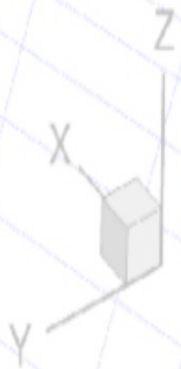# Grand CFD Portfolio Roadmap

Numerical Methods, High Performance Computing (HPC), and Research
Grade Solvers

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Purpose and Research Intent

This portfolio is explicitly designed to demonstrate research level numerical analysis skills, solver development maturity, and high performance computing awareness suitable for advanced graduate study and PhD level research applications. The emphasis is placed on mathematical rigor, algorithmic clarity, scalability, reproducibility, and critical evaluation of numerical methods beyond classroom style implementations.

Each project highlights the ability to independently design, verify, and extend CFD solvers while bridging theory and implementation. The portfolio serves as a structured demonstration of research readiness, self directed learning capability, and long term solver development vision across multiple PDE classes.

This portfolio is additionally oriented toward aerospace-relevant CFD, with validation anchored in canonical aerodynamic and propulsion benchmarks. Emphasis is placed on nondimensional reasoning and flow-regime awareness, including Reynolds and Mach number effects, so that solver behavior is interpreted physically rather than visually. Results are verified through grid refinement, conservation checks, and comparison to published reference solutions. The end goal is to demonstrate solver development skills directly applicable to aerodynamics, propulsion, and aero-thermal engineering workflows.

1. Parabolic Problems: Heat and Diffusion Equations

Summary

$$\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

This project focuses on solving parabolic partial differential equations, specifically transient heat conduction and diffusion problems. The objective is not only to obtain correct temperature fields, but to deeply understand time integration behavior, stability limits, error propagation, convergence trends, and solver performance as dimensionality increases.

The work begins with 1D transient diffusion validated against analytical solutions, advances to 2D heat conduction using Alternating Direction Implicit methods, and prepares the foundation for future 3D extensions. Emphasis is placed on solver structure, boundary condition enforcement, clean modular design, and professional quality visualization.

Key Numerical Methods and Concepts

- Governing equation formulation and nondimensionalization
- Explicit FTCS scheme with Fourier number stability constraints
- Fully implicit FTCS and Crank Nicolson time integration
- ADI splitting for efficient 2D implicit solves
- Thomas algorithm for tridiagonal systems
- Stability analysis and timestep sensitivity studies
- Error norms including L_2 and L_∞
- Grid refinement and convergence verification
- Identical solvers implemented in C++, Python, and Fortran
- Modular and single file reference implementations

Real World Applications

Heat transfer in solid components and layered materials, electronics thermal management and chip cooling, transient thermal stresses in aerospace structures, battery thermal runaway modeling, soil and ground heat diffusion, geothermal energy systems, material diffusion and phase change problems, pollutant diffusion in porous media, biological diffusion processes such as drug transport, and numerical foundations for multiphysics solvers involving thermal coupling.

In aerospace applications, these methods underpin transient thermal analysis of turbine blades, combustor liners, avionics enclosures, satellite thermal control panels, re-entry heat diffusion in solid structures, and coupled aero-thermal simulations where fluid solvers exchange heat fluxes with solid domains.

2. Elliptic Problems: Steady State Diffusion and Poisson Equations

Summary

$$\nabla^2 u = f(x, y)$$

Elliptic PDEs represent steady state equilibrium phenomena and form the mathematical backbone of many CFD algorithms, particularly pressure correction and incompressibility enforcement. This project develops solvers for Laplace and Poisson equations and emphasizes efficient solution of large sparse systems.

These solvers establish the foundation required for pressure velocity coupling in incompressible Navier Stokes solvers and expose the mathematical role of elliptic operators.

Elliptic solvers enforce physical constraints rather than directly advancing flow fields. The Poisson equation arises naturally in pressure correction methods used for incompressible aerodynamics and internal flows. Accurate elliptic solvers are therefore critical for mass conservation, numerical stability, and scalability in aerospace CFD workflows.

Key Numerical Methods and Concepts

- Laplace and Poisson equation formulation

- Finite difference and finite volume discretization

- Jacobi, Gauss Seidel, and Successive Over Relaxation methods

- Conjugate Gradient solvers for symmetric systems

- Residual monitoring and convergence diagnostics

- Grid dependence and solver efficiency comparisons

- Role of elliptic solvers in pressure correction and incompressibility enforcement for aerodynamic flows

Real World Applications

Electrostatics and electric potential fields, steady state heat conduction, pressure correction and incompressibility enforcement in CFD solvers, groundwater flow and seepage modeling, gravitational potential calculations, structural equilibrium and membrane deformation problems, image processing and smoothing operations, steady diffusion in porous media, and core linear system solvers underlying projection based Navier Stokes methods.

3. Hyperbolic Problems: Linear and Nonlinear Wave Systems

Summary

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

Hyperbolic PDEs model wave propagation, advection, and transport dominated phenomena. This project focuses on stability constraints, numerical dissipation, dispersion, and shock handling behavior in time dependent problems.

Both linear and nonlinear wave equations are solved using upwind and flux based schemes, with emphasis on CFL constraints and conservative formulations.

In aerospace applications, hyperbolic systems govern the propagation of pressure waves, acoustic disturbances, shocks, and convective transport of flow quantities. Numerical treatment of these equations directly impacts stability, accuracy, and physical fidelity in aerodynamic simulations. This section emphasizes the relationship between numerical schemes and information propagation, highlighting how discretization choices influence wave speed resolution, numerical dissipation, and shock sharpness.

Key Numerical Methods and Concepts

- Linear advection and wave equations
- Upwind, Lax Friedrichs, and Lax Wendroff schemes
- TVD schemes with flux limiters
- CFL stability analysis
- Characteristics, wave propagation direction, and information transport in hyperbolic systems
- Artificial viscosity and numerical dissipation
- Shock capturing behavior

Real World Applications

Compressible fluid dynamics, acoustic wave propagation, shock wave modeling, traffic flow and crowd dynamics, atmospheric transport and pollutant advection, tsunami and shallow water wave modeling, gas dynamics and aeroacoustics, electromagnetic wave propagation, signal transmission systems, and numerical foundations for conservation law based CFD solvers.

In aerospace engineering, these methods are fundamental to compressible aerodynamics, aeroacoustics, shock wave prediction, gust response analysis, transonic and supersonic flow modeling, and the numerical treatment of convective transport in both inviscid and viscous flow solvers.

4. Incompressible Navier Stokes: Lid Driven Cavity

Summary

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}$$

This flagship project solves the incompressible Navier Stokes equations using the classical lid driven cavity benchmark. Pressure velocity coupling is handled via projection methods such as SIMPLE and PISO style algorithms.

This solver integrates all prior project components and serves as a capstone demonstration of numerical stability, solver maturity, and code architecture quality.

The lid-driven cavity is treated as a canonical benchmark for assessing pressure–velocity coupling, discretization consistency, and stability in incompressible solvers. Emphasis is placed on algorithmic structure, error control, and convergence behavior rather than flow visualization.

Key Numerical Methods and Concepts

- Incompressible Navier Stokes equations

- Fractional step and projection methods

- Pressure Poisson equation solution

- Coupling between elliptic pressure correction and velocity transport operators

- Velocity divergence control

- Grid convergence and benchmark validation

- Residual monitoring and timestep sensitivity

Real World Applications

Internal and external viscous flows, ventilation and indoor airflow modeling, mixing and recirculation flows, lubrication and low Reynolds number flows, biomedical flows such as blood transport in vessels, microfluidic devices, urban wind flow modeling, industrial process flows, benchmark validation for CFD solvers, and research grade incompressible flow algorithm development.

In aerospace and fluid dynamics research, incompressible solvers form the foundation for low-Mach-number flow modeling, algorithm verification, and numerical method development prior to extension to compressible and high-speed regimes.

5. Compressible Flow and Shock Capturing: Euler and Navier Stokes

Summary

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} + \frac{\partial \mathbf{G}(\mathbf{U})}{\partial y} = 0$$

This project targets compressible gas dynamics where shocks and discontinuities appear naturally. The goal is to demonstrate system level conservation laws, characteristic behavior, and robust numerical flux design. Compared to the wave project, this section is explicitly conservative, nonlinear, and designed to handle discontinuities without producing nonphysical oscillations.

Unlike incompressible flow, compressible systems introduce strong nonlinear coupling between mass, momentum, and energy conservation, leading to shock waves, contact discontinuities, and expansion fans. This section treats compressible flow primarily as a numerical challenge, emphasizing conservative formulations, characteristic behavior, and stability under discontinuous solutions rather than smooth-flow accuracy alone.

Key Numerical Methods and Concepts

- Conservative finite volume formulation for Euler and compressible Navier Stokes

- Hyperbolic system eigenstructure and characteristic wave propagation

- Numerical entropy behavior and physically admissible weak solutions

- Riemann problem intuition, wave speeds, and characteristic based thinking

- Shock capturing fluxes such as Rusanov, HLL, HLLC, Roe style

- Higher order reconstruction with limiters such as MUSCL, TVD, WENO

- CFL constraints for compressible systems and stiffness at high Mach

- Verification problems such as Sod tube, Lax problem, Shu Osher, shock vortex interaction

- Diagnostics such as total variation, entropy considerations, conservation error checks

Real World Applications

Supersonic aerodynamics, nozzle and jet flows, shock boundary layer interaction, blast wave modeling, re entry heating coupled with compressible flow, and general high speed aerospace.
Compressible flow solvers are central to aerospace engineering, governing the simulation of high-speed aerodynamic flows, propulsion systems, and shock-dominated environments.

6. Parallelization and Optimization: High-Performance CFD Execution

Summary

This project focuses on scaling CFD solvers beyond single-core execution and into high-performance computing environments. The objective is to demonstrate an understanding of parallel programming models, memory behavior, and performance bottlenecks in scientific computing, rather than simply achieving raw speedup.
Parallelization is treated as a numerical and algorithmic problem, not only a software task.

Key Numerical Methods and Concepts

- Domain decomposition strategies for structured grids

- Strong scaling versus weak scaling behavior

- MPI-based parallelization of finite-difference and finite-volume solvers

- Halo exchange and communication patterns

- OpenMP shared-memory parallelism

- Hybrid MPI + OpenMP execution models

- Cache efficiency and memory access patterns

- Profiling and performance analysis

Implementation Scope

Parallelization is applied incrementally to existing solvers developed in earlier sections, including:

- Parabolic heat equation solvers

- Elliptic Poisson solvers

- Hyperbolic wave solvers

- Incompressible Navier Stokes solvers

- Compressible shock capturing schemes

Each solver is analyzed in serial and parallel to quantify:

- Speedup and efficiency

- Communication overhead

- Scalability limits

Real World Applications

Large-scale CFD simulations in aerospace and energy systems, weather and climate modeling, urban airflow analysis, industrial process simulation, and national supercomputing workloads where solver scalability and efficiency determine feasibility.

7. OpenFOAM and ANSYS Fluent: Industrial CFD Workflows and Validation

Summary

This section focuses on the structured use of established industrial CFD software, specifically Open-FOAM and ANSYS Fluent, to complement first-principles solver development. The objective is not tool proficiency alone, but a deep understanding of how industrial solvers implement numerical methods, turbulence modeling, and pressure velocity coupling, and how these choices relate to underlying mathematical formulations.

Emphasis is placed on verification, validation, solver behavior, mesh sensitivity, and the interpretation of results within the limitations imposed by modeling assumptions. These studies bridge academic solver development with real-world engineering workflows.

Aerospace-Oriented Validation and Case Selection

Industrial CFD solvers are widely used in aerospace applications not because they are universally accurate, but because they balance robustness, scalability, and engineering practicality. In this section, OpenFOAM and ANSYS Fluent are applied to canonical aerospace-relevant flow problems chosen specifically to expose solver behavior rather than to produce visually appealing results.

Representative validation cases include:

- External aerodynamic flows over bluff and streamlined bodies

- Internal duct and channel flows representative of cooling passages

- Transitional and turbulent boundary layer development

- Pressure-driven incompressible flows relevant to low-speed aerodynamics

Key Numerical Methods and Concepts

- Finite volume discretization on unstructured meshes

- Pressure velocity coupling algorithms:

    - SIMPLE, SIMPLEC, PISO, and coupled solvers

- Turbulence modeling assumptions:

    - RANS closures (e.g. k–ε, k–ω, SST)

    - Near-wall treatment and wall functions

- Steady versus transient formulation trade-offs

- Linear solver choices and preconditioning strategies

- Mesh quality metrics and sensitivity analysis

- Boundary condition modeling and physical consistency

- Residual monitoring versus physical convergence

- Verification against analytical solutions and benchmarks

Comparative Insight with In-House Solvers

Results from OpenFOAM and ANSYS Fluent are systematically compared against in-house finite-difference and finite-volume solvers developed in earlier sections of this portfolio. This comparison highlights:

- The role of elliptic pressure Poisson solvers in industrial codes

- Differences between segregated and coupled solution strategies

- Numerical dissipation introduced by turbulence closures

- Sensitivity to timestep and relaxation parameters

- Trade-offs between robustness and physical fidelity

These comparisons reinforce a solver-agnostic understanding of CFD rather than reliance on any single software platform.

Understanding Limitations of Industrial CFD Solvers

A key outcome of this section is recognizing where industrial CFD solvers introduce numerical or modeling compromises. While tools such as OpenFOAM and ANSYS Fluent provide robust frameworks, their accuracy is strongly influenced by turbulence closures, mesh quality, and user-selected numerical parameters.

Key limitations examined include:

- Numerical dissipation introduced by upwind-biased fluxes

- Sensitivity of results to turbulence model selection

- Dependence on under-relaxation and solver tuning for convergence

- Mesh-induced anisotropy and near-wall resolution constraints

Real World Applications

External and internal aerodynamics, HVAC and ventilation systems, urban wind flow modeling, turbomachinery and nozzle flows, vehicle aerodynamics, industrial mixing processes, environmental flow analysis, and validation studies for engineering design workflows in aerospace, energy, and built-environment applications.

For aerospace applications, these studies reinforce that industrial CFD tools must be used with a clear understanding of numerical methods and modeling assumptions. Solver outputs are interpreted as engineering models rather than exact solutions, and assessed through verification and sensitivity studies rather than visual inspection alone.

8. AI-Enhanced CFD: Hybrid Physics-Based and Data-Driven Methods

Summary

This section investigates the integration of machine learning techniques with classical computational fluid dynamics solvers to enhance modeling capability, reduce computational cost, and improve scalability.

The emphasis is placed on hybrid approaches where data-driven models augment physics-based solvers rather than replace them.

Machine learning is treated as a numerical tool that interacts with governing equations, discretization schemes, and solver structure. The objective is to demonstrate a principled understanding of where data-driven methods are beneficial, where they fail, and how they can be rigorously evaluated against traditional CFD techniques.

Key Numerical Methods and Concepts

- Supervised learning for regression of solution fields
- Neural networks as nonlinear function approximators
- Loss functions and optimization in the context of PDE solutions
- Physics-informed learning using PDE residual constraints
- Data-driven surrogate modeling for time-dependent PDEs
- Reduced-order modeling combined with machine learning
- Solver acceleration and parameter prediction using ML
- Stability, generalization, and error analysis for learned models

Implementation Scope

Machine learning models are applied alongside existing CFD solvers developed in earlier sections of the portfolio. The implementation includes:

- Training surrogate models for the 1D and 2D heat equations
- Comparison of ML surrogates against finite-difference solutions
- Physics informed neural networks for enforcing governing equations
- Reduced-order modeling using Proper Orthogonal Decomposition with learned temporal evolution
- Machine learning assistance for elliptic and Poisson solvers, including iteration count prediction and relaxation parameter selection

All machine learning models are validated using quantitative error norms, convergence behavior, and computational cost comparisons against baseline numerical solvers.

Real World Applications

Accelerated CFD simulations for parameter studies and optimization, reduced-order models for real-time prediction and control, data-assisted solvers for large-scale engineering simulations, hybrid physics-data models in aerospace and energy systems, and research-oriented exploration of machine learning techniques for scientific computing and numerical PDEs.

9. Website and PDF Curation: Reproducible Research Presentation

Summary

This section focuses on transforming the technical work of the portfolio into a clear, reproducible, and professionally presented research artifact. The goal is not visual design, but scientific communication, traceability, and long-term maintainability.

The portfolio is structured to allow reviewers to understand methodology, reproduce results, and inspect solver implementations without ambiguity.

Key Concepts and Practices

- Reproducible computational research principles
- Clear separation between theory, implementation, and results
- Consistent documentation of assumptions and limitations
- Version-controlled development workflow

Implementation Scope

- Public Git repositories for each solver family
- Structured directory layout for code, data, and figures
- Automated figure generation where applicable
- PDF portfolio compiled from LaTeX sources
- Portfolio website hosted via GitHub Pages

Each project section includes:

- Governing equations and numerical methods
- Validation and verification results
- Performance and convergence studies
- Clear discussion of numerical behavior

Real World Applications

Academic research portfolios, PhD applications, technical interviews, research grant proposals, and long-term solver development projects where clarity, reproducibility, and documentation quality are as critical as numerical correctness.

High Level Timeline Overview

The timeline milestones below are approximate and may change depending on consistent effort and actual time investment during execution.

Phase	Project	Method	Days
CORE	Parabolic Solvers	1D 2D Finite Difference	15
	Elliptic Solvers	Poisson Laplace	15
	Hyperbolic Solvers	Upwind TVD	15
INTERMEDIATE	Navier Stokes Solver	2D 3D Projection	15
	Compressible Flow	Shock Capturing	30
	Parallelization	MPI OpenMP	30
ADVANCED	OpenFOAM and ANSYS Fluent	Industrial CFD Workflows	15
	AI Enhanced CFD	PINNs ROM Surrogates	70
	Website and PDF Curation	GitHub Pages LaTeX	10
Total			**215**