2023 INCITE Proposal Submission
Proposal

Title: Solution of the Navier-Stokes Equations for Industrial Scale Fluid Dynamics
Principal Investigator: Luigi Martinelli
Organization: Princeton University
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Section 1: PI and Co-PI Information

Question #1

__Principal Investigator:__ The PI is responsible for the project and managing any resources awarded to the project. If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.

Principal Investigator

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Question #2

Co-PI (s)

Question #3

Institutional Contact: *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

Institutional Contact

Institutional Contact Name

Elizabeth Adams

Institutional Contact Phone

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Institutional Contact Email

awards@princeton.edu

Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Engineering: Fluids and Turbulence

Question #2

Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)

Project Summary

The goal is to improve the fundamental understanding of the dynamics of vortex-dominated turbulent flows; such as those encountered by an aircraft at take-off and landing, or on the blades of a wind turbine, by solving the Navier-Stokes equations at the correct physical scales, The results will inform and guide the design process toward improved efficiency and safety.

Section 3: Early Career Track

Question #1

Early Career

Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an Early Career Track in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.

***Who Can Apply**: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

How to Apply:

In the regular application process, there will be a check-box to self-identify as early career.

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.

- *What is the Early Career Track?*
  - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
  - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
  - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.*
- *What review criteria will be used for the Early Career Track?*
  - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.

No

If 'yes', what year was your PhD? If 'no' enter N/A

N/A

If 'yes', how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.

N/A

Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

Question #5

ALCF Theta (Cray XC40) Resource Request - 2023

Question #6

ALCF Polaris Resource Request - 2023

Question #7

ALCF Polaris Resource Request - 2024

Question #8

ALCF Polaris Resource Request - 2025

Question #9

ALCF Aurora (Intel X^e) Resource Request – 2023

Node Hours

76000

Storage (TB)

100

Off-Line Storage (TB)

600

Question #10

ALCF Aurora (Intel X^e) Resource Request – 2024

Node Hours

60000

Storage (TB)

100

Off-Line Storage (TB)

600

Question #11

ALCF Aurora (Intel X^e) Resource Request – 2025

Question #12

List any funding this project receives from other funding agencies.

Funding Sources

Question #13

List any other high-performance computing allocations being received in support of this project.

Other High Performance Computing Resource Allocations

Section 5: Project Narrative and Supplemental Materials

Question #1

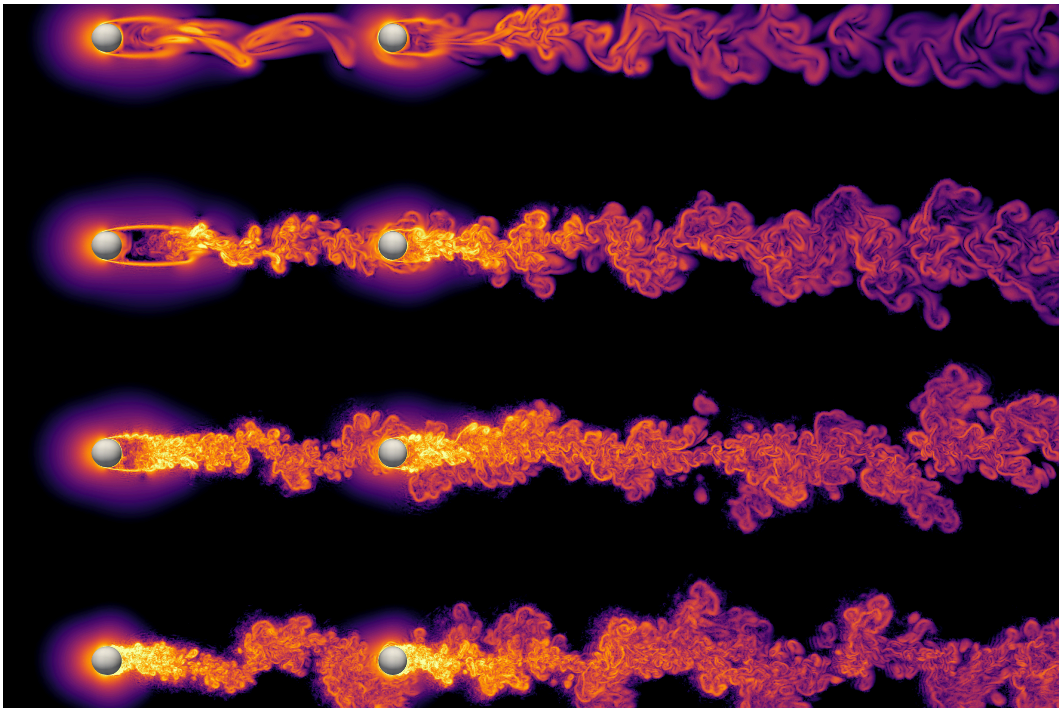
Using the templates provided here, please follow the [INCITE Proposal Preparation Instructions]to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file. Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.

Concatenate all materials below into a single PDF file.

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

INCITE-LM-Collated.pdf
The attachment is on the following page.

SOLUTION OF THE NAVIER-STOKES EQUATIONS FOR INDUSTRIAL SCALE CFD



Incite Project Proposal

Prepared by: Luigi Martinelli, Professor - Department of MAE - Princeton University, Princeton, NJ 08544.

June 14, 2022

PI: Luigi Martinelli

Applying Institution: Princeton University

Resources Name and Number of Node Hours Requested: 76,000 node-hour on the Aurora System in year 1 and 60,000 in year 2.

EXECUTIVE SUMMARY

The ultimate objective of our effort is to enhance the fundamental understanding of the dynamics of vortex-dominated turbulent flows; such as those encountered in the extremes of the flight envelope of an aircraft, at take-off and landing conditions, or in submarine maneuvering. Vortex-dominated flows are ubiquitous in practical engineering and cannot be modeled accurately with the simplified fluid dynamics models (i.e the Reynolds Averaged form of the conservation laws) currently affordable by Industrial CFD; their dynamics must be studied by direct solution of the Navier-Stokes equations.

We are aiming at providing accurate numerical solutions of the Navier-Stokes equations at practical engineering scales, with minimal modeling of the sub grid dynamics. We will use and enhance ***maDG***, a newly developed code designed for the efficient parallel implicit solution of the 3D unstructured nodal discontinuous Galerkin discretization of the unsteady compressible Navier-Stokes equations. The code has been developed at Princeton University by Mark Lohry and Luigi Martinelli to provide an efficient, modular, and maintainable software platform enabling algorithmic and modeling studies in high-resolution CFD. Our code has now reached an advanced stage of development that facilitates its implementation and exploitation on large HPC systems. The current version leverages RAJA for GPU or OpenMP, or pure C++ for serial CPU in such a way that the backend is abstracted from the main code, which enables a quick adoption of new emerging standards.

The result of our effort will provide a new powerful computational tool for both fundamental and applied fluid dynamic research, which will enable more efficient engineering of aircraft, propulsors, and wind turbines.

PROJECT NARRATIVE

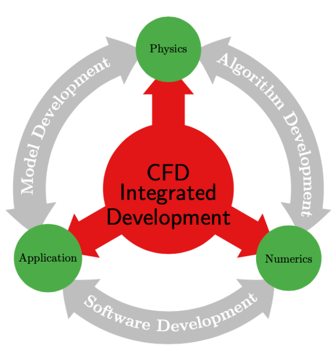
In the first two decades of the 21st century, Computational Fluid Dynamics (CFD) has been generally seen as a mature science. With the gilded age of algorithm development behind, the emphasis shifted primarily toward very large scale simulations of complex industrial problems using an averaged form of the conservation laws complemented by a calibrated turbulence model, with the finite volume formulation being the discretization of choice. In spite of its many successes, traditional finite volume CFD methods have severe limitations that hinder the simulation of wall bounded, vorticity dominated turbulent flows, and progress must be made before robust and accurate simulation of this class of flows, important in many practical engineering application, becomes a reality.

In the past few years, the landscape of high performance computing has once again changed; the available computational resources have increased by orders of magnitude, and exa-scale computing is becoming a reality. For example, with exa-scale performances, a Large Eddy Simulation (LES) of a complete aircraft may become feasible within the next 10 years. However, this increase of performance is realized with a radically different hardware, comprising hierarchical memory systems, which makes existing and well established CFD methods not optimal for current high performance computer (HPC) architectures. This motivated an increase of research interest in high resolution CFD since high order methods may offer a path forward, but further research is needed. Our work address some of the key issues toward the goal of enabling high-resolution CFD analysis in engineering.

Computational efficiency is a necessity for any method to be routinely used in engineering applications. Our work uses efficient numerical methods for implicit time integration of discontinuous Galerkin discretizations based on Jacobian-free Newton-Krylov methods. They have been demonstrated to be significantly more efficient than explicit methods for toy problems up to industrial scale simulations.

Correct, maintainable, and efficient software must also be developed. This is especially necessary for high order methods such as discontinuous Galerkin methods which are inherently more complex than standard second-order methods, and whose formal high accuracy is more easily degraded by minor numerical errors that are safely ignored in traditional methods.

We meet these challenges following a fully integrated approach, since it becomes impossible to filter separately numerical and physical instabilities as more of the scales are resolved by the calculations.



Mark Lohry and Luigi Martinelli have developed ***maDG*** over several years; a usable and extensible software for modern multi-core multiprocessor high performance systems. This flexible framework enables easy experimentation with different methodologies relevant to high-order CFD, while not sacrificing scalable performance for tackling large scale problems: one code fulfilling the needs of both fundamental and applied fluid mechanics research. ***maDG*** is written entirely in modern C++ (at the time of writing, it requires at least a C++14-compliant compiler) using MPI for distributed memory parallelization.

The development of any sufficiently complex software requires the interaction of many different components; successfully managing this complexity is a central challenge of the software engineering discipline. ***maDG*** relies on a number of high quality open source libraries. Several boost libraries are used, in particular the *boost.mpi* library which provides a thin object-oriented interface over the C MPI libraries, as well as the program options and log libraries. The *googletes*t framework is used for automated testing, the *CGNS* library for file handling, *METIS* for parallel partitioning of the mesh, the *eigen* library for dense linear algebra, and *nanoflann* for spatial nearest-neighbor searches used primarily in post-processing. Last but not least, the PETSc library (Portable, Extensible Toolkit for Scientific Computation) provides all the iterative nonlinear and linear algebra solvers used in this work, as well as the implicit time integration methods that use them. PETSc provides high-quality reference implementations of a wide array of numerical methods along with a large community and extensive documentation, making it an ideal base for numerical experiments. Nonetheless, maDG code structure was designed to facilitate the integration of newer libraries and standards as they become available.

The software design philosophy of ***maDG*** reflects the motivation to create a tool suitable for assessing the relative merits of different algebraic solution methods, time integration schemes, and spatial discretization approaches in the context of high performance parallel computing. To this end, the code is highly modular with most components being interchangeable; the same solvers used for the 3D DG discretization of the compressible Navier-Stokes equations on large clusters also work transparently for a serial 1D finite volume discretization of the Poisson equation.

We have demonstrated parallel scaling for both explicit and implicit time integration on up to 1, 920 CPU cores (the largest resources available to us thus far), but at the same time we are able to efficiently run simple verification tests on a workstation.

Implementations must be validated as fit for purpose. This task ranges from verifying that 1D linear problems achieve the formal order of accuracy of a scheme to comparing with experimental results in real turbulent flows. We outline the systematic validation approach leading to high resolution computations of two of the most challenging problems that are a focus of the worldwide CFD research community.

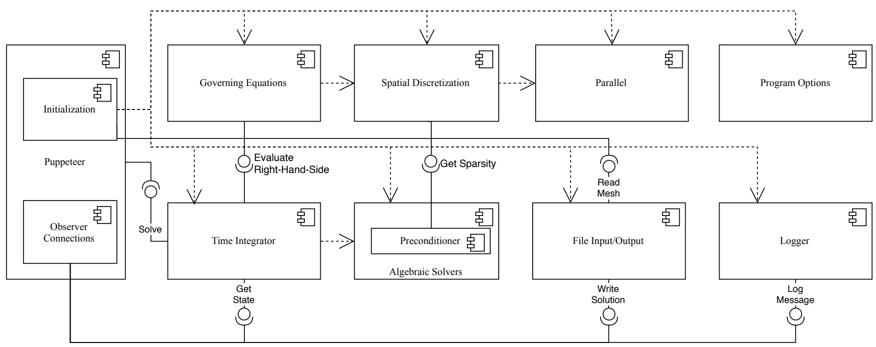
The results obtained by us for the tandem spheres, a recent benchmark problem for high-order methods, represent both the highest resolution known to have been performed as well as at higher Reynolds numbers. Additionally, the accuracy of our code has been benchmarked by participating to the 4th AIAA CFD high lift prediction workshop (HLPW-4) within the high order discretization technical focus group, held in conjunction with the 2021 AIAA SciTech forum: maDG proved to be one of few successful applications of high-order methods to complex aerodynamic flows at this scale.

We believe that our code is now mature enough to be tested and exploited to simulate *ab-initio* more complex turbulent flows. Since ***maDG*** is the keystone of our proposal it will be presented first; we'll conclude the narrative by providing the roadmap for the proposed demonstration study.

maDG

The code solves the compressible form of the Navier-Stokes equation using a nodal Discontinuous Galerkin method as detailed in the thorough text by Hesthaven & Warburton[1] and the many references therein. Presently we use their spatial discretization almost verbatim in both the collocated and quadrature-based discrete differential operators, and so choose to minimize redundant elaboration of the method here. The viscous elliptic terms are handled in the same approach as the original work by Bassi & Rebay[2], by treating them as a system of coupled first order equations. The viscous numerical fluxes in this case follow historically from the finite element literature. The novelty and strength of the code rests on a flexible software design that is maintainable and easily portable to a wide range of HPC architectures.

The code is highly modular with most components being interchangeable; the same solvers used for the 3D DG discretization of the compressible Navier-Stokes equations on large clusters also work transparently for a serial 1D finite volume discretization of the Poisson equation. Similarly, the implementations for evaluating the residual of a specific set of equations should have no knowledge of or dependence on the underlying spatial discretization. This is accomplished in part through object oriented abstraction of the fundamental notions represented by the components listed in the following structural diagram which presents an overview of the major components of ***maDG*** and their interdependencies.



In no particular order, these are

- *Governing Equations*: Evaluates the right hand side of a generic ODE of the form $du/dt = f(u,t)$. Concrete implementations include the compressible Navier-Stokes and Euler equations, the wave equation, and the heat or Poisson equation, as well as simple scalar ODEs useful for testing.
- *Spatial Discretization*: Provides the discrete operators necessary to evaluate the terms required by the governing equations. Primarily this consists of the 3D unstructured tetrahedral DG discretization, but also includes traditional finite volume discretizations, with plans to further extend this to other methods.
- *Parallel*: Provides distributed memory communication capabilities necessary for the spatial discretization.
- *Program Options*: Run-time configurable options with command-line and configuration file input based on the boost.program_options library.
- *Time Integrator*: Drives the solution of the generic ODE $du/dt = f(u,t)$ with the right hand side provided by the governing equations component, with many explicit and implicit variants implemented.

- *Algebraic Solvers*: For the implicit time integrators which require algebraic solvers, this provides a nearly black box interface, where all that is required for preconditioning the JFNK method is the sparsity pattern provided by the spatial discretization.
- *File Input/Output*: Provides parallel input and output of mesh and solution data files, primarily using the standard CGNS library.
- *Logger*: Provides runtime logging facilites to terminal and file as a sink to other components.
- *Puppeteer*: Initializes all of the above components and connects relevant interfaces through use of the C++11 lambda observer pattern.

The "puppeteer" pattern and related "mediator" pattern exist to manage how sets of objects interact with one another. While an overarching design objective is to minimize interdependencies between components, clearly all our components serve a purpose and must interact with one another either directly or indirectly. Each rectangular block represents a single logical component in the structure, and the connections between indicate specific relationships. A dashed line pointing from e.g. component Governing Equations to component Spatial Discretization indicates that Governing Equations depends on Spatial Discretization. Implicit in this relationship is that Spatial Discretization does not depend on Governing Equations, and furthermore that in implementation Spatial Discretization should not even be aware of the existence of Governing Equations. The "ball and socket" UML connection denotes an interface relationship. The component with the ball provides a specific interface, and the component(s) with the connected socket use that interface. Here, the Time Integrator component requires the Governing Equations to provide an interface to evaluate the right hand side of an ODE. The Preconditioner component requires the Spatial Discretization component to provide an interface which defines the sparsity of the linear system. The complete interfaces of all these components are naturally more complex than can be presented in a readable diagram, but the emphasis is on the conceptual design, and encouraging a clear separation of concerns between the components and specific, well defined interactions between them.

Comparing methods that attempt to solve the same problem using different means is a primary task in numerical methods research. A research code should therefor make it as easy as possible to implement new methods in an existing framework. In order to facilitate extension of new capabilities, a design pattern known as the abstract factory method is used. Combining this with automatic static registration of new types allows newly implemented methods to be automatically available through a program options singleton.

Automated testing

Complementary to all of the major solver components is an extensive automated testing framework. Automated testing and continuous integration are essential aspects of modern software development practices that are frequently lacking in academic software. Components and classes are designed to be highly testable in isolation from one another, enabling unit testing of all critical parts which executes in a few seconds after compilation. We make a distinction between automated unit testing, where individual components are tested for correctness, and automated *verification testing*, wherein we are using these integrated components to solve real problems and check their correctness and order of accuracy.

In developing ***maDG*** we have used a test-driven development approach (TDD) which requires that when implementing any new feature, a unit test for the correctness of that feature is implemented *before* the feature itself

The following sections describe automated testing methods used by the authors throughout the development and validation of ***maDG***. We separate the testing into two complementary categories:

- *unit testing*: frequently run, fast tests of simple isolated components used in conjunction with test-driven development (TDD), and
- *verification testing*: longer running tests that verify the full suite of software components combine to correctly solve benchmark problems,

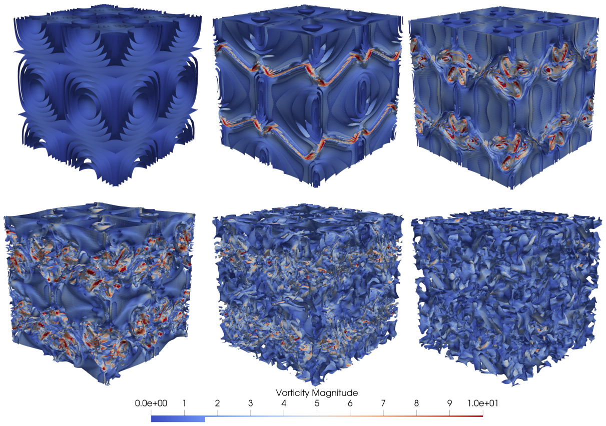
acknowledging the distinction is sometimes blurry.

The bulk of tests when employing TDD are generally very small, almost mundane entities. This entails having many more unit tests than can be communicated in this proposal; what follows is a small sample to hopefully provide a more broad picture.

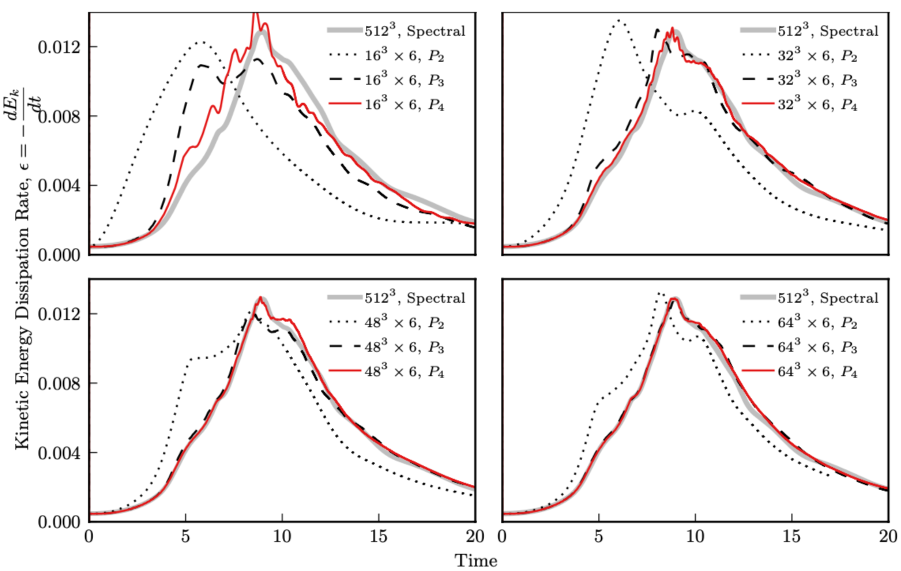
- Basis functions: for the basis sets used in the 1D, triangular, and tetrahedral elements, use a quadrature to ensure the basis functions are all orthonormal to one another for all orders implemented.
- Spatial discretizations: test that gradient, divergence, and integration operators give the expected result for a known analytic input.
- in situ monitoring: test that the integrated enstrophy and kinetic energy values are correct for a known analytic input.
- Inviscid fluxes: test that our Riemann solvers give the expect result of the first step of the Sod shock tube problem.
- Scattered data interpolation: where we use radial basis functions and other methods, check that they correctly interpolate known functions on a mesh.
- Quadrature operators: on a reference element, test that the implementation of volume and surface quadrature operators achieve the correct result to expected accuracy.
- Algebraic solvers: check that the Jacobian-free Newton-Krylov solvers can solve simple nonlinear algebraic systems of equations which have known solutions.
- Governing equations: similar to the above example for testing the Navier-Stokes spatial operator, test the correctness of the Poisson and advection equations.
- File i/o: check that a mesh and solution written to file can be read back into exactly the same state.
- Parallel tests: residual evaluations on arbitrary process counts should be equivalent to serial.

These tests are automatically run when the software is built on a new computer platform.

No matter how thorough our unit testing procedures are, we ultimately still need to solve more “realistic” problems, here taken to mean the solution of a well-posed PDE with some boundary conditions on a parallel computer. We desire these problems to be easily verifiable, either by the existence of an exact solution or by extensive numerical reference material. We also desire these problems to be computationally inexpensive, albeit they will naturally be much more expensive than the unit tests described previously. Problems such the tandem spheres implicit LES from past high order workshops and previously presented by the authors are excellent benchmarks highlighting the advantages of high order methods, but are of limited utility in automated testing due to their computational expense. For this reason, we use a Quasi-3D Couette Flow, a Quasi-3D Driven Cavity, and a Quasi-3D Inviscid Vortex and finally a DNS solution for the Taylor-Green Vortex at Re=1600 as final tests for our software.



The Taylor-Green vortex case consists of a periodic box with an initial laminar vorticity field. The flow field then transitions to homogeneous anisotropic turbulence and subsequently decays. As a validation case for high-order CFD, this serves to assess the accuracy and efficiency of a method for these types of flows in a geometry that permits comparison with benchmark spectral method solutions. The pseudo-spectral solution of Van Rees et al (2001)[3] is used as a reference in the following results.

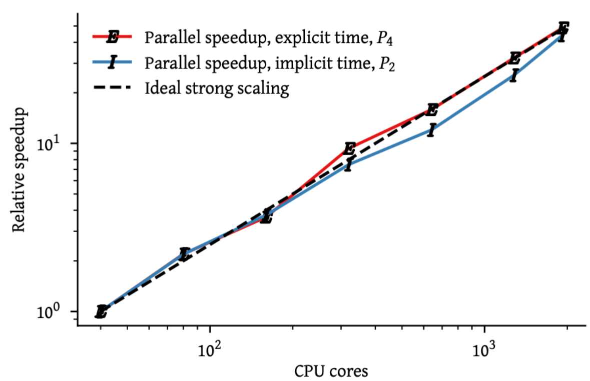


Abstractions

The current version of **maDG** uses RAJA for GPU or OpenMP, or pure C++ for serial CPU abstracted away from the main code, which enables a quick conversion to new emerging standards, and shelters the CFD developer from the details of the backend. The approach we have taken is illustrated in the following figure; for simplicity the coding structure required by the user for a one dimensional model is presented.

Parallel Performance

The parallel scaling of ***maDG*** has been demonstrated to be nearly ideal on the largest computational hardware available to us to date. Parallel scaling for DG methods is aided by the compact high order nature of the discretization's residual evaluation. While the path to parallel scaling for explicit methods is straightforward, parallel scaling for implicit methods is more challenging.   Implicit solvers require the solution of linear and nonlinear systems of equations and introduce algorithmic complexity. The use of a Jacobian-free Newton-Krylov method implies that efficiently parallelized explicit methods translate into efficient implicit methods, at least as far as the computation of the approximate Jacobian matrix-vector product of equation is concerned. The choice of a preconditioner for the Krylov method is also important, as it shouldn't induce additional parallel overhead. The ILU(0) preconditioner, which uses the same sparsity pattern as the underlying problem's sparse Jacobian, in conjunction with the

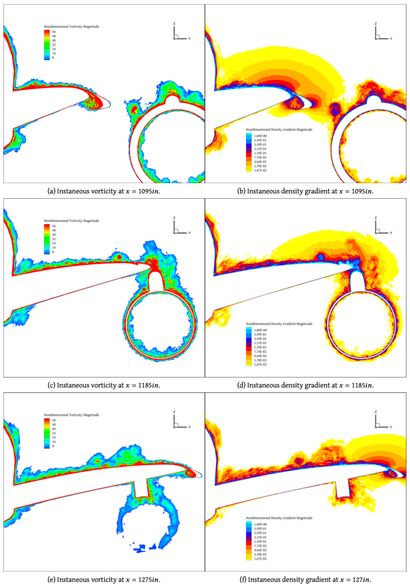


GMRES Krylov solver has been found to be an efficiently scalable solver configuration. The strong scaling achieved by ***maDG*** for the Taylor-Green vortex case using both explicit and implicit time stepping is summarized in the figure above.

COMPUTATIONAL READINESS

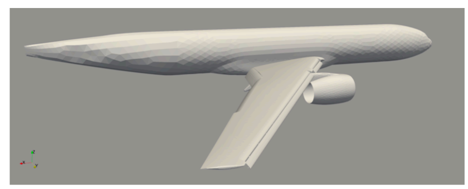
We expect to reach readiness of ***maDG*** on the AURORA system as soon as we are granted access.

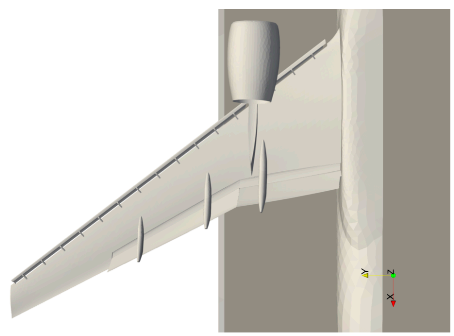
RESEARCH OBJECTIVES, MILESTONES, AND RESOURCES REQUESTED



Prediction of high-lift and stall performance.

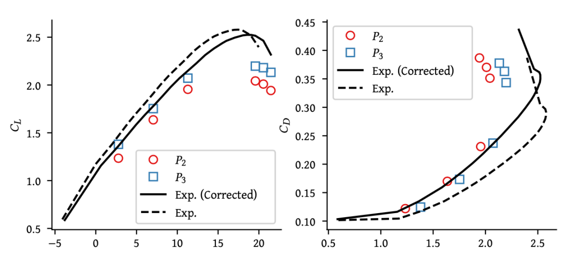
Wall-resolved large eddy simulation of the high-lift configuration model represents something of a holy grail singled out by the motivating CFD Vision 2030 study.[4] High lift devices are one aspect of aerodynamic analysis and design that have seen limited application of computational fluid dynamics, and their performance affect greatly the efficiency of modern airframes, contributing to the weight of the airframe and ultimately on the carbon footprint of air transportation. The NASA High Lift Common Research Model (HL-CRM) is a publicly available geometry intended as a reference point for collaboration and comparison of experimental and computational results. Evans et al[5] provide detailed experimental data for this case, which is one subject of the 3rd and 4th AIAA High Lift Prediction Workshop. Complex transitional and separating unsteady flows are found in this configuration, particularly near CL,max . This is precisely the type of flow where high-order methods are hoped to overcome weaknesses in traditional $2nd$ order RANS and hybrid LES-RANS methods. The geometry is a simplified model of a transport aircraft including leading-edge slats and trailing-edge flaps, an empty nacelle, flap fairings and slat hinges.





The multiscale flow physics result in very challenging and complex numerics. The stability issues are severe for this case, and despite applying over-integration and filtering methods, ***maDG*** has not yet been able to reliably produce stable solutions at the specified Reynolds number of 5.49 × 10E6. It is expected that increased grid refinement will result in effective stabilization, the computational resources required by such computations are

Quantity	Value
Mach number	0.1
Reynolds number (mean aerodynamic chord)	3.84×10^5
Mesh cell count	$2.58M$
Mesh wall resolution	$y^+ \approx 200$
Boundary conditions	Riemann farfield, isothermal no-slip wall, symmetry
Time step	$\Delta t_c = 1.43 \times 10^{-4}$ based on characteristic scale of U_∞ / MAC
Time integration method	BDF2
Iterative solver	GMRES-ILU(0) Jacobian-free Newton-Krylov



commensurate to the resources requested on AURORA. It is estimated that for each angle of attack, the calculations at full Reynolds number require approximately 8,000 node-hour each. Thus a complete polar is estimated to require 48,000 node-hours.

The preliminary calculations run at a lower the Reynolds number and the conditions summarized in the table. The results obtained are very promising: all the vortical structures controlling the flow physics are computed accurately, resulting in good agreement with the experimental forces away from stall.

The results obtained so far and presented here, while not themselves fully resolved, demonstrate that the methods current under development are a path forward for future high resolution simulations of full aircraft configurations. Our work is one of few successful applications of high-order methods to complex aerodynamic flows at this scale. We are planning to extend these calculation to flight Reynolds numbers and move toward the goal of a wall-resolved large eddy simulation of the high-lift configuration model.

Characterization of vortex generators performance.

Vortex generators are ubiquitous passive flow control devices used on airplane wings and wind-turbine blades to control turbulent flow separation and delaying stall, nevertheless not very much is known about the controlling flow physics of these devices.

We are planning to study from first principle (DNS) the flow filed created by vortex generators at Reynolds number characteristics of industrial scale devices, with the aim of discovering scaling laws that would aid their design and optimal deployment. Preliminary calculations performed with ***maDG*** on vortex generators at Reynolds numbers of 400,000 were found in excellent agreement with available PIV measurements, we are planning to extend the study of this problem up to flight Reynolds number (order 1.E7).

It is estimated that this task will require a total of 12,000 node-hours.

Continuous Improvement of *maDG*

We will continue to carry out algorithmic research and improve our computer code. In particular, we are planing to

A. Validate a novel implicit BDF schemes that leverages the efficiency of p-multigrid. Preliminary studies indicate that the convergence rate are comparable to a fully implicit method but a much lower computational cost especially on GPUs, as demonstrated by the following figure illustrating convergence rates of several p-multigrid strategies in comparison to the current implicit scheme. We project the cost of these calculations to be one third of the fully implicit scheme. Thus the calculation of a polar will require 16,000 nodes-hour on AURORA.

B. Extend the code applicability to Hypersonic gas dynamics, by implementing sub grid-models based on a local solution of the Boltzmann equation which will allow the resolution of shock waves at all relevant scales. The estimation of this work, to be carried out in year 2, is estimated to require 60,000 node-hours on AURORA.

REFERENCES

1) J. S. Hesthaven and T. Warburton. *Nodal Discontinuous Galerkin Methods - Algorithms, Analysis, and Appli- cations*. Vol. 54. Texts in Applied Mathematics. New York, NY: Springer New York, 2008

2) F. Bassi and S. Rebay. “High-Order Accurate Discontinuous Finite Element Solution of the 2D Euler Equations”. In: *Journal of Computational Physics* 138.2 (Dec. 1997), pp. 251–285..

3) W. M. van Rees, A. Leonard, D. I. Pullin, and P. Koumoutsakos. “A comparison of vortex and pseudo-spectral methods for the simulation of periodic vortical flows at high Reynolds numbers”. In: *Journal of Computational Physics* 230.8 (2011), pp. 2794–2805.

4) J. Slotnick et al., “CFD Vision 2030 Study : A Path to Revolutionary Computational Aerosciences

5) A. Evans, D. Lacy, I. Smith, and M. Rivers. “Test summary of the nasa semi-span high-lift common research model at the qinetiq 5-metre low-speed wind tunnel”. In: *Aiaa Aviation 2020 Forum* 1 PartF (2020), pp. 1–24 (cited on p. 126).

PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

We are requesting access to AURORA for the two developers of ***maDG:*** the principal investigator Luigi Martinelli and his principal collaborator Mark Lohry. Luigi Martinelli has more than three decades experience in developing CFD methods and codes. He collaborated extensively throughout his career with A. Jameson toward the development of the more recent FLO codes for aerodynamic analysis, and collaborated extensively with J. Alonso in parallelizing the FLO codes in the mid 1990s. Additionally he pioneered continuous adjoint optimization methods based on the solution of the Reynolds Averaged Navier-Stokes equations. Mark Lohry completed his Ph.D. at Princeton under Martinelli's guidance, and he is the originator of the software framework implemented in ***maDG***.

Throughout the initial development of the software we have formed a synergistic partnership that allowed us to design and craft the code with precision while minimizing team management tasks. We are planing to continue following a similar path, which will make it trivial to assign resources to the three prongs of the project. The team holds weekly virtual meetings to review progress and prioritize the work. The principal investigator is ultimately responsible for meeting the project milestones.

MILESTONE TABLES

Year 1 Total number of node-hours for year 1: 76000

Milestone	Description	Dates	Status
NASA High Lift Common Research Model (HL-CRM) at Full Reynolds Number	Compute the polar for the HL-CRM model at full Reynolds number with the implicit scheme. 48,000 node-hour	6/30/2023	
Fluid Dynamics of Vortex generators	Full characterization of vortex generators via DNS 12,000 node-hour	12/30/2023	
Validation of p-mgrid driven scheme	Compute the polar for the HL-CRM model at full Reynolds number with the new solver. 16,000 node-hour	9/30/2023	

Year 2 Total number of node-hours for year 2: 60000

Milestone	Description	Dates	Status
Extension of maDG to hypersonic regime		6/30/2024	
Validation for Hypersonic flow	The BOLT Boundary Layer Transition flight experiment will be used as a benchmark	12/30/2023	

Biographical Sketch: Luigi Martinelli

Department of Mech. & Aerosp. Engineering, Princeton University
Phone: (609) 258-6652, Fax: (609) 258-6123 Email: gigi@princeton.edu Princeton, New Jersey 08544

Professional Preparation

Politecnico di Milano, Milano, Italy *April 1981*
Laurea **(Doctorate) in Aeronautical Engineering**

Princeton University, Princeton, New Jersey *October 1987*
Ph.D. in Mechanical and Aerospace Engineering

Appointments

Princeton University, Princeton, New Jersey *July 2019 -*
Professor in the Department of MAE
Associate Faculty in the Program in Applied and Computational Mathematics (PACM)
Associate Faculty in the Princeton Institute for Computational Science and Engineering (PICSciE)

Princeton University, Princeton, New Jersey *June 2000- June 2019*
Associate Professor in the Department of MAE

Princeton University, Princeton, New Jersey *January 1994 - June 2000*
Assistant Professor in the Department of MAE

Princeton University, Princeton, New Jersey *August 1987- January 1994*
Research Staff Member in the Department of MAE

Products most closely related

MR1 *"Discontinuous Galerkin Implicit Large Eddy Simulation of Tandem Spheres and the High-Lift Common Research Model."* (with Mark Lohry), AIAA Science and Technology Forum and Exposition 2022, (AIAA 2022-1375)

MR2 *"On the development, verification, and validation of a discontinuous Galerkin solver for the Navier–Stokes equations"* (with M. Lohry), Computers & Fluids, Volume 223, 2021, 104921, https://doi.org/10.1016/j.compfluid.2021.104921.

MR3 *" Implicit Time Integration of Discontinuous Galerkin Approximations to the Navier-Stokes Equations"* (with Mark Lohry) , AIAA Science and Technology Forum and Exposition 2020, (AIAA 2020-0774 -Invited Paper), https://arc.aiaa.org/doi/abs/10.2514/6.2020-0774.

MR4 *"Higher-Order Implicit Large Eddy Simulations of a VFE-2 Delta Wing"* (with Tarik Dzanic), AIAA Science and Technology Forum and Exposition 2019, AIAA 2019-0276.

MR5 *"Identification of unsteady aerodynamic models for a generic wide-body aircraft at high angles of attack"*, (with Dirk M. Luchtenburg, Clarence W. Rowley, Mark W. Lohry, and Robert F. Stengel), Journal of Aircraft 52.3 (2015): 890-895.

RESEARCH INTEREST AND EXPERTISE

Martinelli's research is primarily motivated by the desire of improving the aerodynamics efficiency of airplanes, cars, ships, and energy conversion devices, and is concerned with a variety of fundamental problems at the intersection of aerodynamics, computational science and engineering design. He contributed to the development of fast multigrid methods for the solution of viscous conservation laws in both compressible and incompressible regime. He also made noted contributions to the development of efficient shape design optimization methods based on the Reynolds Averaged Navier-Stokes equations, which have been widely used in Industry for the aerodynamic design of contemporary transonic airplanes. In the mid 90's he led the effort of porting the FLO codes to multiprocessor systems, one of the first successful transition of aerodynamic software to parallel computers. For the past 10 years his research has been focus on the simulation of complex, unsteady, vortex-dominated, wall bounded turbulent flows. To this end, he has led the effort of developing modern software for the reliable and efficient implementation of high-order methods on current HPC systems.

SYNERGISTIC ACTIVITIES

SA1 Developed, in collaboration with Antony Jameson, accurate and efficient viscous solvers for compressible and incompressible flow, which form the basis of simulation methods used worldwide by major aerospace companies.

SA2 Developed, in collaboration with Antony Jameson, the first practical aerodynamic design method based on control theory of the RANS for the optimization of transonic wings.

SA3 Extended adjoint based optimization methods to incompressible flow, and demonstrated successful design of low-cavitating airfoil for use in marine propellers and pumps, and ship hull with reduced wave drag.

COLLABORATORS AND OTHER AFFILIATIONS

Collaborators: Juan Alonso (Stanford U.), Antony Jameson (Texas A&M.), Mark Lohry (Princeton U. now at Cadence Design System Inc.) Richard Miles (Princeton U.), Clarence Rowley (Princeton U.), Alexander Smits (Princeton U.)

Section 6: Software Applications and Packages

Question #1

Please list any software packages used by the project, and indicate if they are on open source or export controlled.

Application Packages

Package Name

RAJA, PETSC, METIS, BOOST, EIGEN,NANOFLANN, GOOGLETEST

Indicate whether Open Source or Export Controlled.

Open Source

Section 7: Wrap-Up Questions

Question #1

National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.

The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.

Proprietary Information

Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?

Yes

Will the proposed project use proprietary information, intellectual property, or licensing?

No

Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?

If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.

No

Question #2

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.

PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.

Export Control

Does this project use or generate sensitive or restricted information?

No

Does the proposed project involve any of the following areas?

i. Military, space craft, satellites, missiles, and associated hardware, software or technical data

ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data

iii. Encryption above 128 bit software (source and object code)

iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)

No

Does the proposed project involve International Traffic in Arms Regulations (ITAR)?

No

Question #3

The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.

Health Data

Will this project use health data?

No

Will this project use human health data?

No

Will this project use Protected Health Information (PHI)?

No

Question #4

The PI and designated Project Manager agree to the following:

Monitor Agreement

I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.

Yes

I agree to provide periodic updates of research accomplishments and to

acknowledge INCITE and the LCF in publications resulting from an INCITE award.

Yes

I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.

Yes

I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.

Yes

Section 8: Outreach and Suggested Reviewers

Question #1

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Outreach

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Email Notice.

Question #2

Suggested Reviewers

Section 9: Testbed Resources

Question #1

The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)

The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation.

The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: https://www.alcf.anl.gov/alcf-ai-testbed.

Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.

No-AI.pdf
The attachment is on the following page.

No AI testbed access required for this proposal.