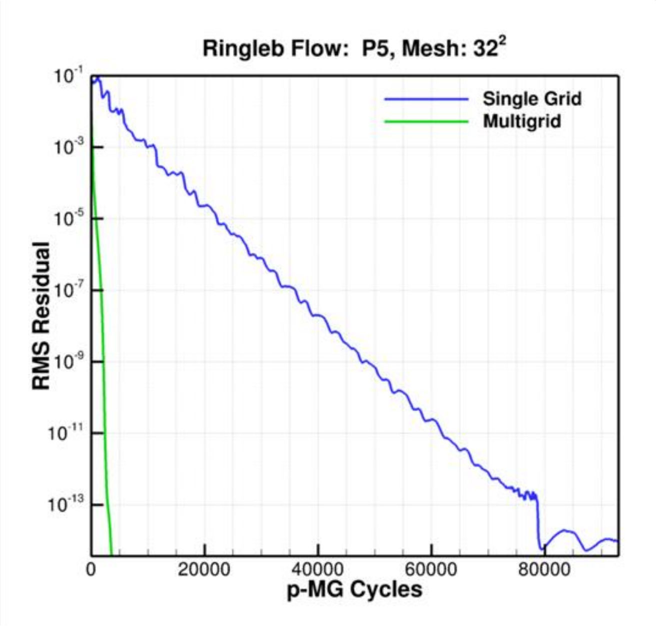
p-multigrid

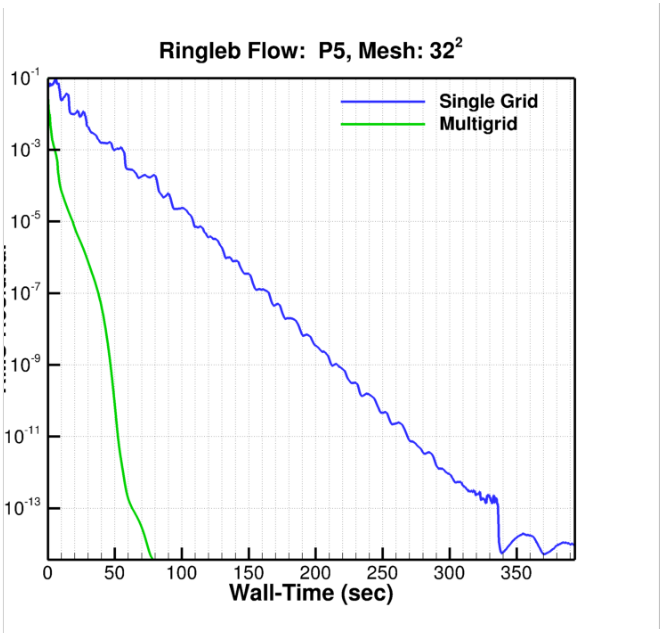


- Use explicit pseudo-time stepping on each level
  - Preserves benefits of tensor product formulation
- Geometric multigrid at p=0 omitted
  - Frequencies greater than cell size not damped
  - Potentially large cell sizes at p=8

p-MG Solution of Ringleb Flow at p=5

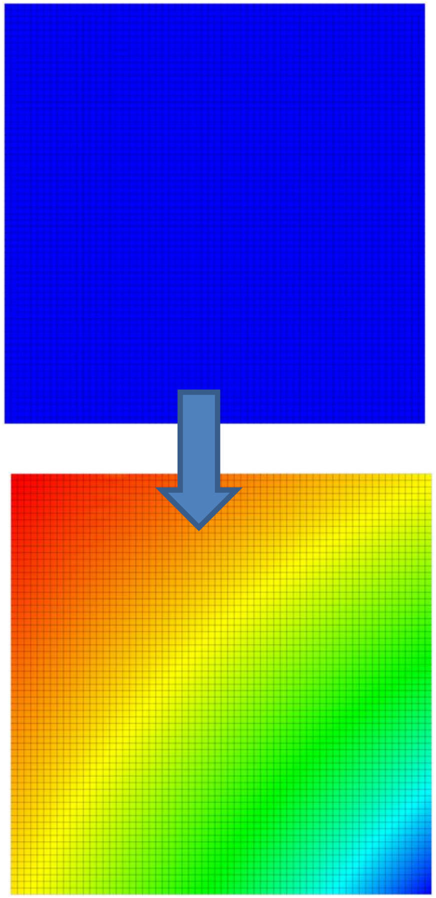


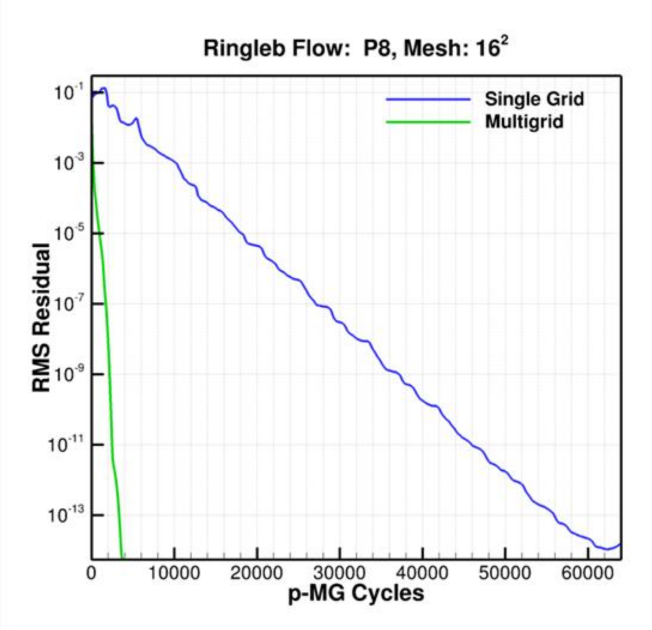


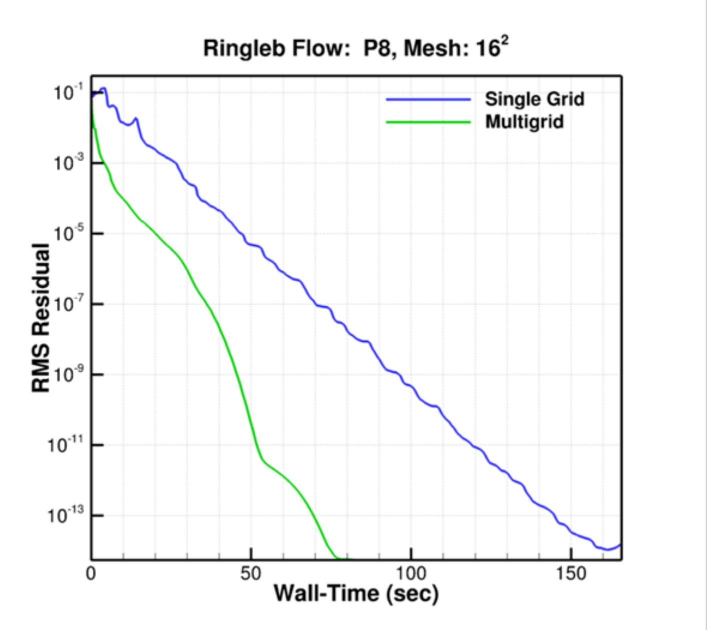


- Cost of p-MG cycle at higher p
- Largest benefits on finer grid

p-MG Solution of Ringleb Flow at p=8





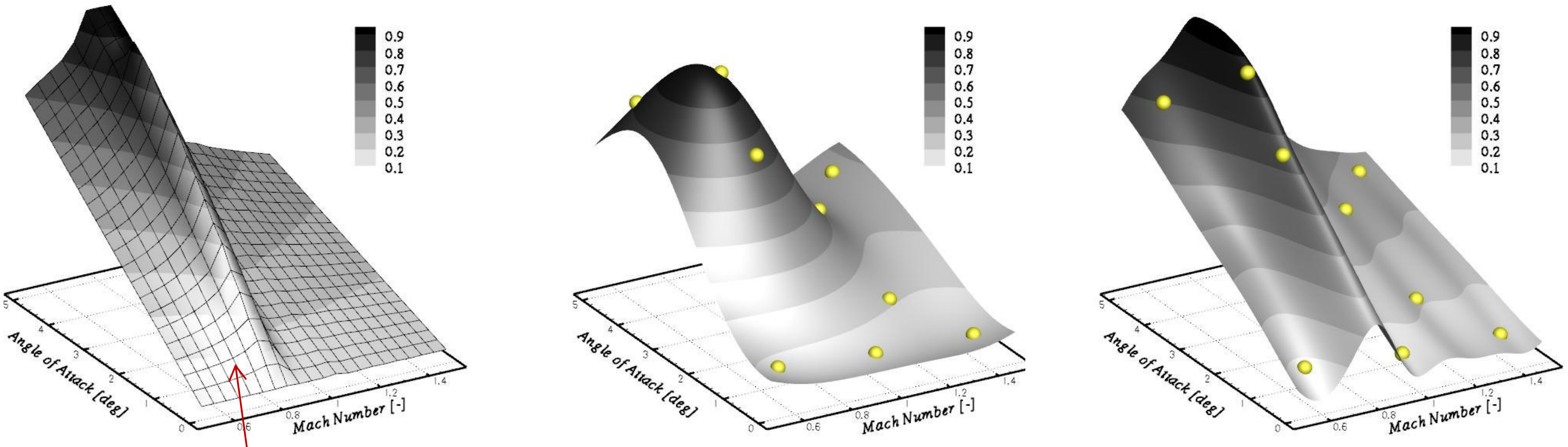


- Cost of p-MG cycle at higher p
- Largest benefits on finer grid

Adjoint Methods

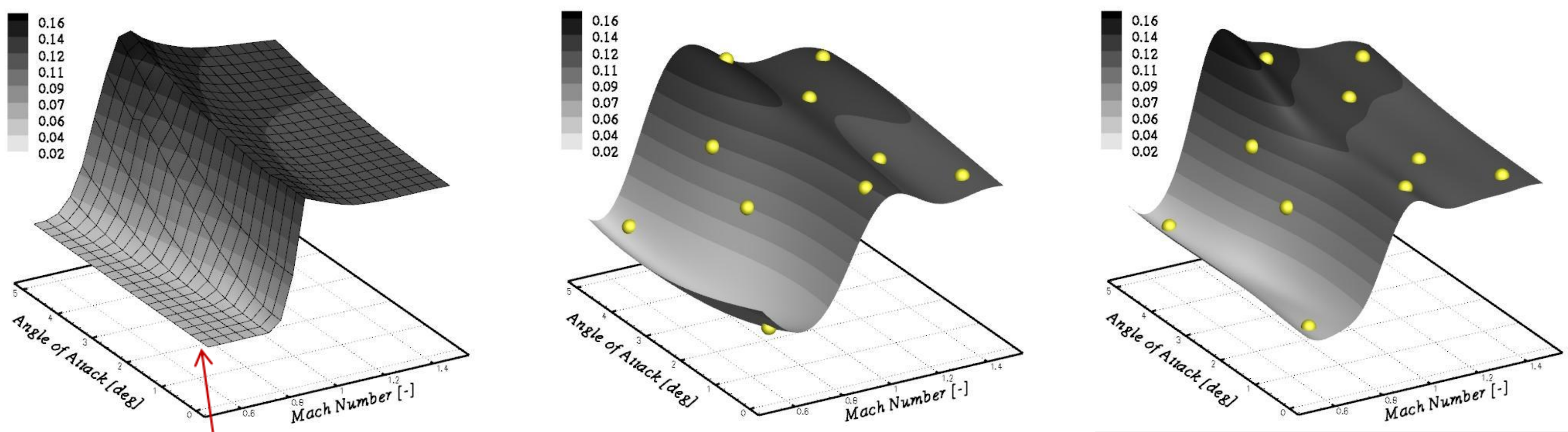
- Pioneered in aerodynamics by A. Jameson
  - Enables sensitivity computation independent of number of design variables
  - Enabled cost-effective high-fidelity MDAO
- Enables AMR based on engineering objectives rather than local error
- Used to compute sensitivities for UQ (CbA)
- Build better response surface models or ROMS

Aerodynamic Data Base Fill In



- Lift = f(Mach,alpha)
  - Exact: 144 steady-state solutions
  - Kriging model : 10 solutions
    - Function, Function + Gradient (Adjoint)

Aerodynamic Data Base Fill In

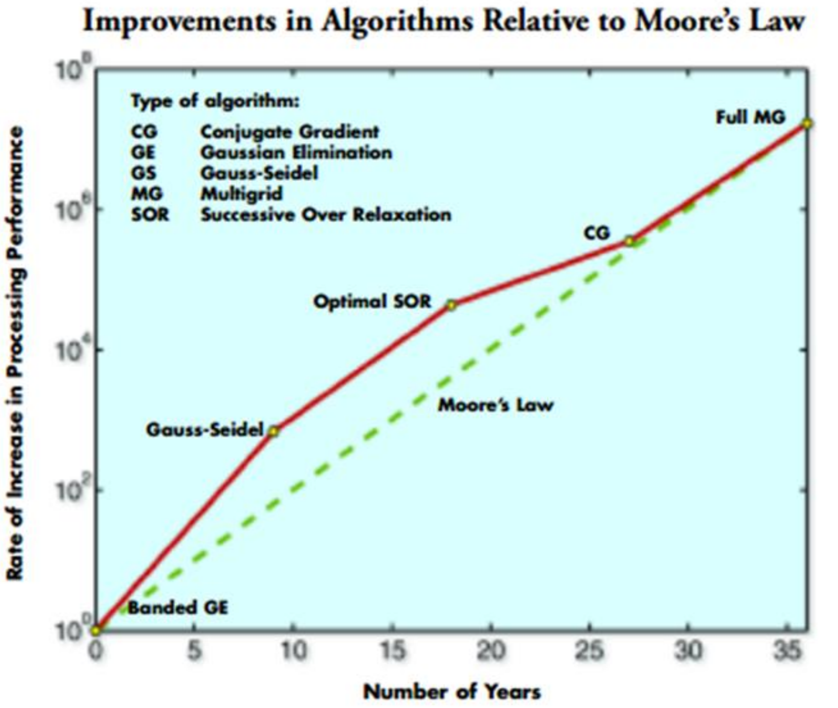


- Drag = f(Mach,alpha)
  - Exact: 144 steady-state solutions
  - Kriging model : 10 solutions
    - Function, Function + Gradient (Adjoint)

Importance of Algorithmic Advances

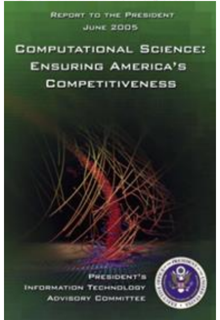
- Increased simulation capabilities due to:
  - More capable hardware (Moore's Law)
  - Advanced algorithms

- Algorithmic advances are asymptotic
  - Provide increasing benefits for larger problems
    - O(N) vs 0(N^2) when N=10^{12}



Improvements in Algorithms Relative to Moore's Law

The relative gains in some algorithms for the solution of an electrostatic potential equation on a uniform cubic grid compared to improvements in the hardware (Moore's Law).



REPORT TO THE PRESIDENT
JUNE 2005

COMPUTATIONAL SCIENCE: ENSURING AMERICA'S COMPETITIVENESS

PRESIDENT'S
INFORMATION TECHNOLOGY
ADVISORY COMMITTEE

A. Jameson Contributions Past and Present

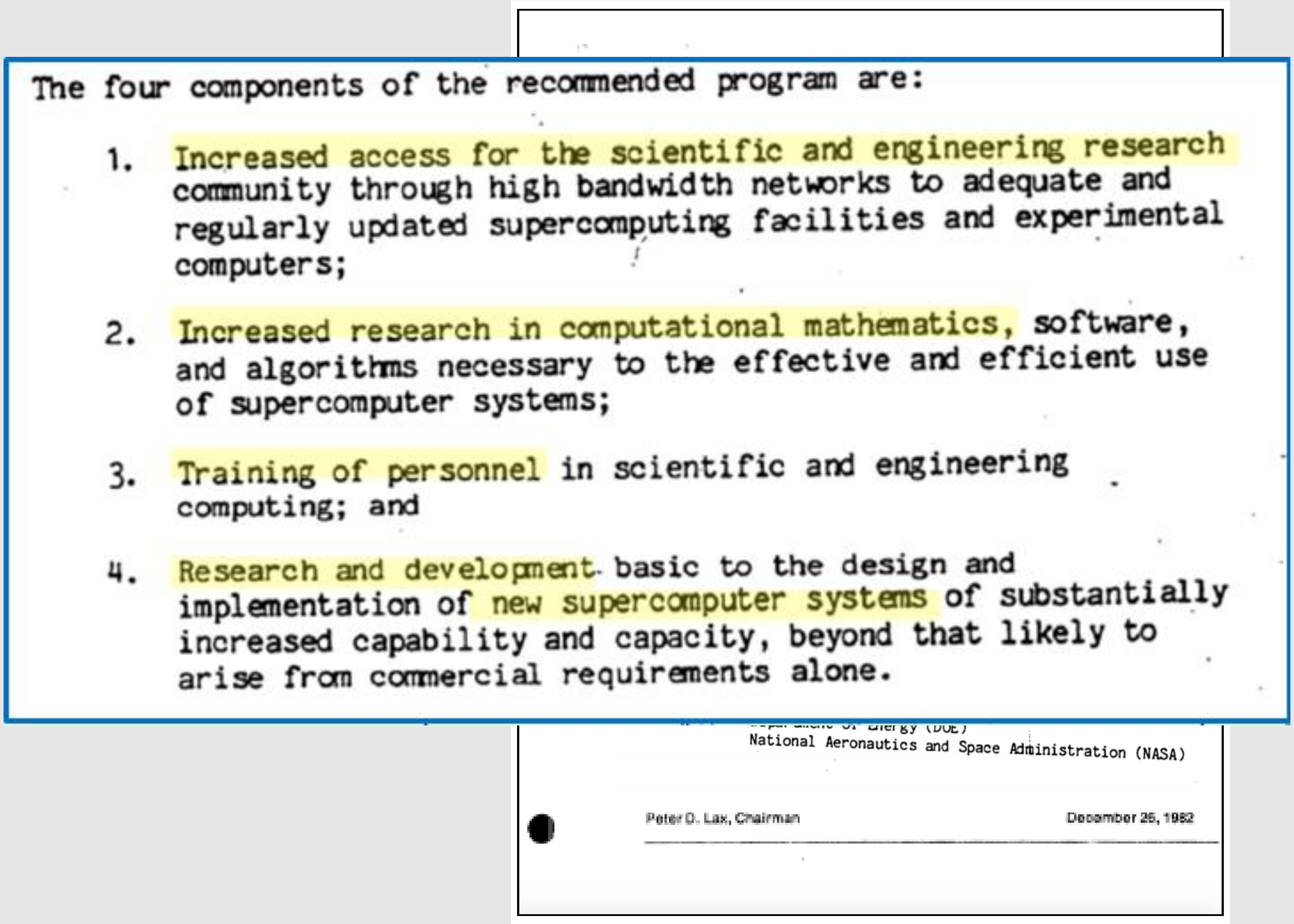
- Full aircraft using unstructured meshes
- Discretizations
  - JST schemes, early extension to unstructured meshes
- Multigrid methods
- Adjoint methods
- High-order methods (DG, FR)

Some Outstanding Algorithmic Challenges

- Predicting smooth body separation
- Reliable transition prediction
- Adjoint techniques for chaotic problems
- High-order nonlinearly stable schemes
  - Explicit and implicit
- Uncertainty quantification

Continued Advocacy for Algorithmic Advances

The Lax Report (1982)



The four components of the recommended program are:

1. Increased access for the scientific and engineering research community through high bandwidth networks to adequate and regularly updated supercomputing facilities and experimental computers;
2. Increased research in computational mathematics, software, and algorithms necessary to the effective and efficient use of supercomputer systems;
3. Training of personnel in scientific and engineering computing; and
4. Research and development basic to the design and implementation of new supercomputer systems of substantially increased capability and capacity, beyond that likely to arise from commercial requirements alone.

National Aeronautics and Space Administration (NASA)

Peter D. Lax, Chairman

December 26, 1982

THANK YOU

List of Ph.D. Students' Theses

Ph.D. Student	University	Year	Dissertation Title
I-Chung Chang	NYU	1981	Unsteady transonic flow past airfoils in rigid body motion
Brian McCartin	NYU	1982	Theory, computation and application of exponential splines
Richard Pelz	Princeton	1983	Transonic flow calculations using triangular finite elements
John Fay	Princeton	1985	On the design of airfoils in transonic flow using the Euler equations
Seokkwan Yoon	Princeton	1985	Numerical solution of the Euler equations by implicit schemes with multiple grids
Craig Streett	Princeton	1987	A spectral method for the solution of transonic potential flow about an arbitrary two-dimensional airfoil
Dimitri Mavriplis	Princeton	1987	Solution of the two dimensional Euler equations on unstructured triangular meshes
Venkat Venkatakrishnan	Princeton	1987	Computation of unsteady transonic flows over moving airfoils
Luigi Martinelli	Princeton	1987	Calculations of viscous flows with a multigrid method
Mohan Jayaram	Princeton	1987	Solution of the three-dimensional Navier-Stokes equations for transonic flow using a multigrid method
Takeshi Sakata	Princeton	1990	Solution of the Euler equations in multibody flow fields using the overlapping-mesh method
Mark Stewart	Princeton	1990	Non-overlapping composite meshes for multi-element airfoils
Feng Liu	Princeton	1991	Numerical calculation of turbomachinery cascade flows
Todd Mitty	Princeton	1993	Development of a Delaunay-based adaption scheme with applications to complex three-dimensional rotational flows
James Farmer	Princeton	1993	A finite volume multigrid solution to the three dimensional nonlinear ship wave problem
James Reuther	UC Davis	1996	Aerodynamic shape optimization using control theory
Juan Alonso	Princeton	1997	Parallel computation of unsteady and aeroelastic flows using an implicit multigrid-driven algorithm
Andrey Belov	Princeton	1997	A new implicit multigrid-driven algorithm for unsteady incompressible flow calculations on parallel computers
Chongam Kim	Princeton	1997	Robust and accurate numerical methods for high speed unsteady flows
Scott Sheffer	Princeton	1997	Parallel computation of supersonic reactive flows with detailed chemistry including viscous and species diffusion effec
Biing-Horng Liou	Princeton	1998	Calculation of nonlinear free surface wave with a fully implicit multigrid method
Paul Lin	Princeton	2001	Two-dimensional implicit time dependent caculations for incompressible flows on adaptive unstructured meshes
Yee Feng Ruan	Stanford	2002	Shock capturing schemes with gas-kinetic methods
Sriram Shankaran	Stanford	2003	Numerical analysis and design of upwind sails
Siva Nadarajah	Stanford	2003	The discrete adjoint approach to aerodynamic shape optimization
Matthew McMullen	Stanford	2003	The application of non-linear frequency domain methods to the Euler and Navier-Stokes equations
John Hsu	Stanford	2005	An implicit-explicit flow solver for complex unsteady flows
Kasidit Leoviriyakit	Stanford	2005	Wing planform optimization via an adjoint method
Balaji Srinivasan	Stanford	2006	The BGK and LRS schemes for computing Euler and Navier Stokes flows
Georg May	Stanford	2006	A kinetic scheme for the Navier-Stokes equations and high-order methods for hyperbolic conservation laws
Arathi Gopinath	Stanford	2007	Efficient Fourier-based algorithms for the time-periodic unsteady problems
Karthik Palaniappan	Stanford	2007	Algorithms for automatic feedback control of aerodynamic flows
Nawee Butsuntorn	Stanford	2008	Time spectral method for rotorcraft flow with vorticity confinement
Aaron Katz	Stanford	2009	Meshless methods for computational fluid dynamics
Jen-Der Lee	Stanford	2009	NLF wing design by adjoint method and automatic transition prediction
Rui Hu	Stanford	2009	Supersonic biplane design via adjoint method
Sachin Premasuthan	Stanford	2010	Towards an efficient and robust high order accurate flow solver for viscous compressible flow
Sean Kamkar	Stanford	2011	Mesh adaption strategies for vortex-dominated flows
Kwan Yu Chiu	Stanford	2011	A conservative meshless framework for conservation laws with applications
Yves Allaneau	Stanford	2012	Energy conserving numerical methods for the computation of complex
Patrice Castonguay	Stanford	2012	High-order energy stable flux reconstruction schemes for fluid flow simulations on unstructured grids
Kui Ou	Stanford	2012	High-order methods for unsteady flows on unstructured dynamic meshes
Andre Chan	Stanford	2012	Control and suppression of laminar vortex shedding off two-dimensional bluff bodies
Yi Li	Stanford	2013	Automatic mesh adaptation using the continuous adjoint approach and the spectral difference method
Matthew Culbreth	Stanford	2013	High fidelity optimization of flapping airfoils and wings
David Williams	Stanford	2013	Energy stable high-order methods for simulating unsteady, viscous, compressible flows on unstructured grids
Joshua Leffell	Stanford	2014	An overset time-spectral method for relative motion
George Anderson	Stanford	2015	Shape optimization in adaptive search spaces
Manuel Lopez-Morales	Stanford	2016	Towards industry-ready high-order flow solvers: increasing robustness and usability
Kartikey Asthana	Stanford	2016	Analysis and design of optimal discontinuous finite element schemes
Abhishek Sheshadri	Stanford	2016	An analysis of stability of the flux reconstruction formulation with applications to shock capturing
Joshua Romero	Stanford	2017	On the development of the direct flux reconstruction scheme for high-order fluid flow simulations
Jerry Watkins	Stanford	2017	Numerical analysis and implicit time stepping for high-order, fluid flow simulations on GPU architectures
Jacob Crabill	Stanford	2018	Towards industry-ready high-order overset methods on modern hardware
David Manosalvas-Kjono	Stanford	2018	Aerodynamic design of active flow control systems aimed towards drag reduction in heavy vehicles