// blastFEM: a GPU-accelerated, very high-performance and energy-efficient solver for highly compressible flows

Synthetik applied technologies

// MFEM COMMUNITY WORKSHOP
October 25, 2022

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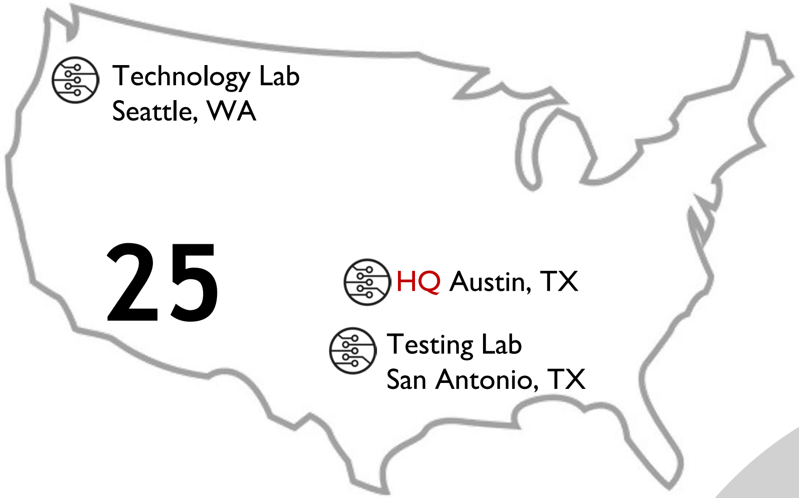
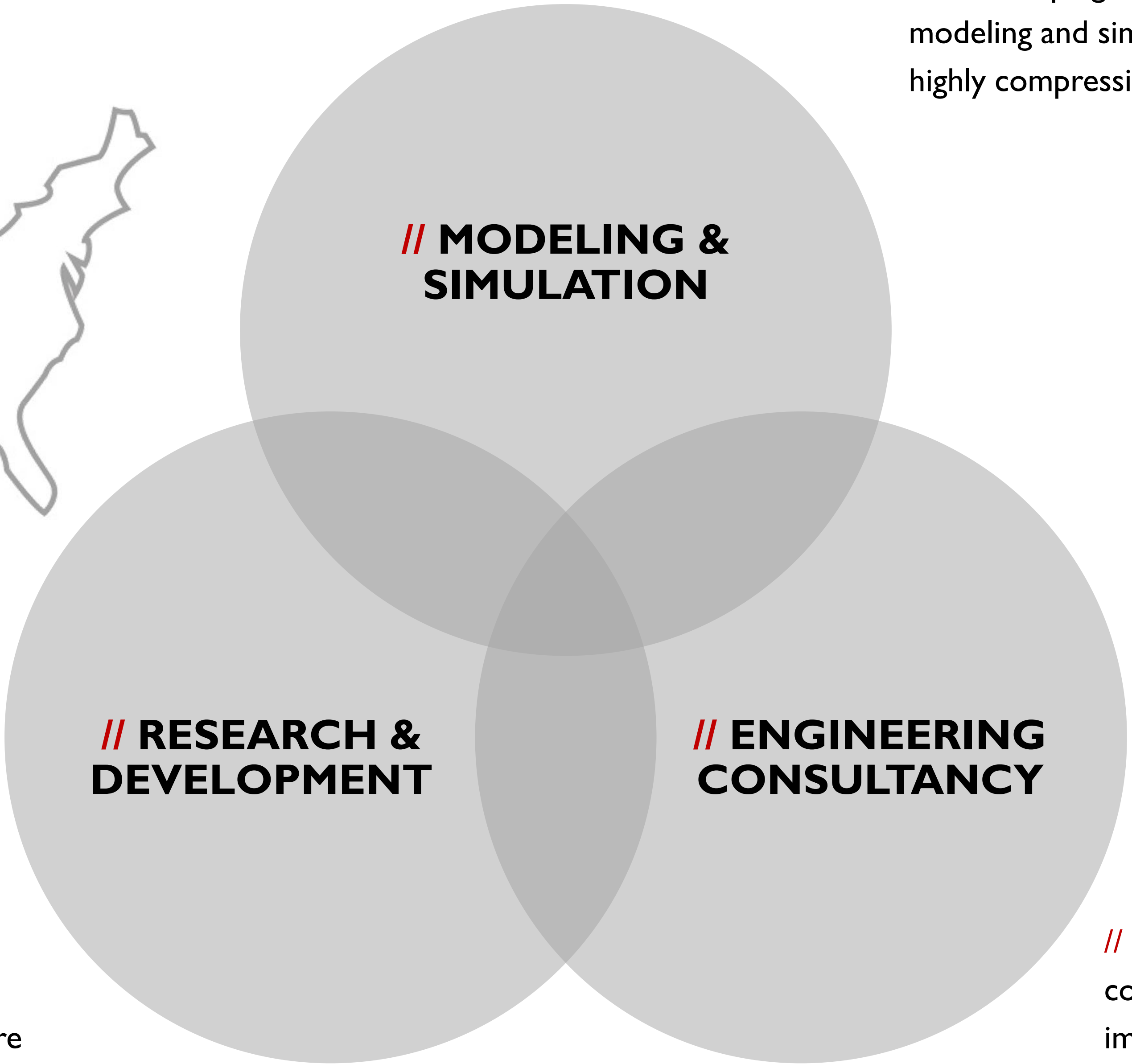


// Developing world-class first-principles-based modeling and simulation (M&S) codes with a focus on highly compressible reactive flows.



// Uniquely skilled and experienced in the conduct of R&D programs across multiple diverse technology areas. We are currently working with several US government agencies and commercial clients.

// Synthetik provides engineering consultancy services related to shock and impact - working with commercial and federal clients on global landmark infrastructure projects.

// Synthetik Modeling & Simulation Team

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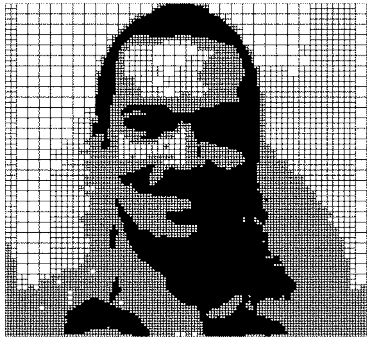

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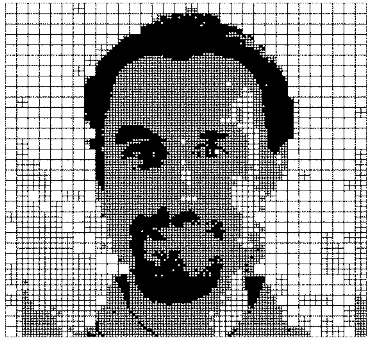
Principal Investigator

PhD, Mechanical Engineering, Iowa State University, Ames, IA



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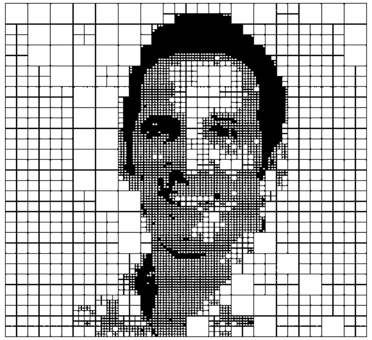
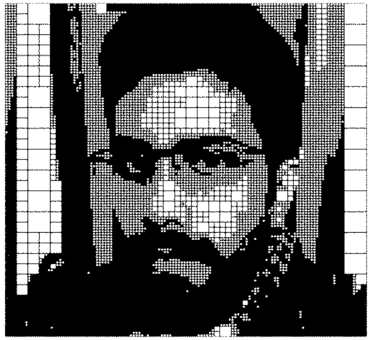
PhD, Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign, Urbana, IL



Tim Brewer
Project Manager

Professionally Licensed Engineer and Practitioner



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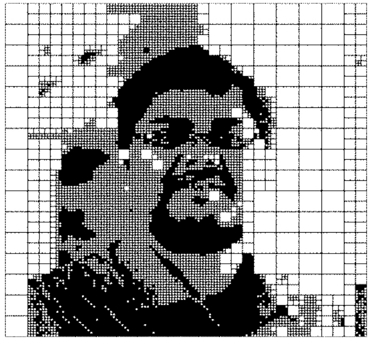

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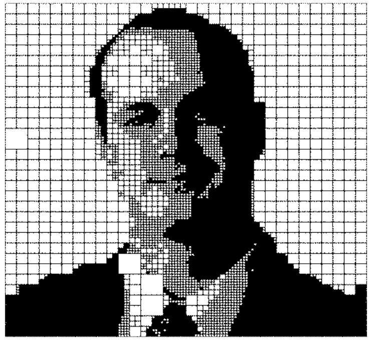

Peter Vonk
SME

Developer of CFD codes and CAD-integrated tools for simulation driven design

DEVELOPMENT HISTORY

/ / Where have we been, and where are we going?

- **blastFoam** first presented at OpenFOAM Users Conference in Germany and USA, 2016/17.
- **blastFoam v2** first public release of blastFoam as an opensource project.
- **blastFoam v6** Addition of support for mesh motion, fluid structure interaction, a comprehensive AMR library, and coupling to external solid dynamics solvers using preCICE.
- **blastCFD** a GPU-accelerated and optimized commercial code for modeling highly compressible reactive flows.
- **blastFEM** DOE Phase I SBIR to integrate blastFoam and the ASCR-funded MFEM libraries to deliver blastFEM:
  - Higher order FEM-DG solutions
  - GPU support
  - Scalability

blastFoam (10/16)

blastFoam v2 (5/19)

blastFoam v6 (7/22)

blastCFD (8/22)

blastFEM (10/22)

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BRIEFING FORMAT

// A high-performance and energy-efficient solver for highly compressible flows

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Part I: Solver Development

1. Starting with MFEM
2. Addition of a two-phase system of equations
3. Relevant equations-of-state (EOS)
4. Integration of MFEM adaptive mesh refinement (AMR)
5. Leveraging MFEM load balancing
6. Load balancing
7. Improved time stepping
8. Development of limiters
9. Leveraging artificial viscosity
10. Generalize case creation for arbitrary geometries
11. Artificial Viscosity
12. Preprocessing utilities

Part II: Initial Phase I Results

1. Single Phase
2. Validations
3. Two-Phase

STARTING WITH MFEM

/ / A high-performance and energy-efficient solver for highly compressible flows

- MFEM Example 18 used as the reference implementation
- Uses a compressible Euler system of equations
- Transient non-linear hyperbolic PDE
- Discontinuous Galerkin (DG) formulation
- System of equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = 0$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho \boldsymbol{u} \\ \rho E \end{pmatrix}$$

$$\mathbf{F} = \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbf{I} \\ (\rho E + p)\boldsymbol{u} \end{pmatrix}$$

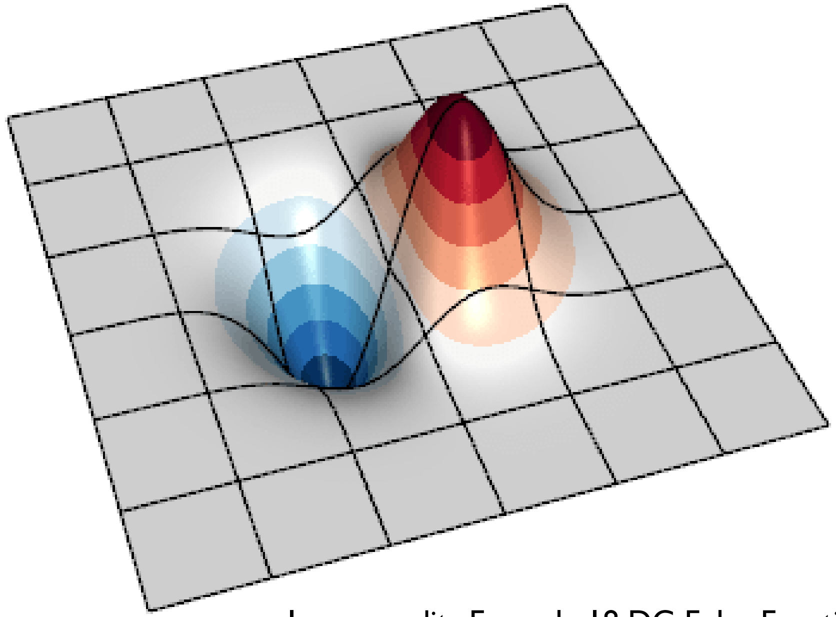

Image credit : Example 18 DG Euler Equations
https://mfem.org/examples/

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// ADDITION OF A TWO-PHASE SYSTEM OF EQUATIONS

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Volume fraction, α, phase tracking function

The alpha equation can be written as the material derivative:

$$\frac{\partial \alpha}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha = 0$$

This is implemented into blastFEM using MFEM's ConvectionIntegrator and NonconservatriveDGTraceIntegrator.

The total density ρ,

$$\rho = \alpha \rho_1 + (1-\alpha)\rho_2$$

For the two-phase Euler compressible the momentum and energy source terms are 0.

Pressure solved through the equation of state

System of equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S} \qquad \mathbf{U} = \begin{pmatrix} \alpha \\ \alpha\rho_1 \\ (1-\alpha)\rho_2 \\ \rho\boldsymbol{u} \\ \rho E \end{pmatrix}$$

$$\mathbf{F} = \begin{pmatrix} \alpha\boldsymbol{u} \\ \alpha\rho_1\boldsymbol{u} \\ (1-\alpha)\rho_2\boldsymbol{u} \\ \rho\boldsymbol{u} \otimes \boldsymbol{u} + p\mathbf{I} \\ (\rho E + p)\boldsymbol{u} \end{pmatrix} \qquad \mathbf{S} = \begin{pmatrix} \alpha\nabla\cdot\boldsymbol{u} \\ 0 \\ 0 \\ \dot{\mathrm{M}} \\ \dot{\mathrm{E}} \end{pmatrix}$$

Zheng HW, Shu C, Chew YT, Qin N. A solution adaptive simulation of compressible multi-fluid flows with general equation of state. *International Journal for Numerical Methods in Fluids*. 2011;67(5):616-637. doi:10.1002/fld.2380

RELEVANT EQUATIONS-OF-STATE (EOS)

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The user can select from a collection of EOSs for each phase:

- Pressure is computed from the equation of state
- Currently implemented EOS:
  - Ideal gas $p = (\gamma - 1)\rho e$
  - Stiffened gas $p = (\gamma - 1)\rho e - \gamma a$
  - Van der Waals $p = \frac{\gamma-1}{1-b\rho}(\rho e + a\rho^2) - (a\rho^2 + c)$

Zheng HW, Shu C, Chew YT, Qin N. A solution adaptive simulation of compressible multi-fluid flows with general equation of state. *International Journal for Numerical Methods in Fluids*. 2011;67(5):616-637. doi:10.1002/fld.2380

// INTEGRATION OF MFEM ADAPTIVE MESH REFINEMENT (AMR)

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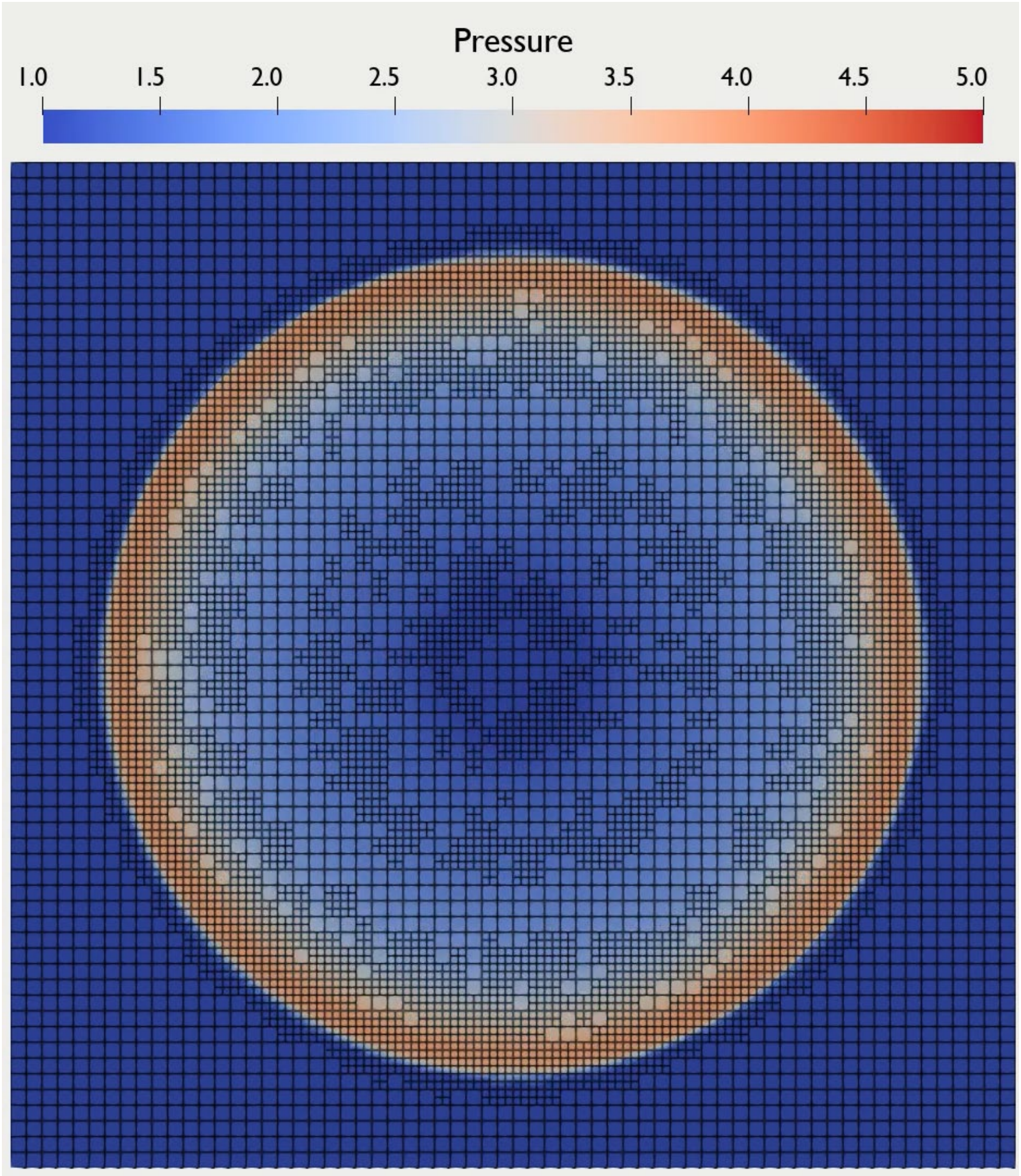
- Integrated MFEM's AMR capability into blastFEM
- Refinement and relaxation for moving shocks
- Error estimator based on gradient of field of interest: density or pressure
- Initial higher pressure concentrated at the center



// LEVERAGING MFEM LOAD BALANCING

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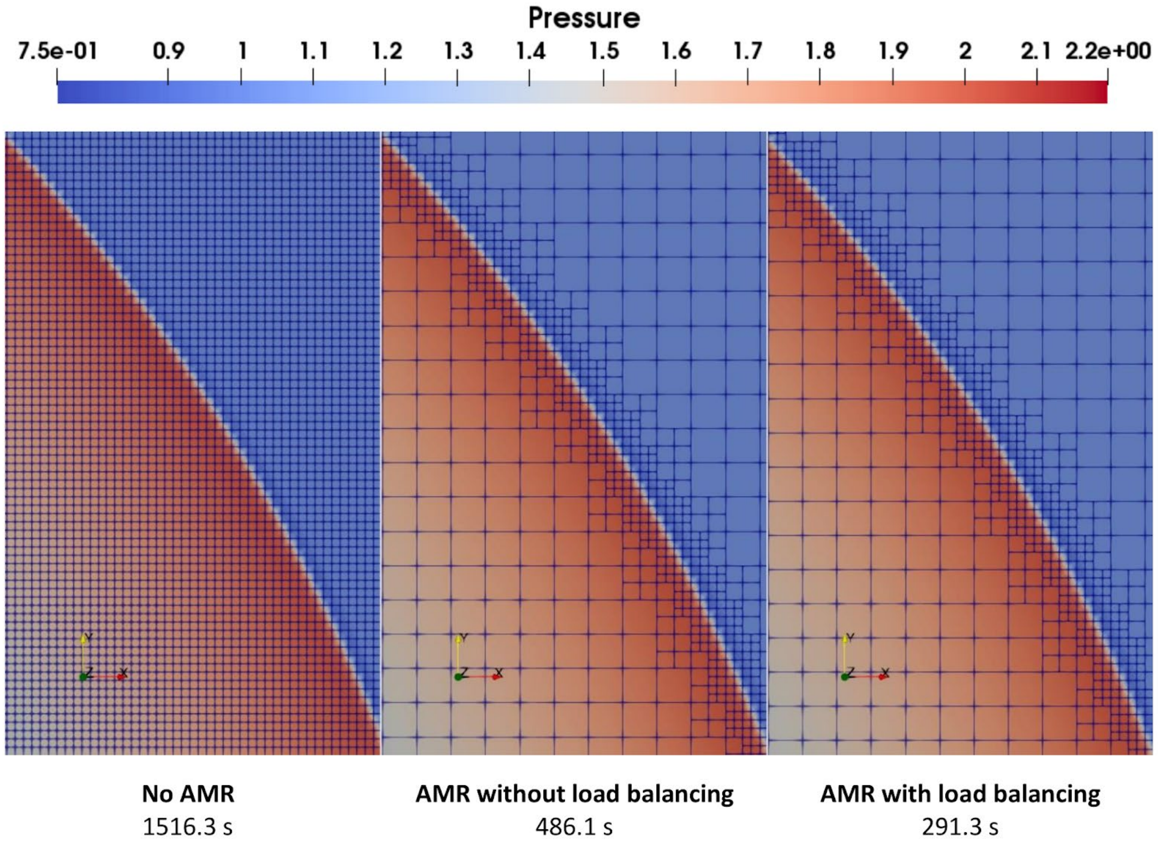
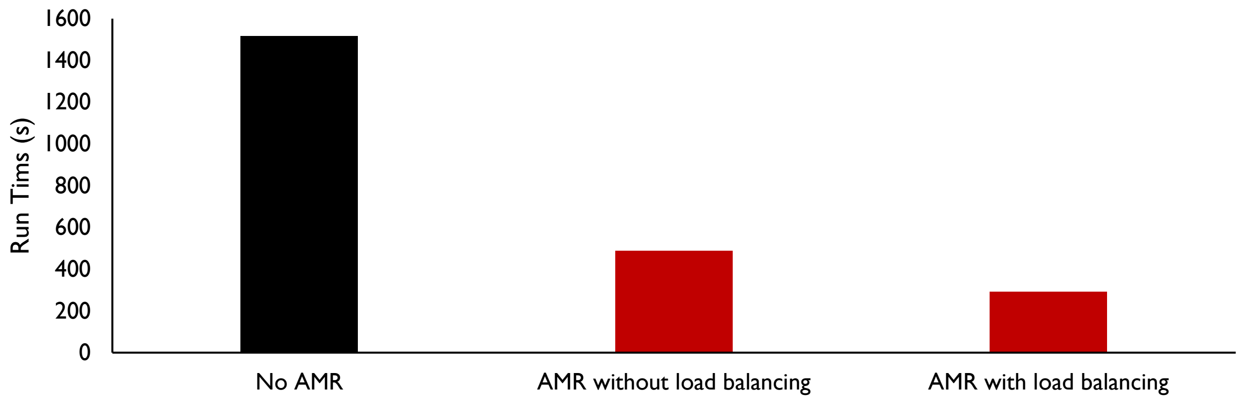
- Uses the load balancing available in MFEM for non-conforming meshes
- Computational execution time comparison:
  1. No AMR with max refinement everywhere
  2. AMR without load balancing
  3. AMR with load balancing
- Max refinement used to resolve the shock front
- Simulation end time: 0.5s
- Parallel simulation on 12 CPUs
- First order basis functions





IMPROVED TIME STEPPING

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Previous implementation based on Cockburn and Shu

Computed from the ratio of smallest element size, h to largest velocity magnitude, u in the entire domain:

$$\Delta t = CFL \times \frac{\min(h)}{\max(u)} \frac{1}{2k+1}$$

New implementation computes the ratio of element size and velocity for each element and the time step is computed as:

$$\Delta t = CFL \times \min\left(\frac{h_e}{u_e}\right) \frac{1}{2k+1}$$

Avoids over constraining the time step size.

Cockburn B, Shu CW. Runge–Kutta Discontinuous Galerkin Methods for Convection-Dominated Problems. *Journal of Scientific Computing*. 2001;16(3):173-261. doi:10.1023/A:1012873910884

DEVELOPMENT OF LIMITERS

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- Can lead to unphysical oscillations near regions of large gradients in hyperbolic problems
- Numerical instabilities
- Negative density and pressure
- Shock capturing limiters are used to mitigate this unphysical behavior
- Limiters based on Moe et al were implemented in blastFEM
- The extent of limiting can be set by the user.

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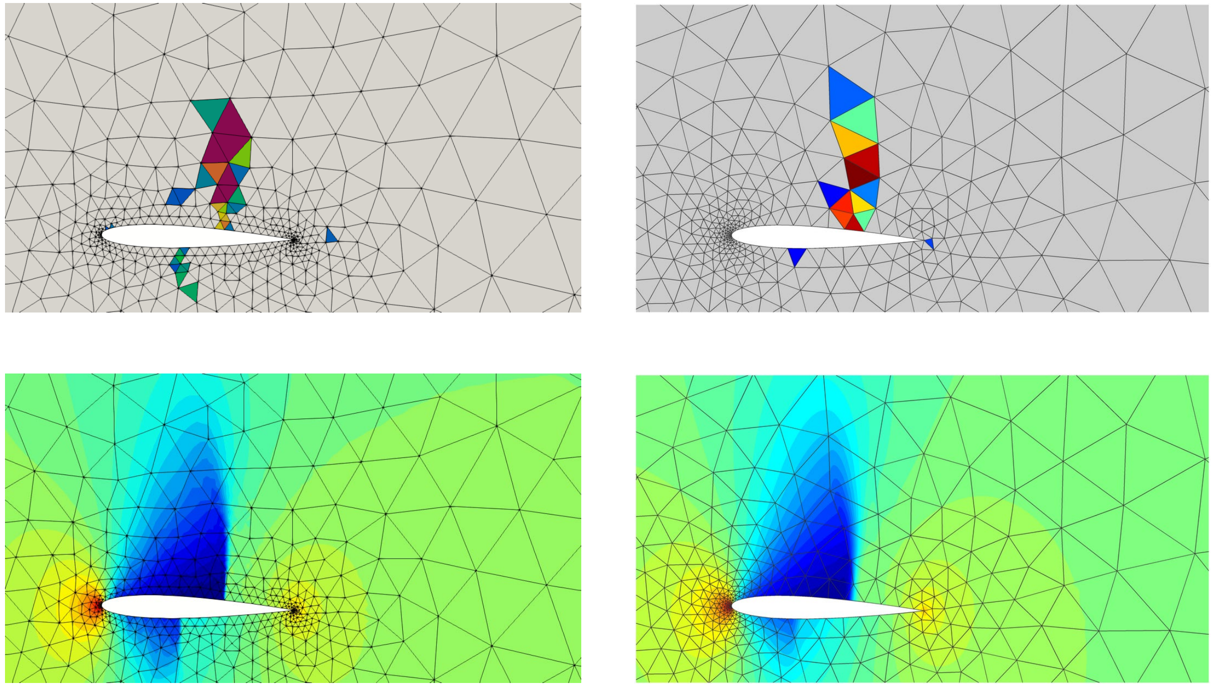
Moe SA, Rossmanith JA, Seal DC. A Simple and Effective High-Order Shock-Capturing Limiter for Discontinuous Galerkin Methods. Published online July 10, 2015. doi:10.48550/arXiv.1507.03024

// LEVERAGING ARTIFICIAL VISCOSITY

- Artificial diffusion can help improve the stability of the shock on the interior of higher order elements.
- Implemented a discontinuity sensor which projects the field to lower order (*p-1*) FE system, and measures the difference between the original and projected field
- The difference indicated the regions of strong gradients/ discontinuities.
- Based on the magnitude of the difference, diffusivity is added to the elements
- The threshold at which diffusion is added can be controlled with an additional free parameter κ
- NACA airfoil at Mach 0.8, 1.5 ° angle of attack
- Fourth order basis functions



Comparison between blastFEM (left) and literature (right) for the NACA0012 airfoil at Mach 0.8.

Top images show the presence of artificial diffusion, where gray elements contain no added diffusion. The bottom images show the corresponding pressure field.

Persson PO, Peraire J. Sub-Cell Shock Capturing for Discontinuous Galerkin Methods. In: *44th AIAA Aerospace Sciences Meeting and Exhibit.* Aerospace Sciences Meetings. American Institute of Aeronautics and Astronautics; 2006. doi:10.2514/6.2006-112

// GENERALIZED CASE CREATION FOR ARBITRARY GEOMETRIES

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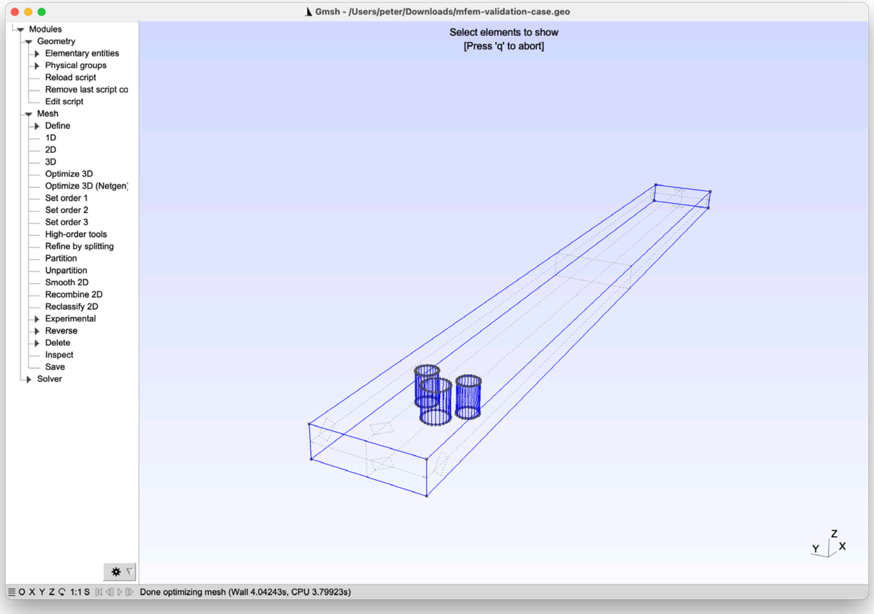
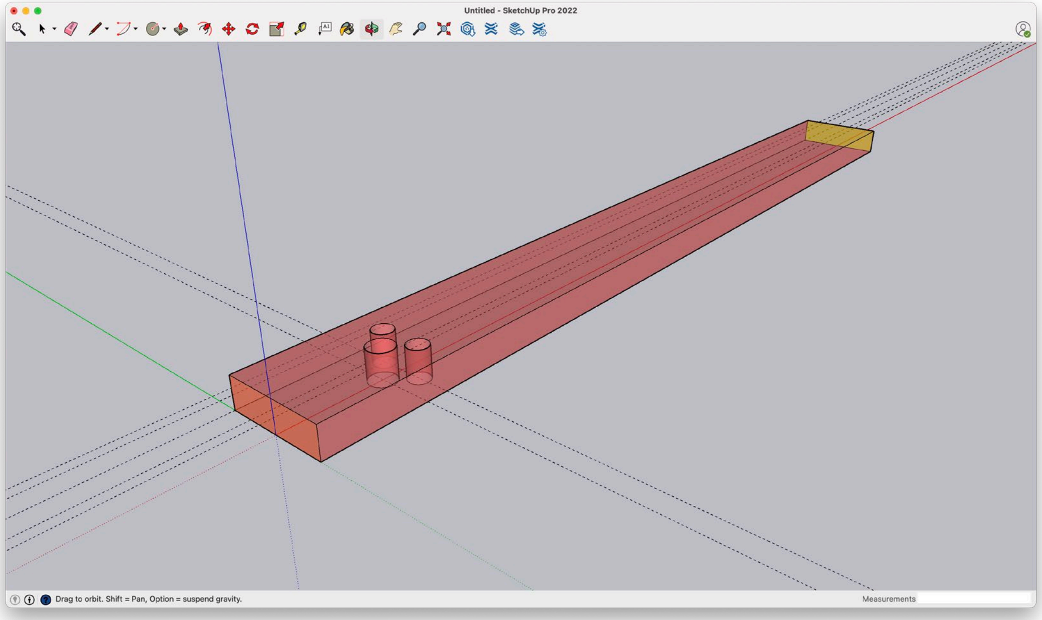
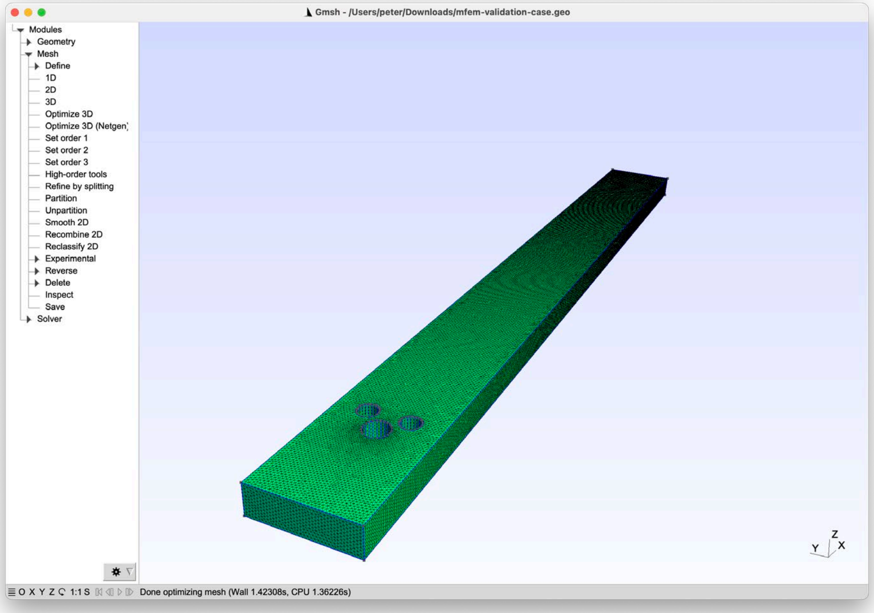
- CAD integration as a step towards using MFEM for general industry/industrial problems
- Verified our *Sketchup MeshKit* plugin for compatibility with Sketchup 2022 and the latest version of GMSH
- Set named boundaries and meshing options from within SketchUp
- Export .geo files and generate mesh with GMSH (GUI, CLI)
- Import case and run with MFEM







// PREPROCESSING UTILITIES

A configuration file is used to set parameters for running simulations:

- Time controls
- Mesh:
  - Mesh file read and boundary conditions prescribed
  - Quadrature rule
  - Refinement levels
  - AMR setting
- ODE solver options
- Flux schemes
- Limiter control
- Phases
- Thermos
- Initial conditions

```
// Time controls
controls {
    endTime 0.25;
    deltaT 1e-4;
    visualization paraview; // "visit", "glvis"
    writeInterval 0.01;
    maxCo 0.5;
}

// Mesh information
mesh {
    basisFunctionOrder 2;
    nRefine 4;
    meshFile "../data/inline-quad.mesh";

    boundary (bottom {
            type noPenetration;
        }

        top {
            type extrapolated;
        }

        left {
            type extrapolated;
        }

        right {
            type noPenetration;
        }

    );
    useAMR yes;

    AMR {
        ncLimit 1;
        estimator delta;
        fieldName p;
        unrefineLevel 0.1;
        refineLevel 0.1;
        maxLevel 5
    }
}
```

```
// Schemes
fluxScheme HLLC;
odeSolver RK2SSP;
alphaLimiter 0;
kappa 3;
caseType custom;

// Phases
phases (gas1 gas2);

gas1 {
    thermoType {
        equationOfState idealGas;
    }
    equationOfState {
        gamma 1.4;
    }
}
gas2 {
    thermoType {
        equationOfState stiffenedGas;
    }
    equationOfState {
        gamma 1.6;
        a 0.0;
    }
}

//Initial Conditions
defaultFieldValues (
    scalar alpha.gas1 1.0
    scalar rho.gas1 1.0
    scalar rho.gas2 2.0
    scalar p 1
    //vector U (0.0 0.0 0.0)
);
initialConditions (
    sphere
    {
        centre (0.5 0.5 0.5);
        radius 0.1;
        fieldValues
        (
        scalar alpha.gas1 0.0
        scalar rho.gas2 3.0
        scalar p 20.0);
    }
);
```

// RESULTS: SINGLE PHASE

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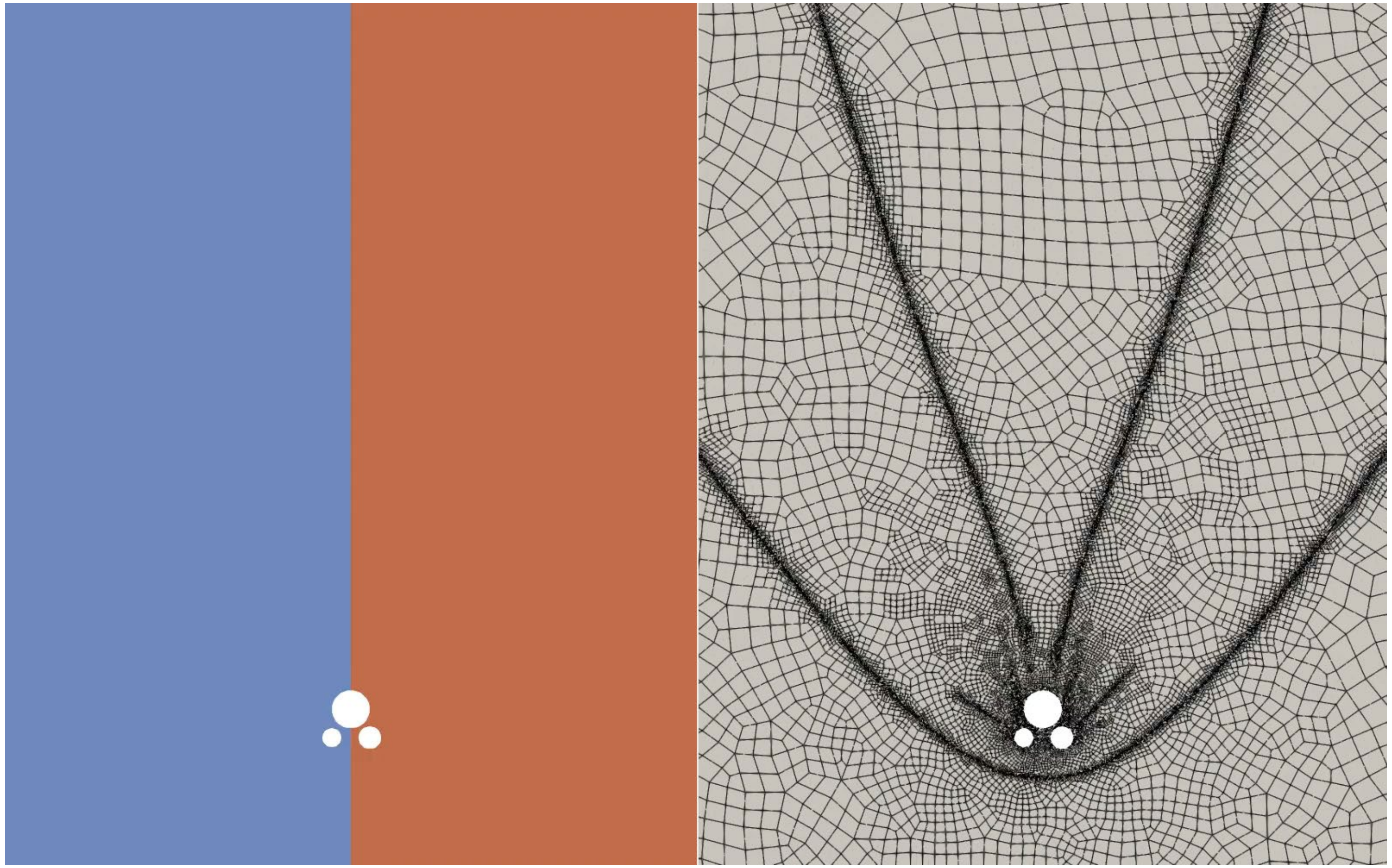
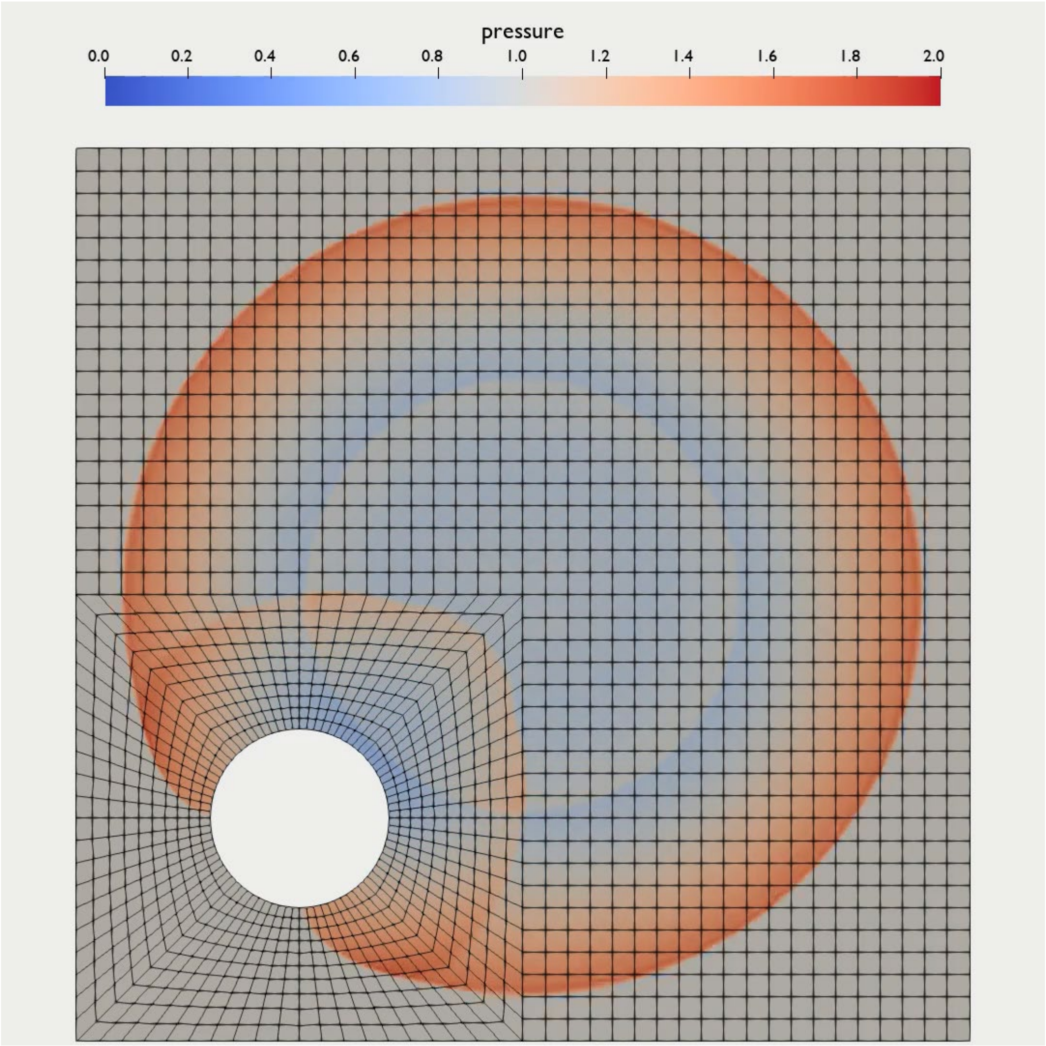


Pressure Velocity AMR

- External flow
- Second order basis functions
- AMR with load balancing



- Fourth order basis functions
- Shock resolution across coarse discretization

// RESULTS: SINGLE PHASE VALIDATION

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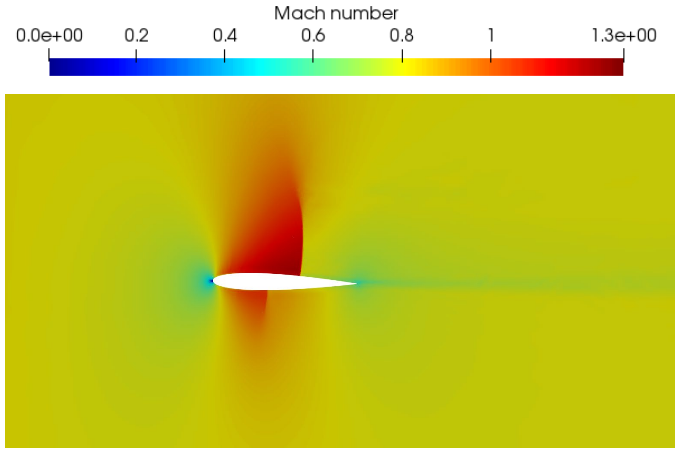
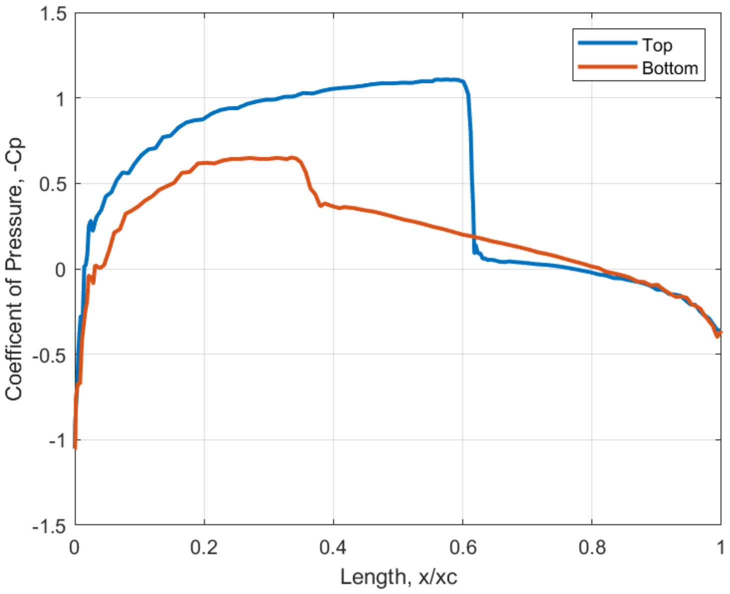
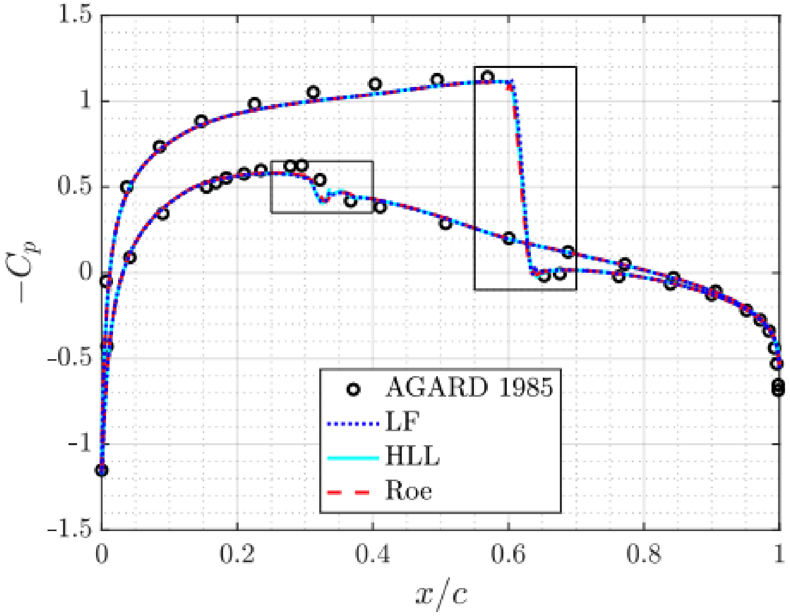
- NACA 0012 Airfoil geometry
- Transonic flow: Mach 0.8
- 1.25° Angle of Attack
- Comparison of the Coefficient of pressure across the surface of the airfoil





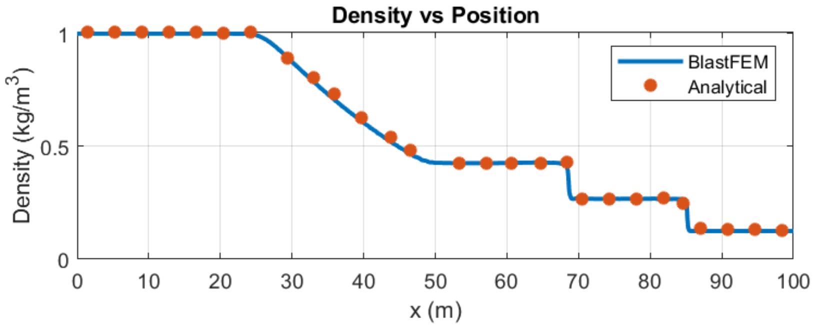
BlastFEM

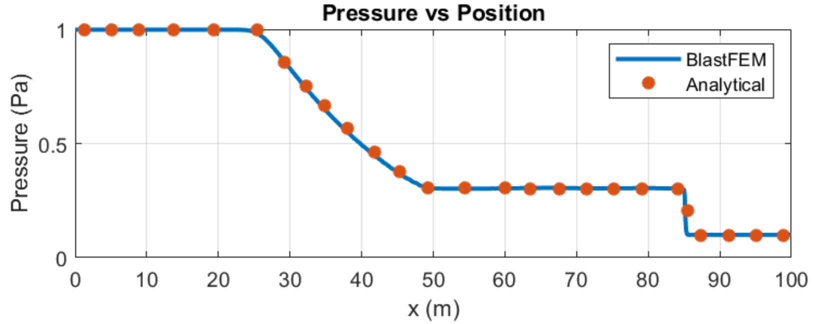


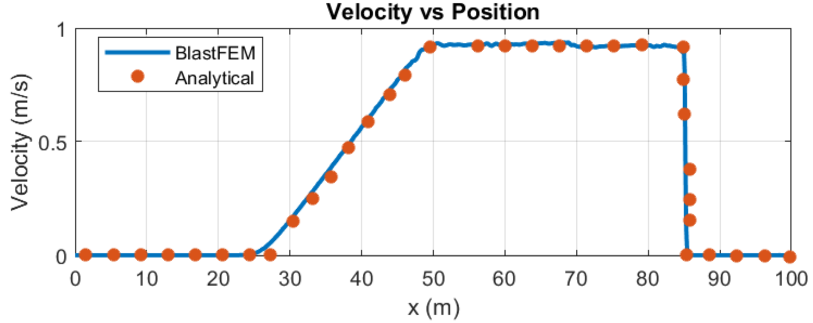
Literature

Vila-Pérez, Jordi & Giacomini, Matteo & Sevilla, Ruben & Huerta, Antonio. (2019). An HLL Riemann solver for the hybridised discontinuous Galerkin formulation of compressible flows. https://doi.org/10.48550/arXiv.1912.00044

- Sod Shock Tube: BlastFEM vs exact solution for density, pressure, and velocity.

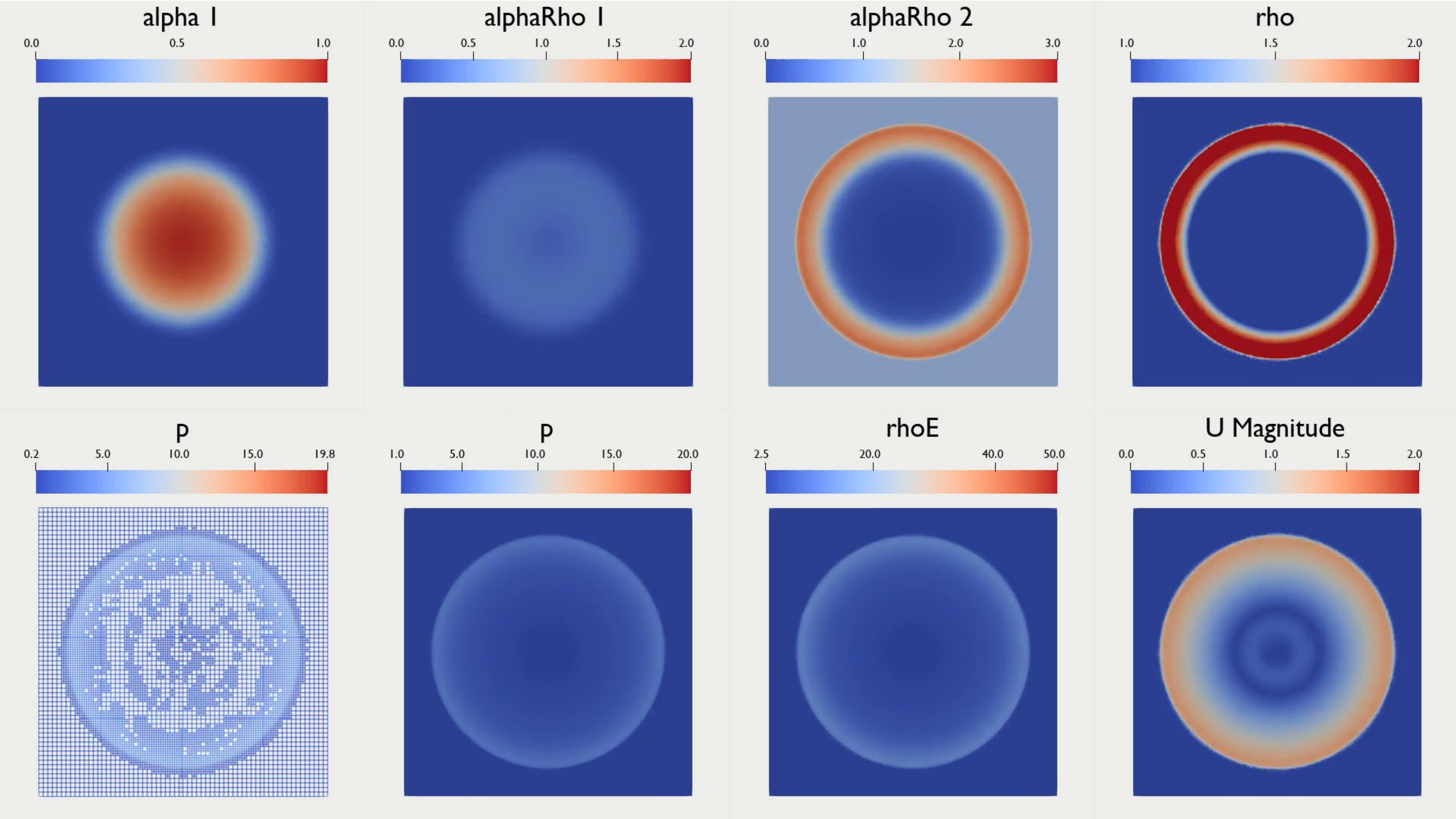






Sod, Gary A. "A Survey of Several Finite Difference Methods for Systems of Nonlinear Hyperbolic Conservation Laws." Journal of Computational Physics 27, no. 1 (April 1, 1978): 1–31. https://doi.org/10.1016/0021-9991(78)90023-2.

// RESULTS: TWO PHASE



- Both phases use ideal gas EOS
- AMR with load balancing
- Density ratio of 2:1
- Pressure ratio 20:1

QUESTIONS / DISCUSSION

/ / A high-performance and energy-efficient solver for highly compressible flows

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