SIMULATION AND ADJOINT-BASED DESIGN FOR VARIABLE DENSITY INCOMPRESSIBLE FLOWS WITH HEAT TRANSFER

Dr. Thomas D. Economon

Multiphysics Modeling and Simulation

Robert Bosch LLC

3rd Annual SU2 Developers Meeting

2018.09.17

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Agenda

1. Background

2. Modeling & Implementation

3. Results (V&V)

4. Conclusions

BACKGROUND

Bosch – technology to enhance quality of life

- Some 59,000[1] researchers and developers work at Bosch: at 120[2] locations worldwide, in a single network.
- Bosch is one of the world's leading international providers of technology and services.
- Over the past six years, Bosch has invested more than 27 billion euros in research and development.
- Our objective: to develop innovative, useful, and exciting products and solutions to enhance quality of life – technology that is "Invented for life."

[1] As of 12.16 [2] R&D locations with >50 associates, as of 12.16

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Bosch – Four business sectors
Key figures 2016*

Bosch Group	▶ 73.1 billion euros in sales ▶ 389,281 associates

Mobility Solutions
- One of the world's largest suppliers of mobility solutions

60% share of sales

Industrial Technology
- Leading in drive and control technology, packaging, and process technology

Energy and Building Technology
- One of the leading manufacturers of security and communication technology
- Leading manufacturer of energy-efficent heating products and hot-water solutions

40% share of sales

Consumer Goods
- Leading supplier of power tools and accessories
- Leading supplier of household appliances

* As of 12.16

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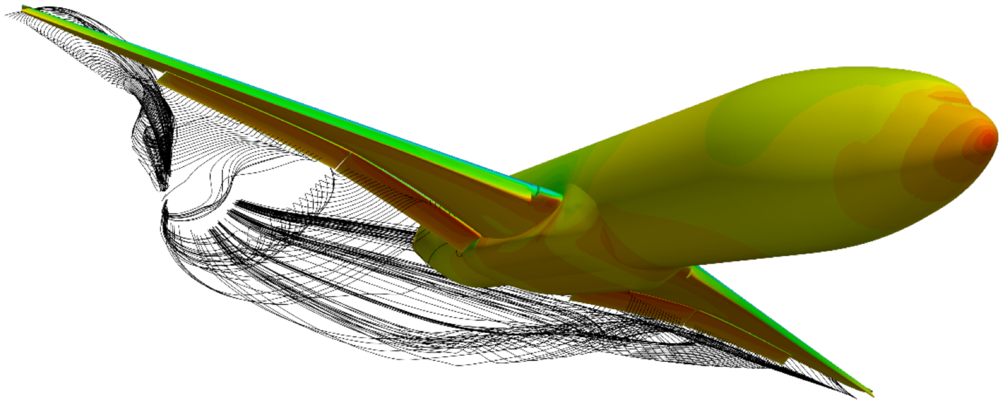
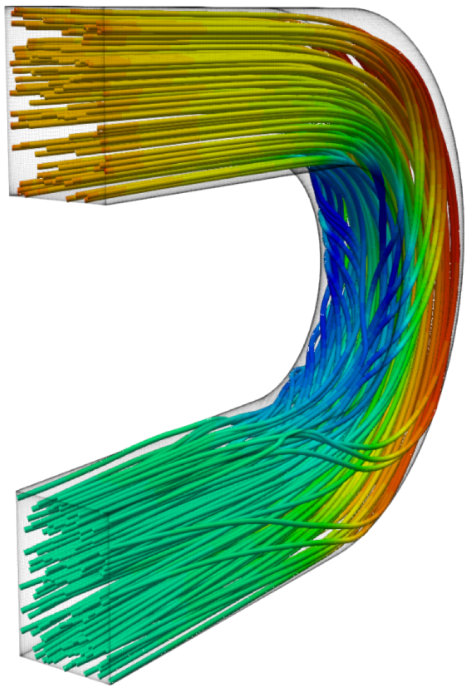
Background
Some SU2 History



External, Compressible Aerodynamics

✓



Internal, Incompressible Flows with Heat Transfer

?

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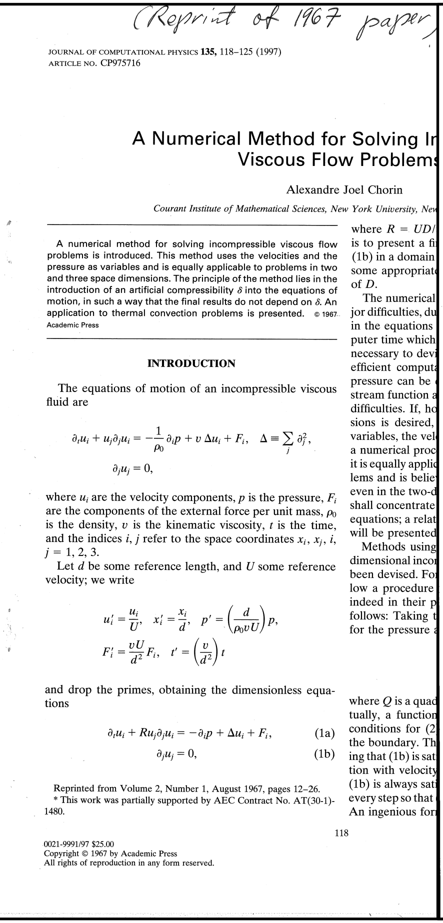
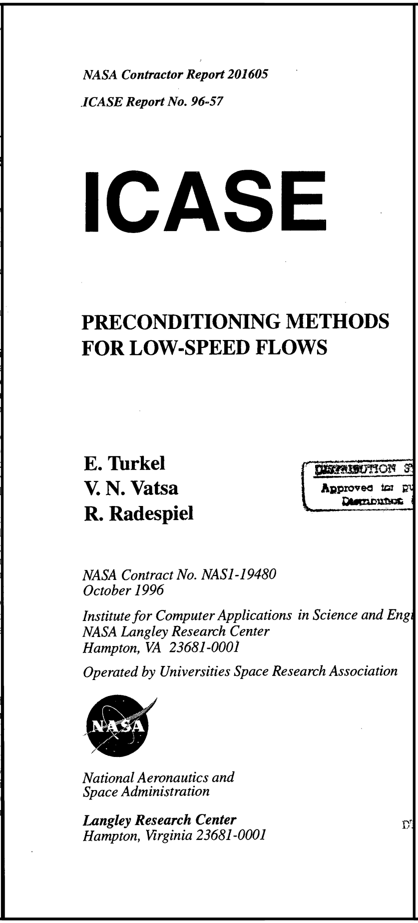
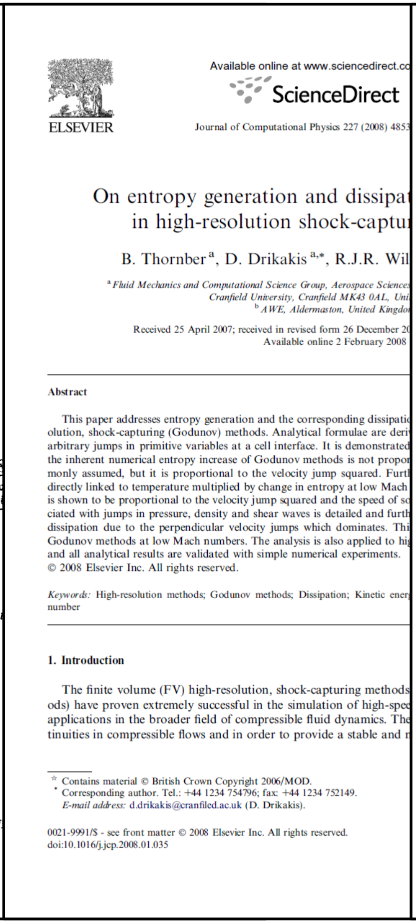
Background

Coupled Approaches (Density-based) in SU2







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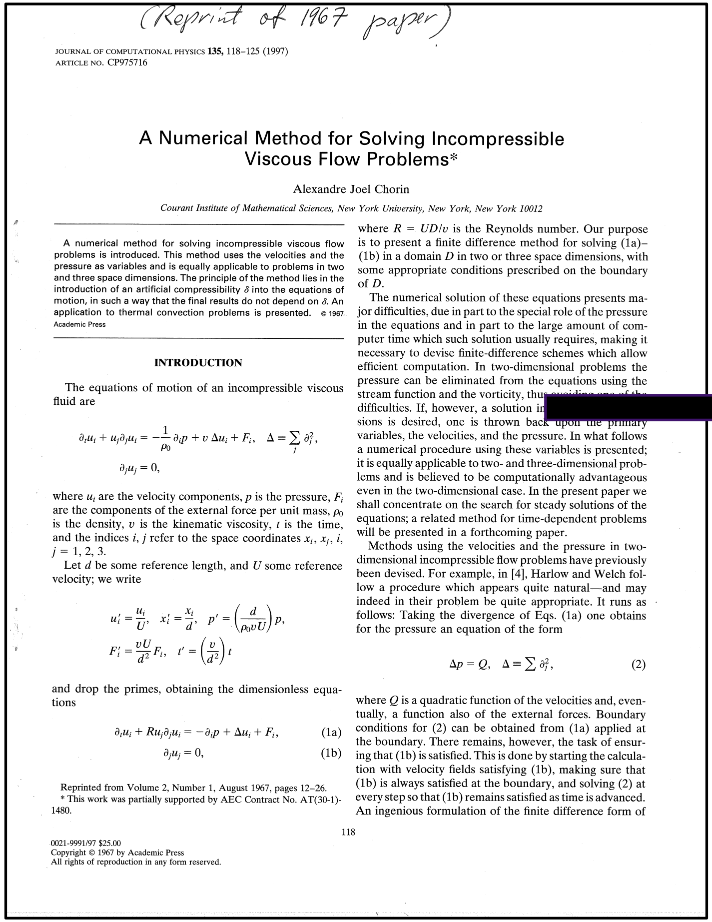
Background

Coupled Approaches (Density-based) in SU2



(Reprint of 1967 paper)

JOURNAL OF COMPUTATIONAL PHYSICS 135, 118–125 (1997)
ARTICLE NO. CP975716

A Numerical Method for Solving Incompressible Viscous Flow Problems*

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A numerical method for solving incompressible viscous flow problems is introduced. This method uses the velocities and the pressure as variables and is equally applicable to problems in two and three space dimensions. The principle of the method lies in the introduction of an artificial compressibility δ into the equations of motion, in such a way that the final results do not depend on δ. An application to thermal convection problems is presented.

INTRODUCTION

The equations of motion of an incompressible viscous fluid are

$$\partial_t u_i + u_j \partial_j u_i = -\frac{1}{\rho_0}\partial_i p + v\,\Delta u_i + F_i, \quad \Delta \equiv \sum_j \partial_j^2,$$
$$\partial_j u_j = 0,$$

where u_i are the velocity components, p is the pressure, F_i are the components of the external force per unit mass, ρ_0 is the density, v is the kinematic viscosity, t is the time, and the indices i, j refer to the space coordinates x_i, x_j, $i, j = 1, 2, 3$.

Let d be some reference length, and U some reference velocity; we write

$$u_i' = \frac{u_i}{U}, \quad x_i' = \frac{x_i}{d}, \quad p' = \left(\frac{d}{\rho_0 v U}\right) p,$$
$$F_i' = \frac{vU}{d^2} F_i, \quad t' = \left(\frac{v}{d^2}\right) t$$

and drop the primes, obtaining the dimensionless equations

$$\partial_t u_i + R u_j \partial_j u_i = -\partial_i p + \Delta u_i + F_i, \qquad (1a)$$
$$\partial_j u_j = 0, \qquad (1b)$$

where $R = UD/v$ is the Reynolds number. Our purpose is to present a finite difference method for solving (1a)–(1b) in a domain D in two or three space dimensions, with some appropriate conditions prescribed on the boundary of D.

The numerical solution of these equations presents major difficulties, due in part to the special role of the pressure in the equations and in part to the large amount of computer time which such solution usually requires, making it necessary to devise finite-difference schemes which allow efficient computation. In two-dimensional problems the pressure can be eliminated from the equations using the stream function and the vorticity, thu difficulties. If, however, a solution in sions is desired, one is thrown back upon the primary variables, the velocities, and the pressure. In what follows a numerical procedure using these variables is presented; it is equally applicable to two- and three-dimensional problems and is believed to be computationally advantageous even in the two-dimensional case. In the present paper we shall concentrate on the search for steady solutions of the equations; a related method for time-dependent problems will be presented in a forthcoming paper.

Methods using the velocities and the pressure in two-dimensional incompressible flow problems have previously been devised. For example, in [4], Harlow and Welch follow a procedure which appears quite natural—and may indeed in their problem be quite appropriate. It runs as follows: Taking the divergence of Eqs. (1a) one obtains for the pressure an equation of the form

$$\Delta p = Q, \quad \Delta \equiv \sum \partial_j^2, \qquad (2)$$

where Q is a quadratic function of the velocities and, eventually, a function also of the external forces. Boundary conditions for (2) can be obtained from (1a) applied at the boundary. There remains, however, the task of ensuring that (1b) is satisfied. This is done by starting the calculation with velocity fields satisfying (1b), making sure that (1b) is always satisfied at the boundary, and solving (2) at every step so that (1b) remains satisfied as time is advanced. An ingenious formulation of the finite difference form of

Reprinted from Volume 2, Number 1, August 1967, pages 12–26.
* This work was partially supported by AEC Contract No. AT(30-1)-1480.

0021-9991/97 $25.00

Let's develop a robust coupled method more general than Artificial Compressibility w/out complexity of fully compressible N-S.

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Preconditioning Applied to Variable and Constant Density Flows

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A time-derivative preconditioning of the Navier–Stokes equations, suitable for both variable and constant density fluids, is developed. The ideas of low-Mach-number preconditioning and artificial compressibility are combined into a unified approach designed to enhance convergence rates of density-based, time-marching schemes for solving flows of incompressible and variable density fluids at all speeds. The preconditioning is coupled with a dual time-stepping scheme implemented within an explicit, multistage algorithm for solving time-accurate flows. The resultant time integration scheme is used in conjunction with a finite volume discretization designed for unstructured, solution-adaptive mesh topologies. This method is shown to provide accurate steady-state solutions for transonic and low-speed flow of variable density fluids. The time-accurate solution of unsteady, incompressible flow is also demonstrated.

Introduction

THE use of computational fluid dynamics (CFD) technologies is expanding throughout industry, academia, and the research community. As such, numerical flow solvers are relied upon to solve a wide class of flow problems ranging from incompressible, low-Reynolds-number flows to high-speed compressible flows at high Reynolds numbers. In addition, the flowfields of interest are becoming more geometrically complex and contain flow features that span um of length scales. Because it is more practical to self with a single code, designers, experimentalists, and other end-users of CFD software look to a single flow solver that can address this wide range of flow conditions.

Historically, incompressible low-Reynolds-number flows were first addressed by pressure-based solution algorithms.[1] In these methods the equations of motion are solved in a segregated (uncoupled) manner, relying on diagonal dominance for convergence. Pressure-based algorithms have since been extended to solve flows at high Reynolds numbers and compressible flows[2] as well. Alternatively, density-based schemes were developed in the context of transonic, external aerodynamic applications.[3] These methods employ time-marching procedures, both implicit[4,5] and explicit,[6] to solve the hyperbolic system of governing equations. Density-based methods have also been extended to solve low-Reynolds-number and incompressible flows.[7,8] The similarities and differences between the pressure-based and density-based approaches are discussed in further detail in Ref. 9.

To meet the demand of CFD users cited earlier, a density-based flow solver is developed based on an unstructured, solution-adaptive mesh topology. The algorithms employed here are designed to compute steady-state and time-dependent flows of incompressible and variable density fluids at all speeds over a wide range of Reynolds numbers.

We have chosen to use unstructured meshes because they provide great flexibility in discretizing geometrically complex domains and offer the potential for solution adaption to resolve the various length scales of an evolving flowfield. Optimizing computational efficiency is especially important for numerical flow solvers based on unstructured meshes because these schemes are generally used in conjunction with explicit, multistage solution algorithms such as Runge–Kutta.[6] Explicit schemes provide a low operation count per iteration but suffer from serious time-step limitations relative to their implicit counterparts. Time steps are limited even further by equation stiffness when solving low-Mach-number compressible flows and by time-accuracy constraints in unsteady problems. The effect of decreased time-step size is realized by low convergence rates that in turn result in higher computational costs per solution.

Time-marching schemes provide good stability and convergence characteristics when solving compressible flows at transonic and supersonic Mach numbers. At low speeds, however, system stiffness resulting from disparate particle and acoustic velocities (i.e., large condition number) causes convergence rates to deteriorate. Convergence can be made independent of Mach number by altering the acoustic speeds of the system such that all eigenvalues become of the same order and the condition number is made to approach unity. Several approaches to normalizing eigenvalues via time-derivative preconditioning have been proposed[10–13] and shown to enhance convergence of flows with low Mach numbers.

In their fundamental form, time-marching schemes are useless for solving incompressible flows because the incompressible system is not fully hyperbolic, and pressure cannot be updated from an equation of state. This deficiency is overcome by employing an artificial-compressibility approach[7,8] wherein a pressure time derivative is introduced into the continuity equation. With the artificial pressure term, the system becomes hyperbolic and a means to update pressure is provided. When solving the equations in conservative form, it has been recommended that this term be included in all of the equations.[11] In either case, the pressure time derivative is normalized by a pseudoacoustic speed (squared). The pseudoacoustic speed is typically set to about twice the local velocity, such that a pseudo-Mach number of one-half is achieved, thereby providing optimal convergence.

It is our objective to combine the ideas of low-Mach-number preconditioning and artificial compressibility into a unified approach and produce a preconditioning matrix that will provide for efficient solution of both constant and variable density flows at all speeds. The derivation of this new preconditioning follows closely with that given in Ref. 12 for compressible flows with three notable exceptions: 1) derivatives of density with respect to pressure and temperature are carried through without the assumption of an ideal gas law equation of state, 2) the pseudoacoustic speed used to condition the eigenvalues of the system is written in terms of a characteristic reference velocity as opposed to a local speed of sound and reference Mach number, and 3) derivatives of density with respect to temperature are retained. It has been our experience that this latter exception is necessary for solving flows in which density is a function of temperature only.

Because time-derivative preconditioning destroys the time accuracy of the governing equations, the solution of unsteady flow is not possible by these means alone. To overcome this limitation, we employ a dual time-stepping[13,14] procedure. This involves an inner iteration loop in pseudotime that is wrapped by an outer loop stepping through physical time. Thus, the flowfield at each physical time

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*R&D Engineer. Member AIAA.

MODELING & IMPLEMENTATION

Modeling & Implementation

Governing Equations: low-Mach N-S (variable density)

- Eqns. in conservative form in a domain Omega with solid wall boundary S and inlet/outlet boundaries:

$$
\begin{cases}
R(U) = \frac{\partial U}{\partial t} + \nabla \cdot \bar{F}^c(U) - \nabla \cdot \bar{F}^v(U, \nabla U) = 0, & \text{in } \Omega, \\
\bar{v} = 0, & \text{on } S, \\
T = T_S, & \text{on } S, \\
(W)_{\bar{v}} = W_{in}, & \text{on } \Gamma_{in}, \\
(W)_{\bar{P}} = W_{out}, & \text{on } \Gamma_{out},
\end{cases}
$$

$$U = \{\rho, \rho\bar{v}, \rho c_p T\}^{\mathsf{T}} \qquad \bar{F}^c(U) = \begin{Bmatrix} \rho\bar{v} \\ \rho\bar{v} \otimes \bar{v} + \bar{\bar{I}}p \\ \rho c_p T\bar{v} \end{Bmatrix}, \quad \bar{F}^v(U, \nabla U) = \begin{Bmatrix} \cdot \\ \bar{\bar{\tau}} \\ \kappa \nabla T \end{Bmatrix},$$

$$\rho = \frac{p_o}{RT}$$

$$\bar{\bar{\tau}} = \mu \left(\nabla\bar{v} + \nabla\bar{v}^T \right) - \mu \frac{2}{3} \bar{\bar{I}} \left(\nabla \cdot \bar{v} \right).$$

Research and Technology Center North America | CR/RTC5.2-NA-Economon | 09.17.2018

Modeling & Implementation
Coupled Approach I/II

- We follow the approach of Weiss & Smith [1995] with some notable differences… in the end we have:

$$R(V) = \Gamma \frac{\partial V}{\partial t} + \nabla \cdot \bar{F}^c(V) - \nabla \cdot \bar{F}^v(V, \nabla V) = 0$$

$$\Gamma = \begin{bmatrix} \frac{1}{\beta^2} & 0 & 0 & 0 & \rho_T \\ \frac{u}{\beta^2} & \rho & 0 & 0 & \rho_T u \\ \frac{v}{\beta^2} & 0 & \rho & 0 & \rho_T v \\ \frac{w}{\beta^2} & 0 & 0 & \rho & \rho_T w \\ \frac{c_p T}{\beta^2} & 0 & 0 & 0 & \rho_T c_p T + \rho c_p \end{bmatrix}$$

Modeling & Implementation
Coupled Approach II/II

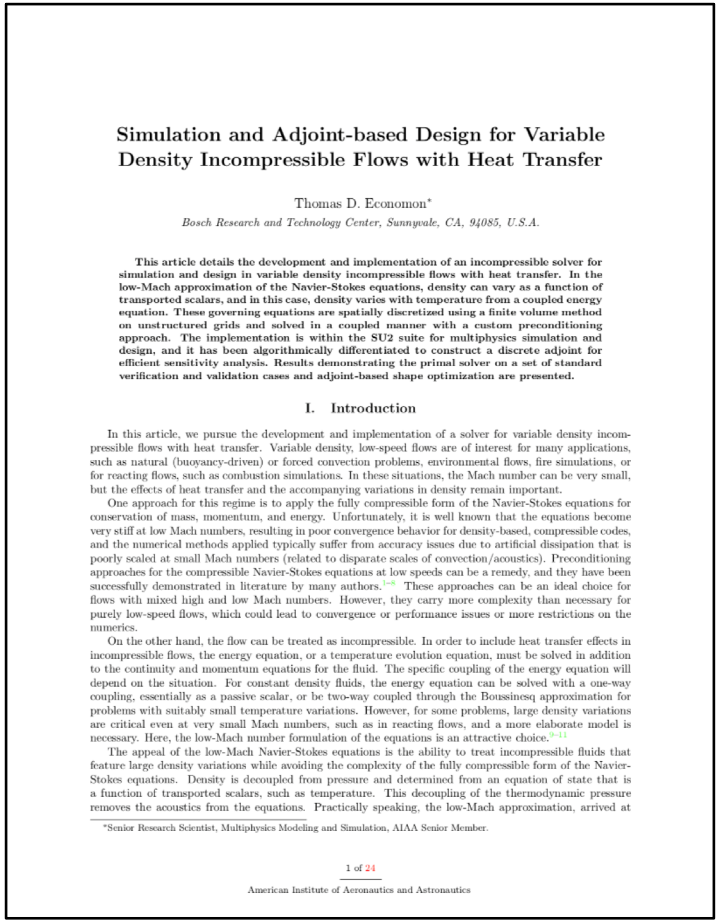
- What exactly is Beta?
  - It is an artificial sound speed
  - We can see this clearly by comparing the eigenvalues of convective flux Jacobian to the compressible case.
  - **Draws clear link between the Artificial Compressibility and preconditioning approaches.**

$$\lambda\left(\Gamma^{-1}\frac{\partial \bar{F}^c}{\partial V}\right) = \lambda\left(\Gamma^{-1}\bar{A}^c\right) = \begin{bmatrix} \bar{v}\cdot\bar{n} & 0 & 0 & 0 & 0 \\ 0 & \bar{v}\cdot\bar{n} & 0 & 0 & 0 \\ 0 & 0 & \bar{v}\cdot\bar{n} & 0 & 0 \\ 0 & 0 & 0 & \bar{v}\cdot\bar{n}-\beta\left|\bar{n}\right| & 0 \\ 0 & 0 & 0 & 0 & \bar{v}\cdot\bar{n}+\beta\left|\bar{n}\right| \end{bmatrix}$$

$$\beta^2 = \epsilon^2(\bar{v}\cdot\bar{v})_{max}$$

Modeling & Implementation
Present Developments

- A custom preconditioning method for low speed flows with heat transfer:
  - Simplicity: fully compressible N-S not required
  - Euler, N-S, and RANS (low-Mach, decoupled energy, or isothermal)
  - Conservative formulation
  - Primitive variable-based, V = {p, u, v, w, T}
  - Custom Flux Difference Splitting (upwind) and centered schemes
  - Implicit & explicit time integration for steady relaxation, time-accurate flows with dual time-stepping
- Enables variable density incompressible flows:
  - Introduces 2 new fluid models: constant density fluid, incompressible ideal gas
- Includes energy equation:
  - New energy eqn. options: disable, solve decoupled, apply Boussinesq approximation, or couple for variable density



Simulation and Adjoint-based Design for Variable Density Incompressible Flows with Heat Transfer

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This article details the development and implementation of an incompressible solver for simulation and design in variable density incompressible flows with heat transfer. In the low-Mach approximation of the Navier-Stokes equations, density can vary as a function of transported scalars, and in this case, density varies with temperature from a coupled energy equation. These governing equations are spatially discretized using a finite volume method on unstructured grids and solved in a coupled manner with a custom preconditioning approach. The implementation is within the SU2 suite for multiphysics simulation and design, and it has been algorithmically differentiated to construct a discrete adjoint for efficient sensitivity analysis. Results demonstrating the primal solver on a set of standard verification and validation cases and adjoint-based shape optimization are presented.

I. Introduction

In this article, we pursue the development and implementation of a solver for variable density incompressible flows with heat transfer. Variable density, low-speed flows are of interest for many applications, such as natural (buoyancy-driven) or forced convection problems, environmental flows, fire simulations, or for reacting flows, such as combustion simulations. In these situations, the Mach number can be very small, but the effects of heat transfer and the accompanying variations in density remain important.

One approach for this regime is to apply the fully compressible form of the Navier-Stokes equations for conservation of mass, momentum, and energy. Unfortunately, it is well known that the equations become very stiff at low Mach numbers, resulting in poor convergence behavior for density-based, compressible codes, and the numerical methods applied typically suffer from accuracy issues due to artificial dissipation that is poorly scaled at small Mach numbers (related to disparate scales of convection/acoustics). Preconditioning approaches for the compressible Navier-Stokes equations at low speeds can be a remedy, and they have been successfully demonstrated in literature by many authors.[1–8] These approaches can be an ideal choice for flows with mixed high and low Mach numbers. However, they carry more complexity than necessary for purely low-speed flows, which could lead to convergence or performance issues or more restrictions on the numerics.

On the other hand, the flow can be treated as incompressible. In order to include heat transfer effects in incompressible flows, the energy equation, or a temperature evolution equation, must be solved in addition to the continuity and momentum equations for the fluid. The specific coupling of the energy equation will depend on the situation. For constant density fluids, the energy equation can be solved with a one-way coupling, essentially as a passive scalar, or be two-way coupled through the Boussinesq approximation for problems with suitably small temperature variations. However, for some problems, large density variations are critical even at very small Mach numbers, such as in reacting flows, and a more elaborate model is necessary. Here, the low-Mach number formulation of the equations is an attractive choice.[9–11]

The appeal of the low-Mach Navier-Stokes equations is the ability to treat incompressible fluids that feature large density variations while avoiding the complexity of the fully compressible form of the Navier-Stokes equations. Density is decoupled from pressure and determined from an equation of state that is a function of transported scalars, such as temperature. This decoupling of the thermodynamic pressure removes the acoustics from the equations. Practically speaking, the low-Mach approximation, arrived at

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American Institute of Aeronautics and Astronautics

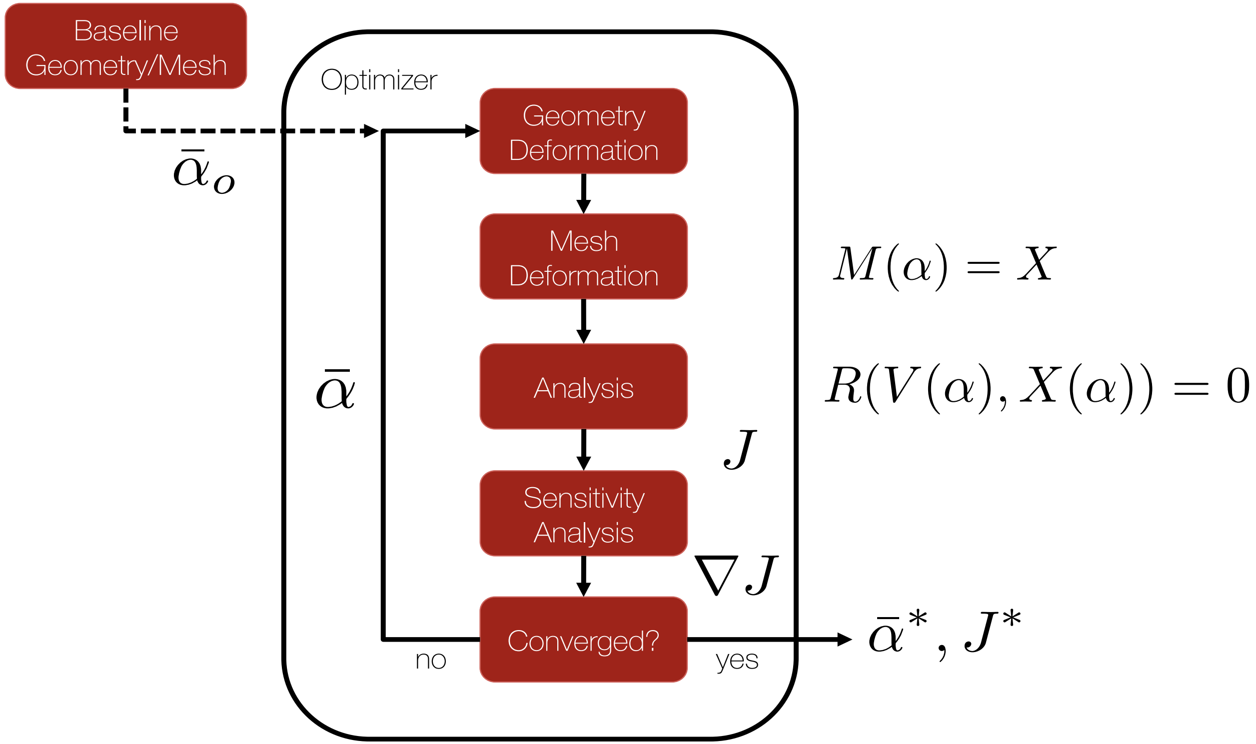
All features released to the public in SU2 v6.1

Modeling & Implementation

Gradient-based Optimal Shape Design

- Input: a baseline geometry/mesh and a chosen parameterization (alpha) controlling shape, and J.
- Primal gives us J, adjoint gives us the gradient efficiently.
- Meshes are deformed with pseudo-structural approach (operator M).
- Numerical optimizer drives the problem to a local optimum J* with final geometry alpha*.
- See Albring et al. 2015, Albring et al. 2016 for full details of discrete adjoint in SU2 with CoDiPack.

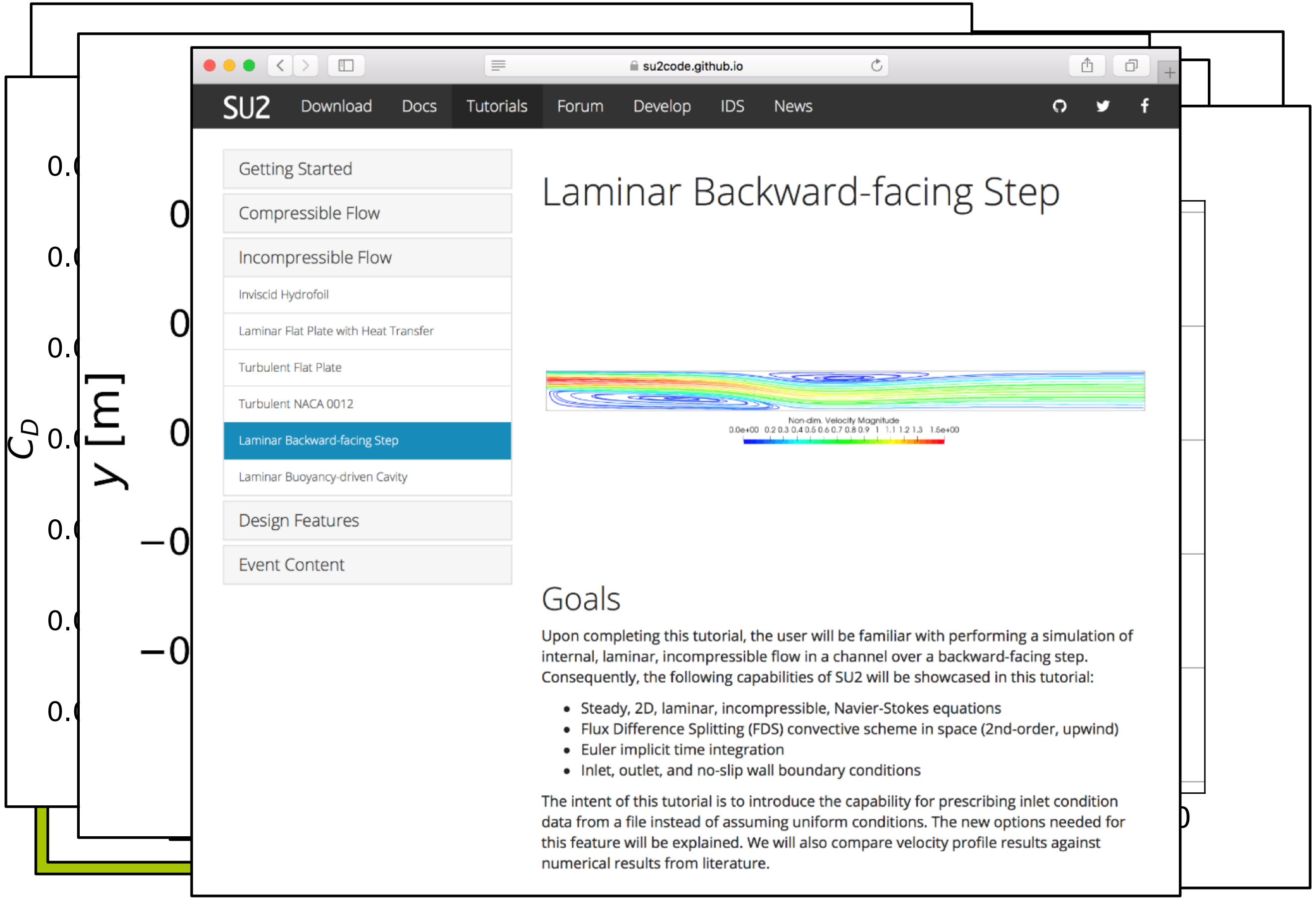
$$\begin{aligned} \min_{\alpha} \quad & J(V(\alpha), X(\alpha)) \\ \text{subject to} \quad & R(V(\alpha), X(\alpha)) = 0 \end{aligned}$$



M. Sagebaum, T. Albring, and N. R. Gauger. *High-Performance Derivative Computations using CoDiPack*. arXiv preprint arXiv:1709.07229, 2017.

RESULTS (V&V)

Results
Verification & Validation (V&V)

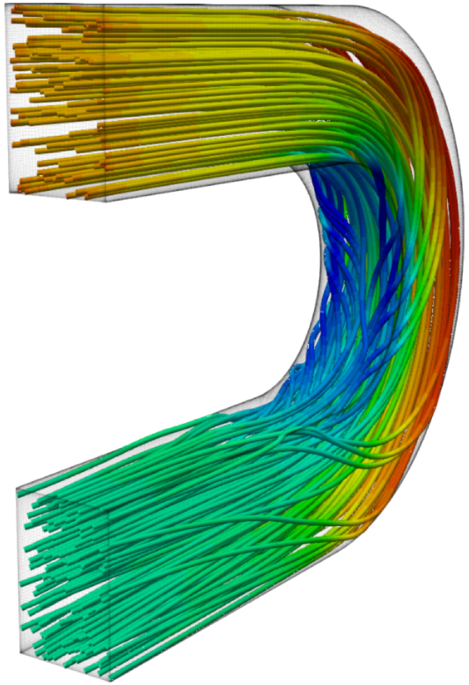


- Inviscid Hydrofoil
- Buoyancy-driven Cavity
- Laminar Flat Plate
- Turbulent Flat Plate
- Turbulent NACA 0012
- Turbulent 3D Bump-in-Channel
- Axisymmetric Pipe
- Laminar Backward-facing Step

- Excellent agreement for all comparisons against theory, well established codes, and experiment.

Tutorials released to the public with SU2 v6.1

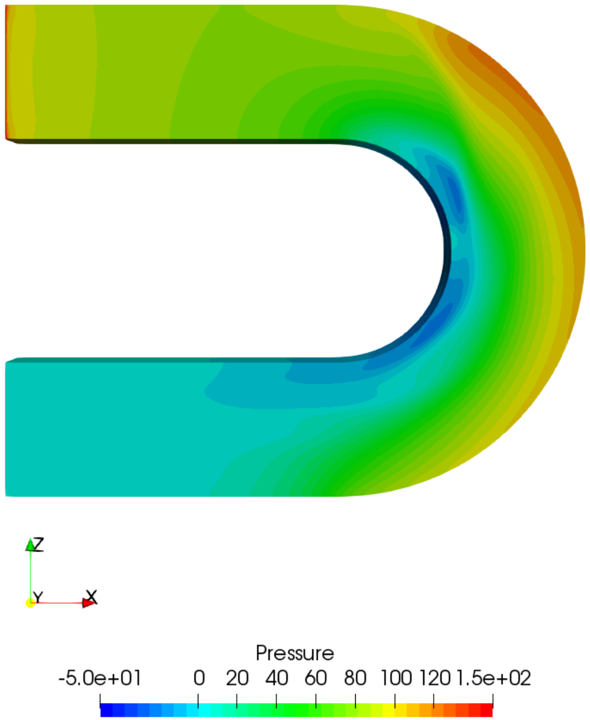
Results
Code Comparison

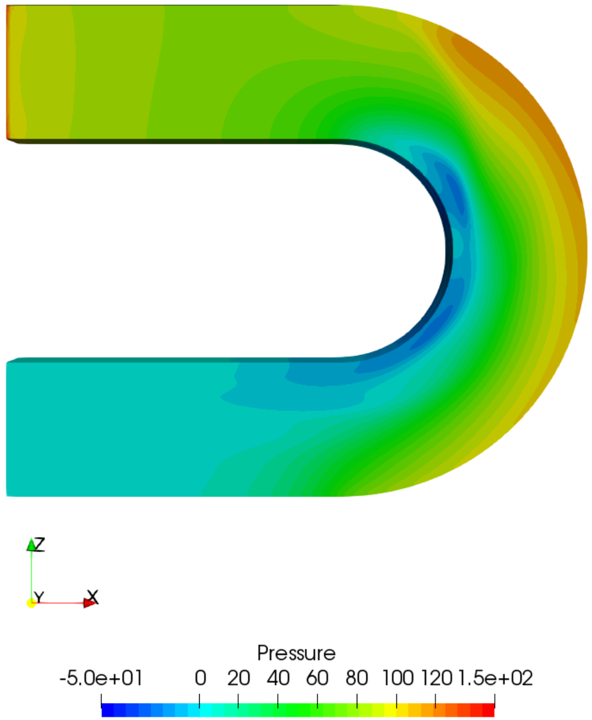


Turbulent flow through a rectangular u-bend.

Re ~ 4300.

SU2 | Fluent





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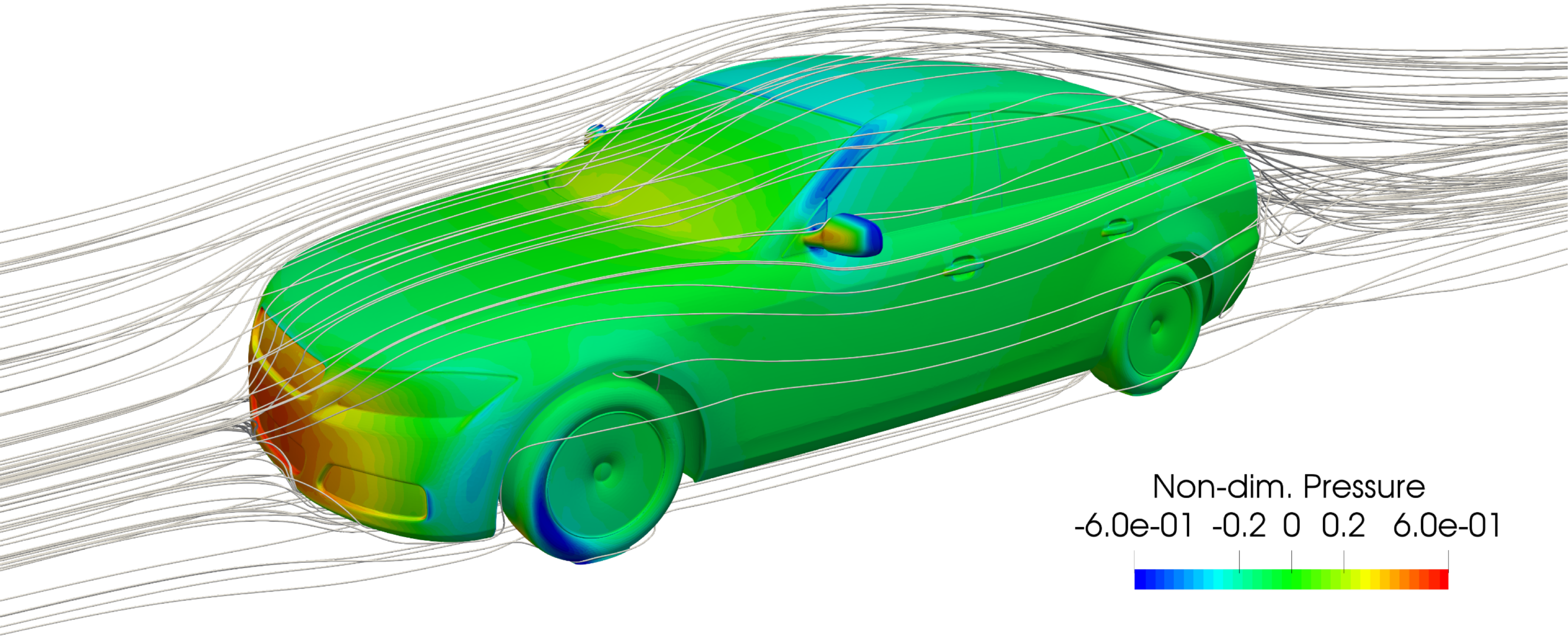
Results
Complex Geometry



DrivAer model. Re ~ 6mio

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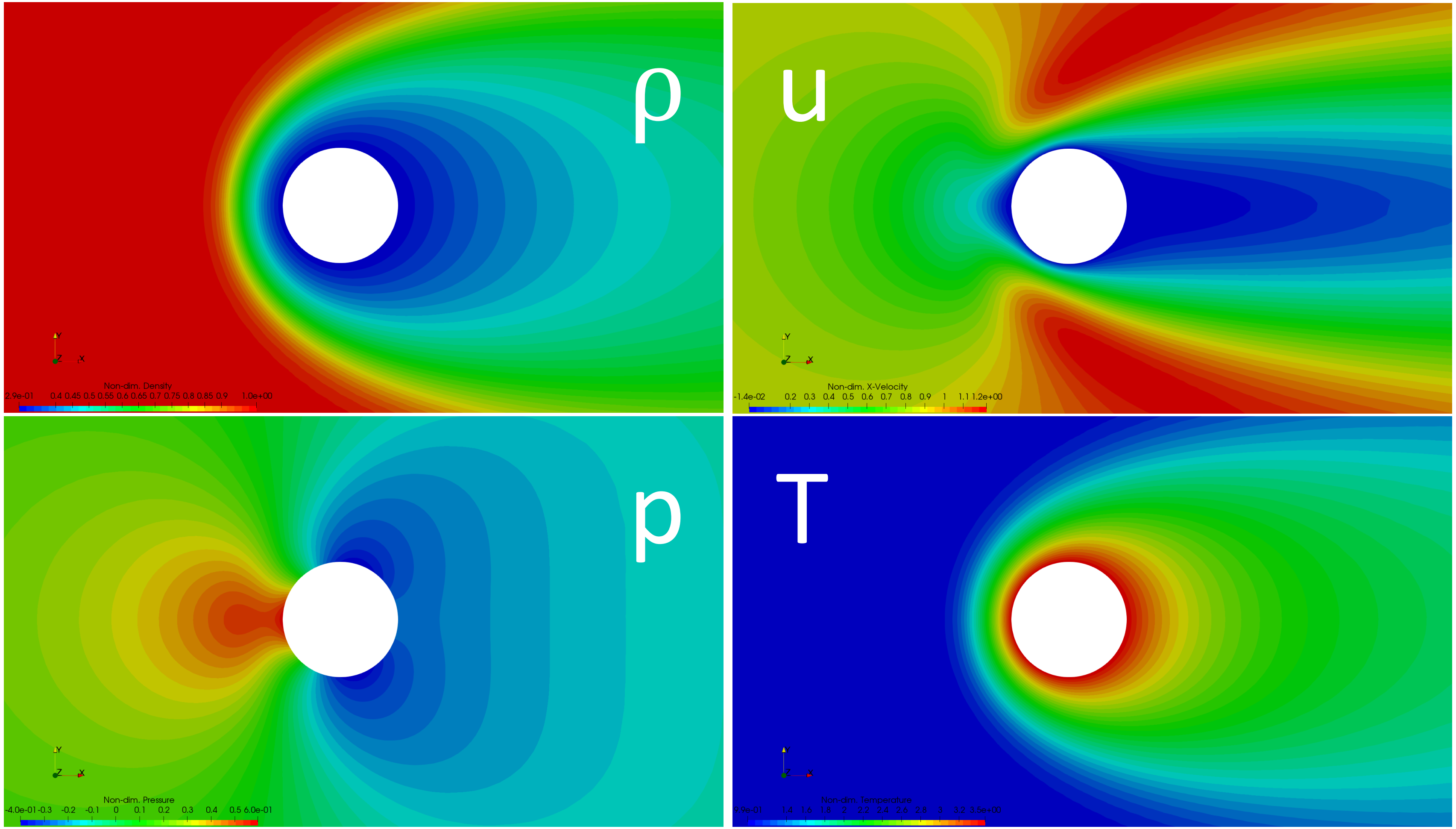
Results

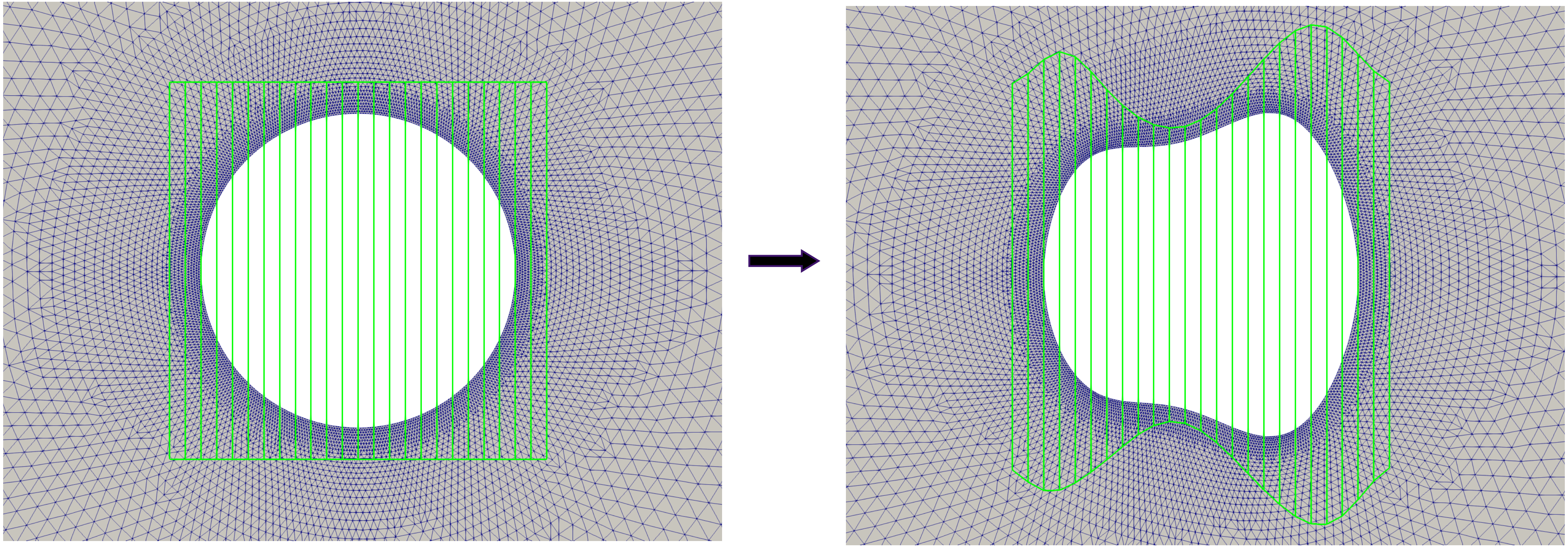
Shape Optimization of a Heated Cylinder: Primal



Re = 40, Tw = 1000 K, Tinf = 288.15, variable density (ideal gas), T-dependent props.

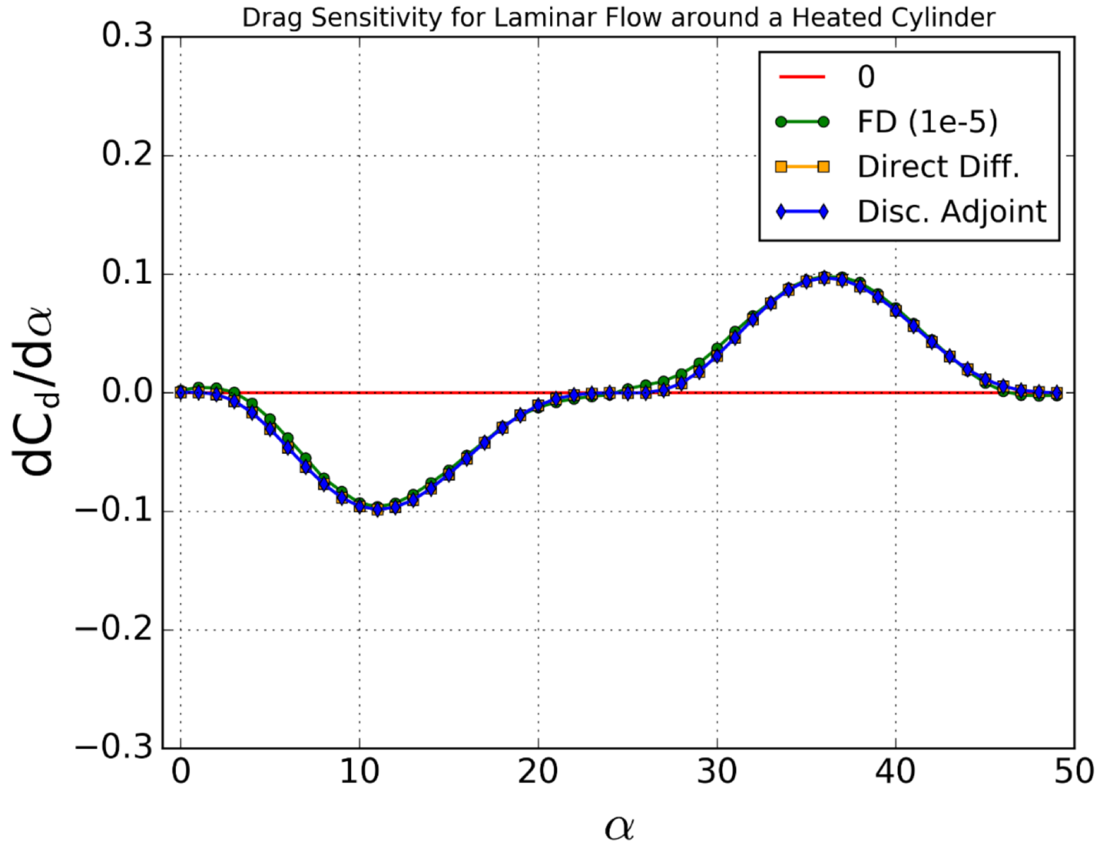
Results

Shape Optimization of a Heated Cylinder: Parameterization



50 free-form deformation control points (25 upper, 25 lower). Vertical movement only.

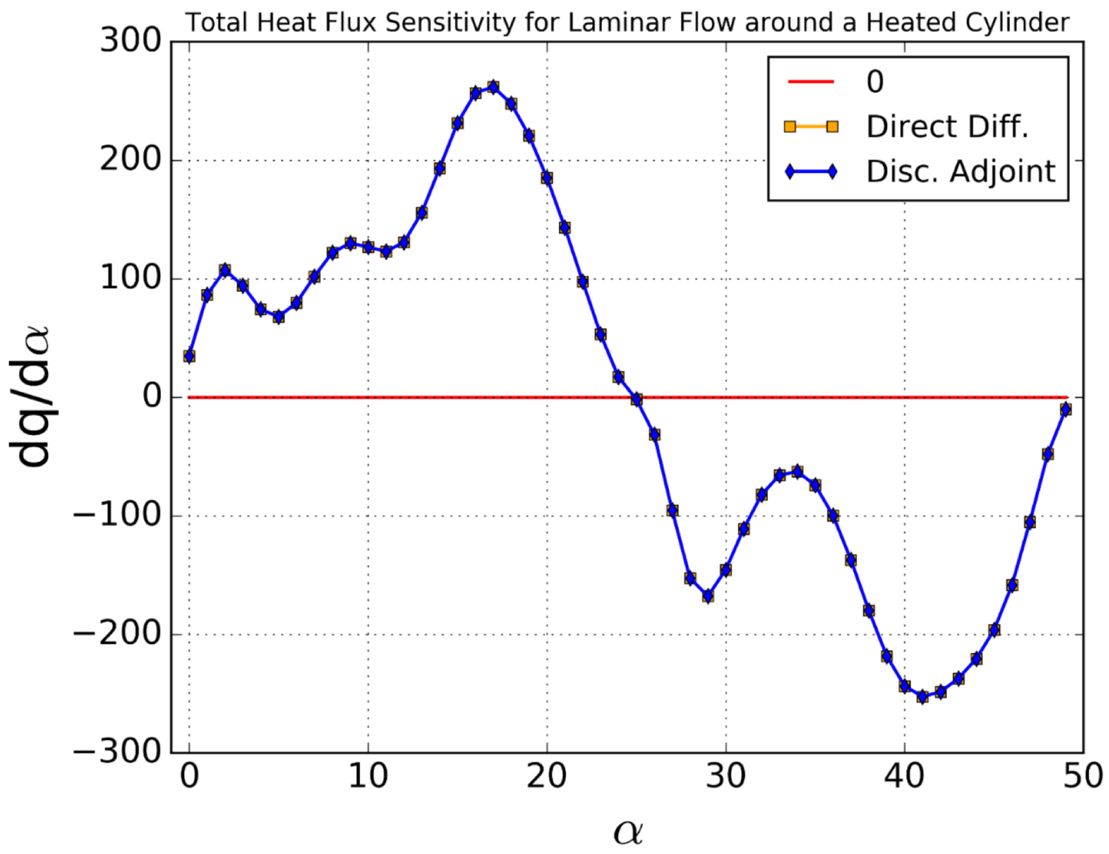
Results
Shape Optimization of a Heated Cylinder: Drag Sens. Verification



50 free-form deformation control points (25 upper, 25 lower). Vertical movement only.

Results

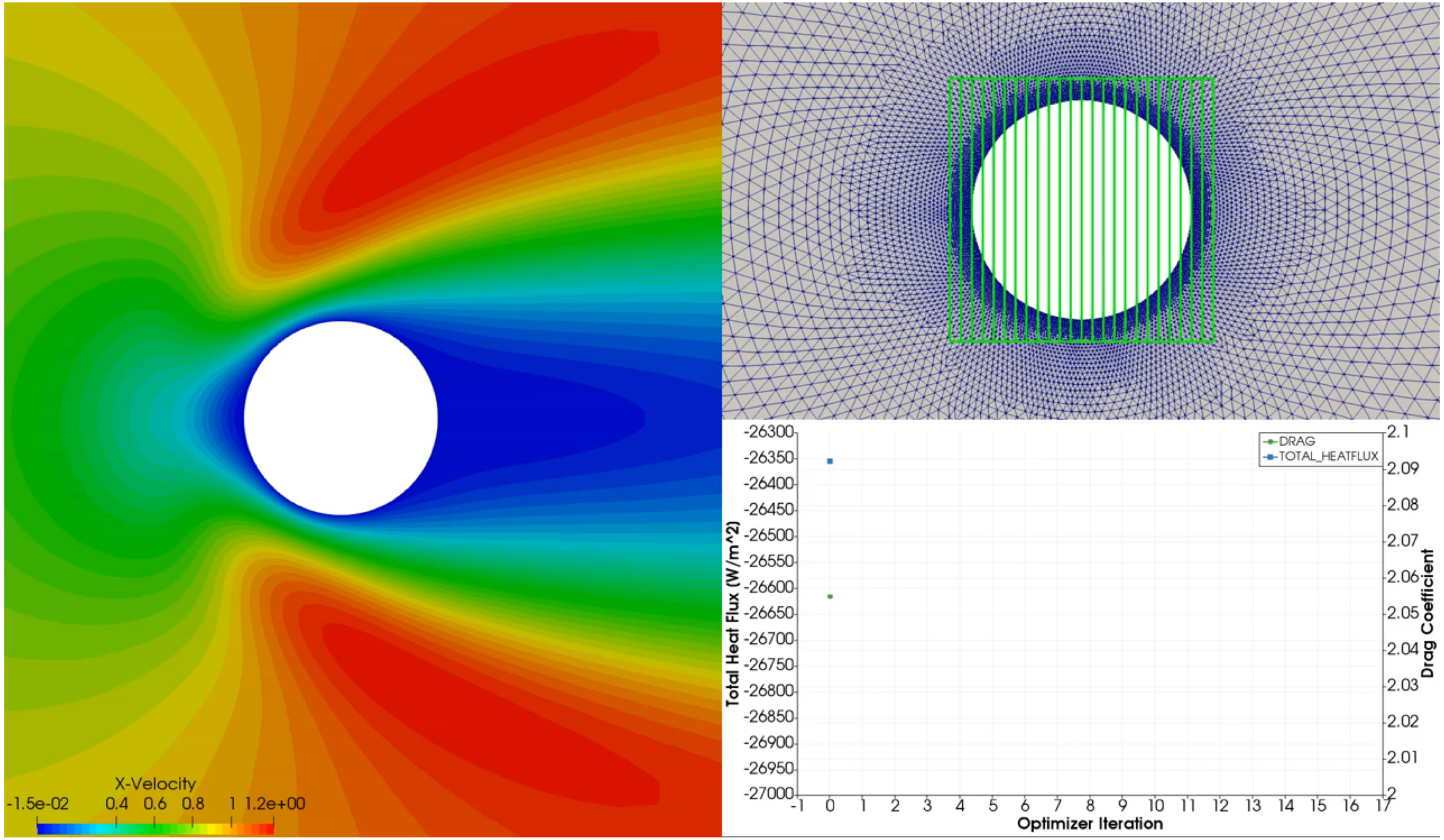
Shape Optimization of a Heated Cylinder: Heat Flux Sens. Verification



50 free-form deformation control points (25 upper, 25 lower). Vertical movement only.

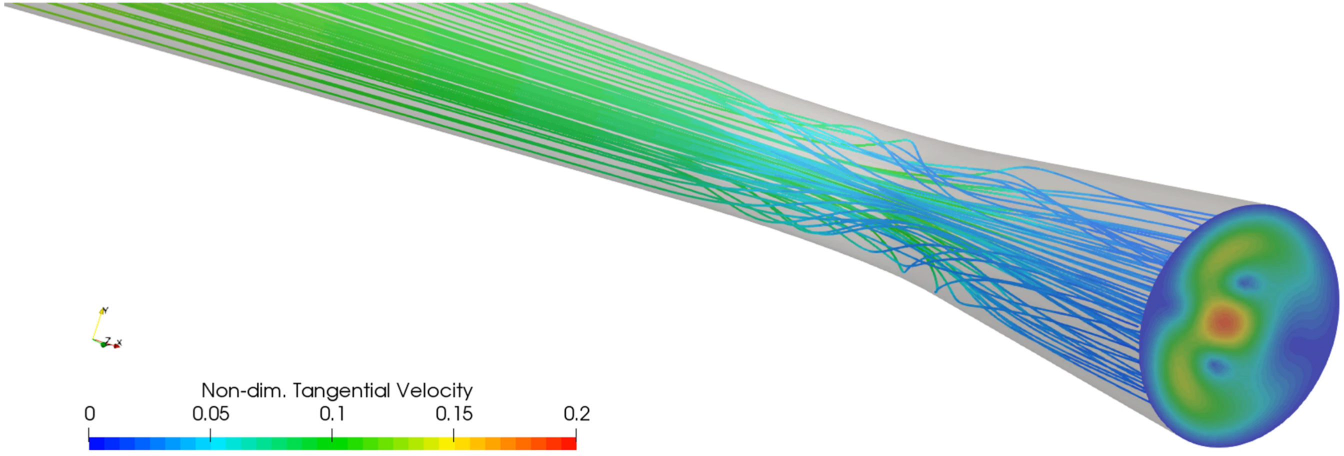
Results

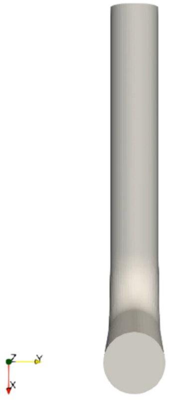
Shape Optimization of a Heated Cylinder: Heat Flux w/ Cd Constraint

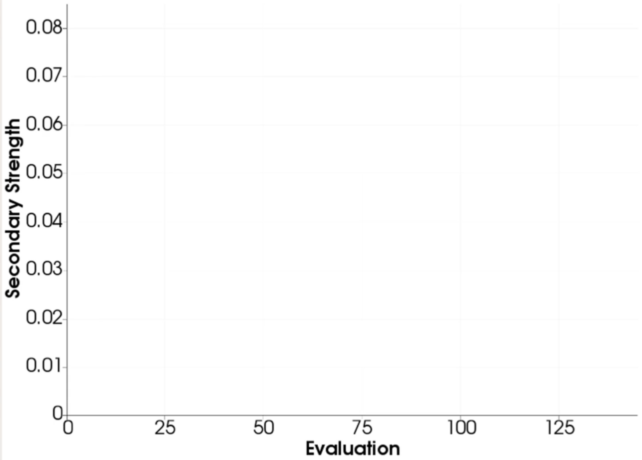


Animation.

V&V
90 Degree Bend Optimization Example

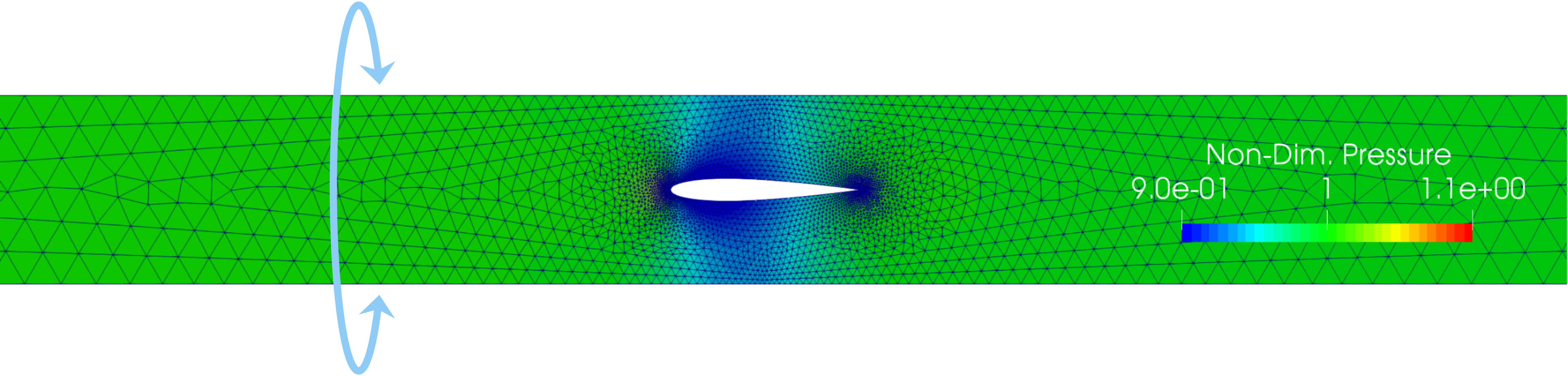






Animation.

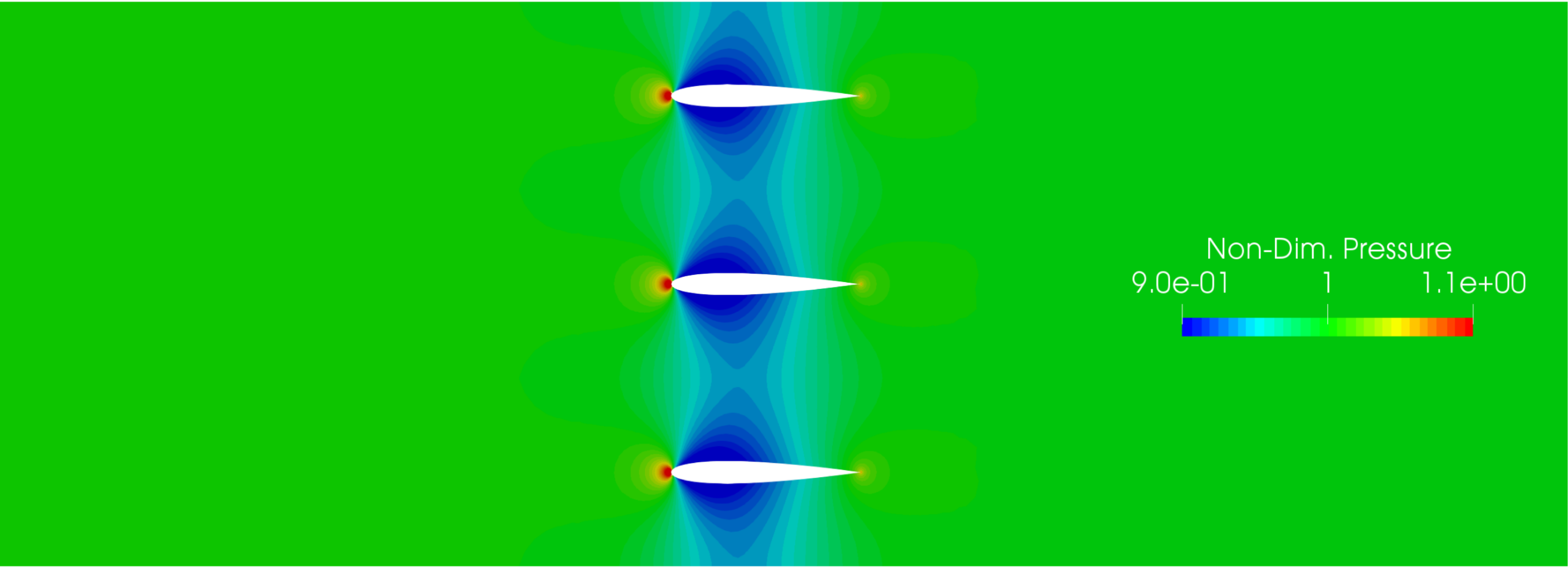
One more thing…
Periodic Boundary Condition



periodic boundary condition now based on concept of completing the residual rather than halo cells

One more thing…

Periodic Boundary Condition



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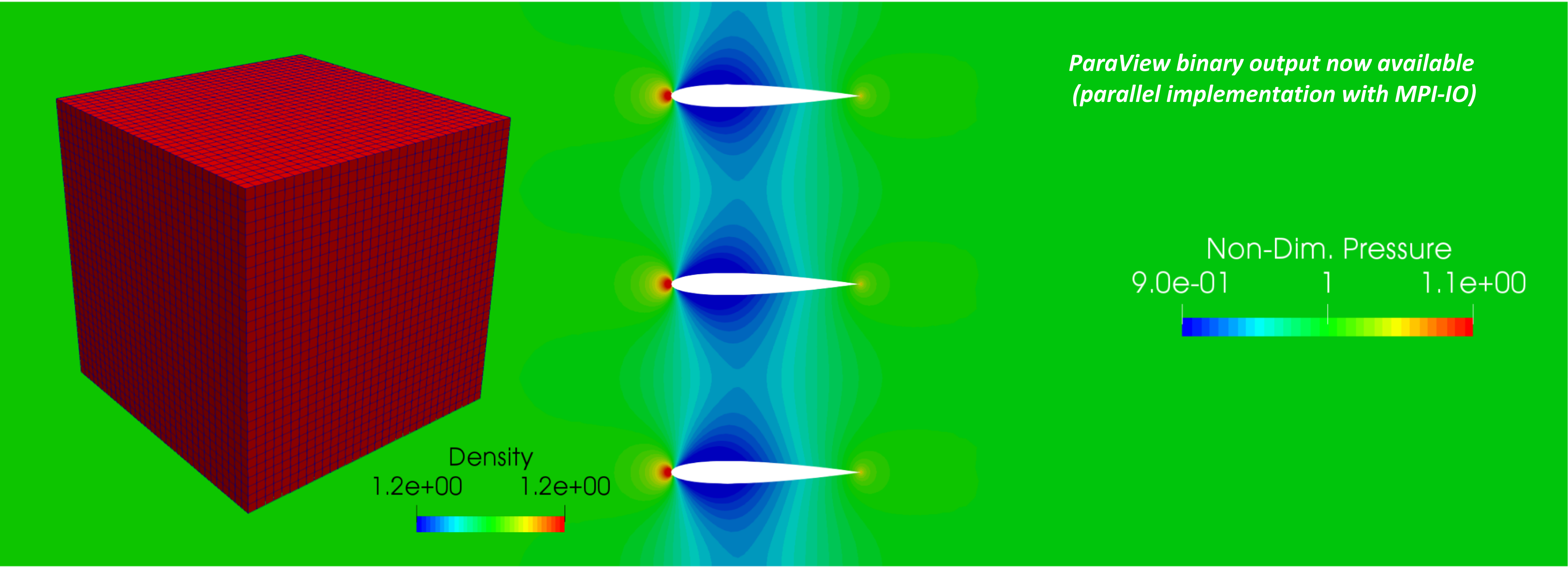
One more thing…
Periodic Boundary Condition



ParaView binary output now available (parallel implementation with MPI-IO)

adjacent periodic surfaces now possible, e.g., triply periodic cube

Conclusions
Key Messages from Today

- Showed a density-based preconditioning approach for a range of incompressible flows.
  - Seen as either a generalization of Artificial Compressibility or simplification of Weiss & Smith [1995].
  - In author’s experience, preconditioning all eqns. is critical for robustness when adding energy eqn. or turbulence model.
- Showed V&V of method with classic and NASA turbulence modeling cases. Demonstrated shape design.
- V&V results are reproducible with open data, source code available to public, tutorials covering usage online.
- Meant as a reference for the SU2 community to build on for incompressible flows.