Composable Multiphysics: From Solvers to Quantities of Interest

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University of Texas at Austin

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Composable

- Rarely know ideal linear solver for complex problem
- **MUST** experiment
- Want to be able to choose at runtime
- Extend idea beyond solver to multiphysics simulation as a whole:
  - Modeling
  - Discretization/Formulation, Mesh
  - Quantity of Interest
  - Boundary/Initial Conditions
  - Solvers
- Heavily influenced by PETSc*,**

* P. Brune, M. G. Knepley, B. F. Smith, X. Tu, "Composing Scalable Nonlinear Algebraic Solvers", 2013

**J. Brown and M. G. Knepley and D. A. May and Lois Curfman McInnes and B. F. Smith,

"Composable Linear Solvers for Multiphysics", 2012

Extensible

- Cannot anticipate every need for every simulation
- Must be able to provide interface to extend capabilities for user's needs
- Examples:
  - Modeling kernels
  - Boundary/Initial conditions
  - Solvers (lots of dirty tricks here)
  - Quantities of Interest
  - Error Estimation
- Encourage incorporation of extensions for reuse if sensible

Goals

Software Abstractions for Multiphysics FEM

- **Runtime** decisions through input file and/or command line
- **Reuse** developed (**and tested!**) modeling kernels
- **Reuse** existing libraries where feasible, practical
- **Extensible** interface for adding new/extending existing kernels
- **Modular** framework for multiphysics simulation
    - Physics Modeling
    - Boundary Conditions
    - Initial Conditions
    - Solvers (Linear, Nonlinear, Timestepping, etc.)
    - Quantities of Interest (functionals)
    - Error Estimation, Adaptive Mesh Refinement/Coarsening

libMesh FEMSystem Framework

Overview

- Developed as part of Stogner Ph.D. work*
- Abstraction for facilitating FEM applications based on libMesh

Problem Class: First Order in Time

$$\begin{aligned} M(\boldsymbol{u})\dot{\boldsymbol{u}} &= F(\boldsymbol{u}), & \text{in } \Omega \times (0,T) \\ G(\boldsymbol{u}) &= 0, & \text{in } \Omega \times (0,T) \\ \boldsymbol{u}(\mathbf{x},0) &= \boldsymbol{u}_0(\mathbf{x}) & \forall \mathbf{x} \in \overline{\Omega} \\ \boldsymbol{u}(t) &= \mathbf{g}(t), & \text{on } \Gamma_d \times (0,T) \\ \sigma(\boldsymbol{u},t) \cdot \mathbf{n} &= h(t), & \text{on } \Gamma_n \times (0,T) \end{aligned}$$

Problem Class: Second Order in Time

$$M(\boldsymbol{u})\ddot{\boldsymbol{u}} + C(\boldsymbol{u})\dot{\boldsymbol{u}} = F(\boldsymbol{u}), \qquad \text{in } \Omega \times (0,T)$$

libMesh FEMSystem Framework

- User supplies **element** level evaluations of weak forms of $F(\boldsymbol{u})$, $G(\boldsymbol{u})$, $M(\boldsymbol{u})$, $C(\boldsymbol{u})$ operators
- Parallel (distributed and threaded) partitioning handled upstream
- Modularity provides flexibility in solver algorithms
  - Steady solvers only need $F(\boldsymbol{u})$, $G(\boldsymbol{u})$
  - First order systems additionally need $M(\boldsymbol{u})$
  - Second order systems additionally (may) need $C(\boldsymbol{u})$
- Adheres to “strategy” pattern
  - Context object provides all necessary data, algorithms for residual evaluation
- Automatically computes finite differenced derivatives if user does not supply

GRINS Multiphysics Framework*

- Builds on FEMSystem framework
- MultiphysicsSystem subclasses FEMSystem
- Modularity in Physics objects, QoI objects, Solver objects, Boundary Conditions, etc.
- Factory objects for easy extension

$$\sum_{p=1}^{N_p} M_p\left(\boldsymbol{u}_h, \dot{\boldsymbol{u}}_h; \boldsymbol{v}_h\right) = \sum_{p=1}^{N_p} F_p(\boldsymbol{u}_h; \boldsymbol{v}_h) \quad \forall \boldsymbol{v}_h \in V^h$$

$$\sum_{p=1}^{N_p} G_p(\boldsymbol{u}_h; \boldsymbol{v}_h) = 0 \quad \forall \boldsymbol{v}_h \in V^h$$

* P. T. Bauman, R. H. Stogner, "GRINS: A Multiphysics Framework Based on the libMesh Finite Element Library", SISC, 38(5), S78–S100, `https://grinsfem.github.io`

GRINS Multiphysics Framework

Reusability

- **Reuse** developed infrastructure
    - Physics, QoIs, Boundary Conditions, Solvers, etc.
- **Reuse** testing of that infrastructure

Runtime Experimentation

- If capability exists, can be selected in input file/command line at **runtime**
- Make heavy use of FunctionParser library
    - Parse mathematical string into code
    - JIT compilation for efficiency
    - Some AD capabilities (ongoing, driven by INL)
- FunctionParser can be used in boundary conditions, initial conditions, source terms, ...

GRINS Multiphysics Framework

Flexibility/Extensibility

- Can standalone, but adhere to “librarization of software” principles*
- Flexible object-oriented design to make it easy to add something that’s missing
    - Physics, QoI, solver, boundary conditions, initial conditions, etc.
    - Can make Physics finer grained, more complex (e.g. AD)
- User subclasses object(s), adds construction to instance of factory. **Done.**
- Particularly useful for ITAR/NDA type applications

*J. Brown, M. G. Knepley, B. F. Smith, “Run-time extensibility and librarization of simulation software”, arXiv:1407.2905

GRINS Multiphysics Framework

Key Aspect: Automatic Discrete Adjoints

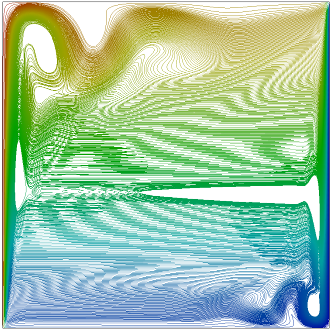
- Information for adjoint solves is already there
    - Steady problems require transpose of Jacobian
    - Unsteady problems require evaluations of these operators
    - Derivatives of QoI w.r.t. forward solution
- Gain QoI-based error estimation/AMR and QoI sensitivities/Hessian **automatically**
    - Derivatives all computed via finite difference if not implemented by the user
    - Includes special boundary QoIs
- Unsteady case still needs work (i.e. checkpointing schemes)

GRINS Example: Fluid Mechanics

Comments

- Variable density (low Mach) Navier-Stokes equations
- Very similar to INS, $\nabla \cdot \boldsymbol{u}$ now depends on temperature
- Flow driven by hot wall/cold wall
- $Ra = 10^8 \Rightarrow$ Stabilization

Cavity Benchmark*



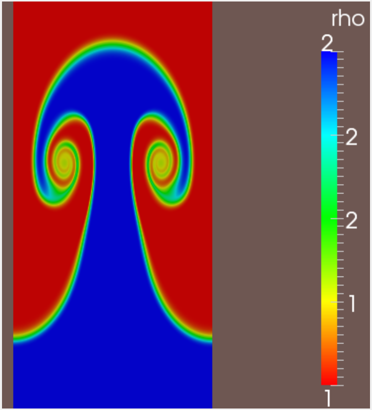
[*] P. Le Quéré et al, "Modelling Of Natural Convection Flows with Large Temperature Differences: A Benchmark Problem for Low Mach Number Solvers. Part 1. Reference Solutions", ESAIM: M2AN, 39(3), 2005

GRINS Example: Fluid Mechanics

Comments

- Variable density (low Mach) Navier-Stokes equations
- Initial temperature field gives differing densities
- Flow driven by buoyancy
- Periodic boundary conditions

Rayleigh-Taylor Instability

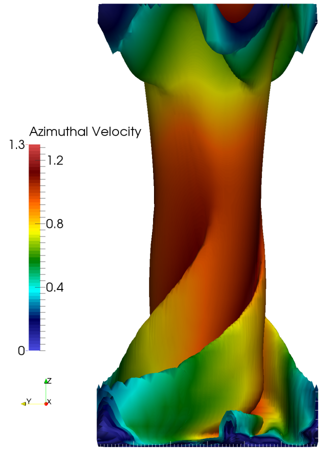


GRINS Example: Fluid Mechanics

Comments

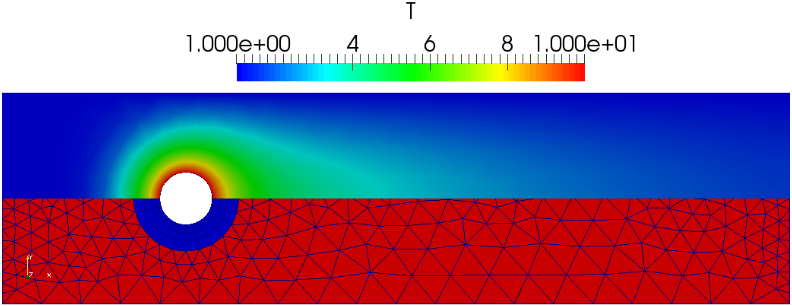
- Thermally driven vortex
- Georgia Tech project on alternative energy
- INS, heat transfer, boussinesq, “interesting” forcing functions
- All set at runtime

Thermally Driven Vortex*



* Image courtesy Nicholas Malaya, U. of Texas at Austin

GRINS Example: Conjugate Heat Transfer

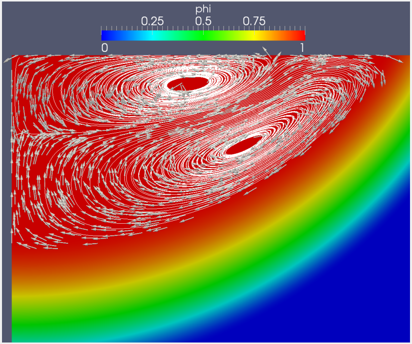


GRINS Example: MHD

Comments

- Model of manufacturing process (vacuum arc remelting)
- INS, heat transfer, boussinesq, solidification, electrostatics, magentostatics (HCurl)
- NDA on boundary conditions ⇒ standalone application
- All set at runtime

Vacuum Arc Remelting

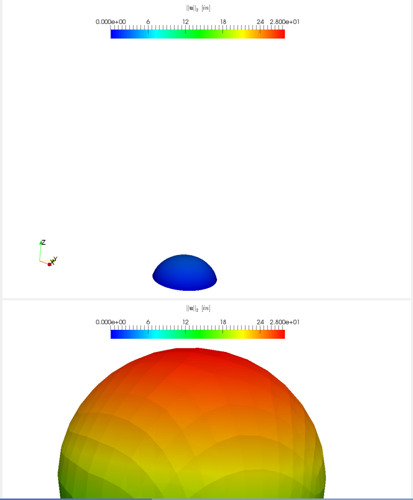


GRINS Example: Solid Mechanics on Manifolds

Comments

- Large deformation nonlinear elasticity
- Rubber (Mooney-Rivlin) membrane
- Constant pressure (normal to surface ⇒ additional geometric nonlinearity
- Incremental pressure solver (quasi-static)

Inflating Membrane

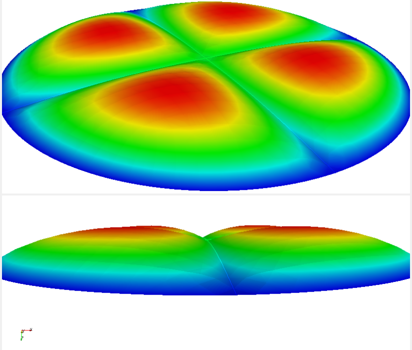


GRINS Example: Solid Mechanics on Manifolds

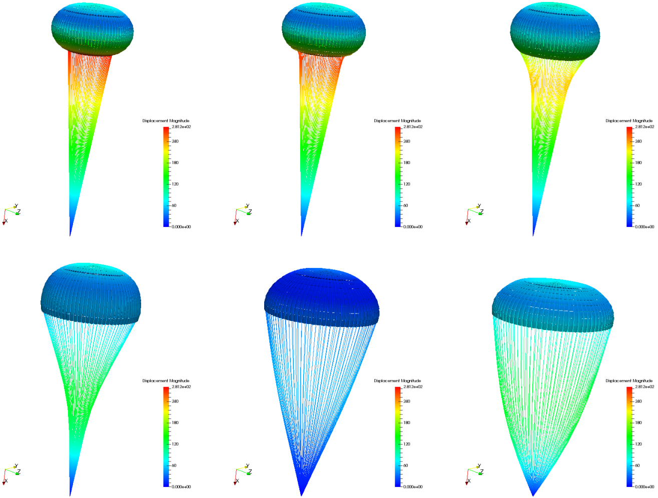
Comments

- Now add elastic rod stiffeners, Hookean
- Large deformation formulation for membrane and rod
- Constant pressure loading
- Incremental pressure solver (quasi-static)

Inflating Membrane with Stiffener



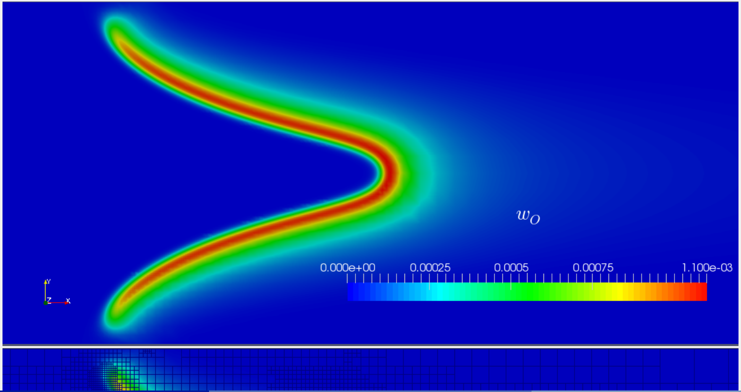
Disreefing: Constant Uniform Pressure



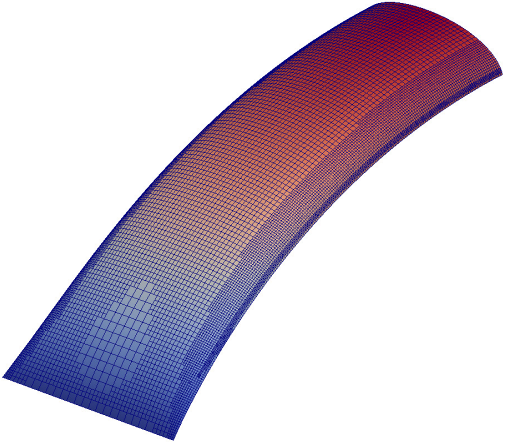
GRINS Example: Laminar Flame AMR

- Reacting low Mach Navier-Stokes ⇒ combustion
- Reuse thermochemistry, transport libraries

Ozone Flame

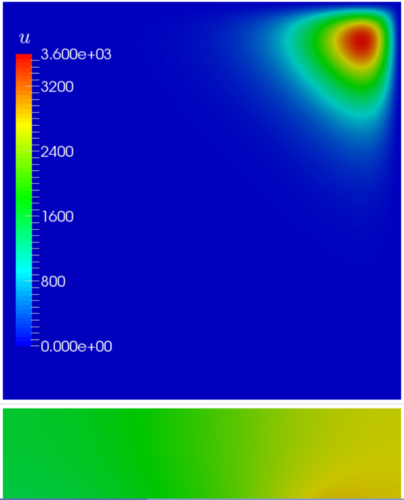


GRINS Example: AMR on Mixed-Dimensional Manifolds



GRINS Example: Point QoIs AMR

Point Value AMR*



Comments

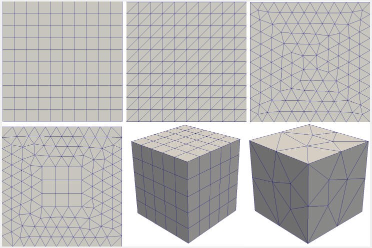
- Laplace equation with specified loading
- Want to drive AMR to control error at point value of solution
- Specify Physics, QoI, error, adaptive algorithm at runtime

Linear and Nonlinear Solver Composability

PETSc DM Infrastructure

- Facilitates field split solvers
- Facilitates geometric multigrid
    - Automated construction of grid hierarchy in `libMesh`, unstructured grids
    - Includes parallel distributed meshes
    - MPI-3 provides path to more scalable algorithm
- Can do GMG on fieldsplit blocks

Coarse Grids



Beyond Forward Problems: Inverse Problems

Bayesian Approach

- Need to determine PDFs of parameters, not just scalar values (deterministic inverse problem)
- Requires advancement in:
    - Calibration algorithms
    - Interaction with experimentalists
- GRINS+QUESO* provides a framework to achieve this
    - MCMC using multiphysics PDEs

Bayes Theorem

$$P(B|A) = \frac{P(B \cap A)}{P(A)}$$

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

Let $A =$ data,
$B =$ parameters

Then $P(A|B) =$ the model

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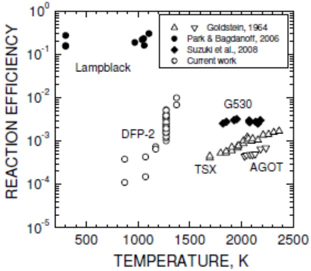
* `https://libqueso.com`

Example: Nitridation Data Reduction Model

Motivation

- Surface/wall catalysis plays a critical role in surface heat flux on a re-entry vehicle
- Reported estimates of surface reaction efficiency vary by few orders of magnitude[1] (often supercatalytic wall is assumed[2])



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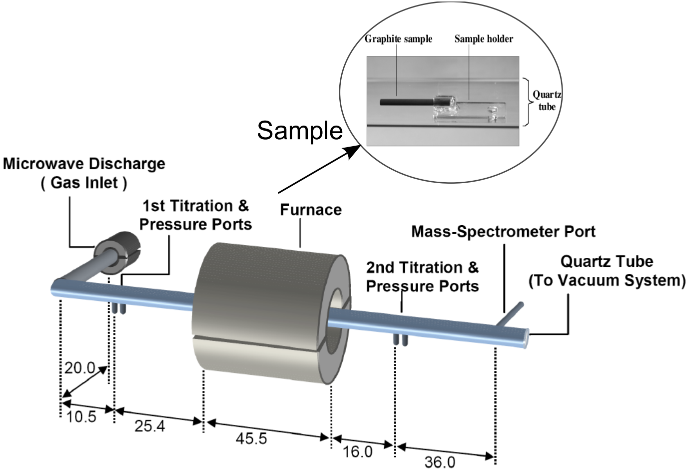
[1] Zhang et. al., “Laboratory Investigation of Active Graphite Nitridation by Atomic Nitrogen”, AIAA-2009-4251

[2] Wright et. al. “Uncertainty and Sensitivity Analysis of Thermochemical Modeling for Titan Atmospheric Entry”, AIAA-2004-2455

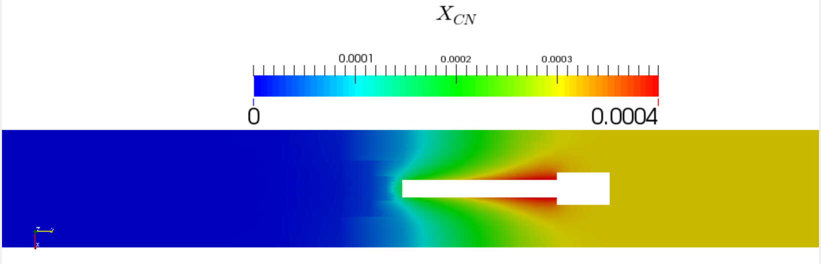
Example: Nitridation Data Reduction Model



* Zhang et. al., “Laboratory Investigation of Active Graphite Nitridation by Atomic Nitrogen”, AIAA-2009-4251

Example: Nitridation Data Reduction Model

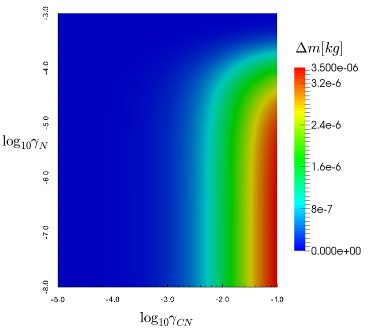
CN-species mass fraction



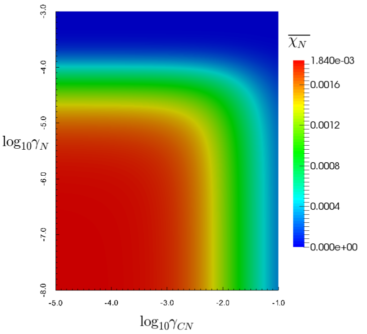
Adapted Grids

Example: Nitridation Data Reduction Model

Δm

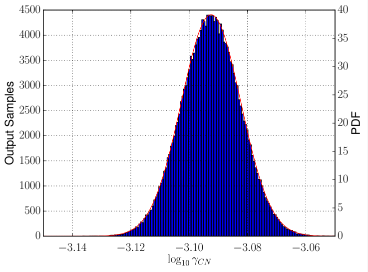


$\overline{\chi}_N$

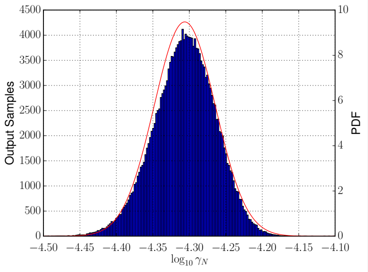


Example: Nitridation Data Reduction Model

γCN



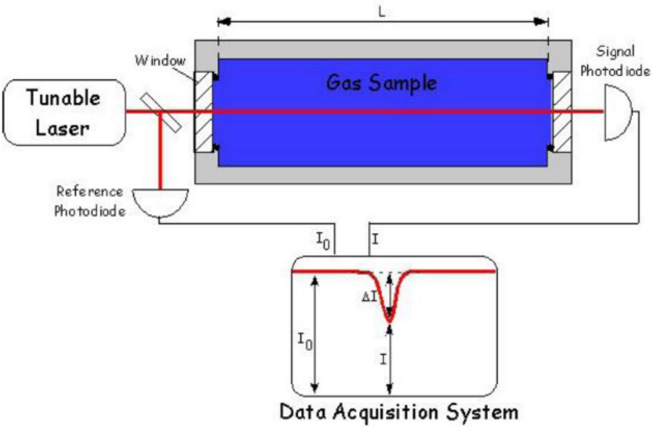
γN



P. T. Bauman, “Enabling Statistical Calibration of Active Nitridation of Graphite by Atomic Nitrogen”, 45th AIAA Thermophysics, 2015, AIAA Paper 2015-2665

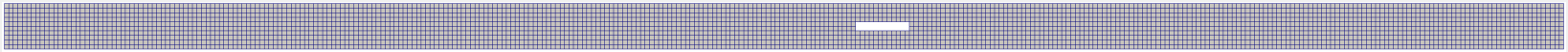
Laser Absorption Spectroscopy

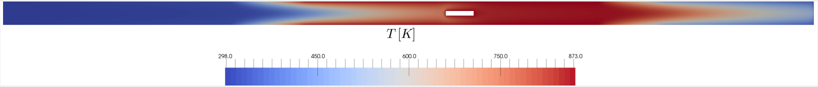
Schematic

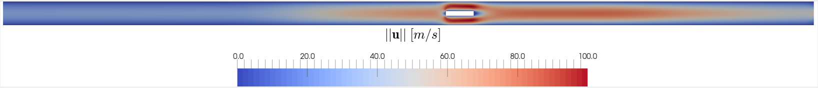


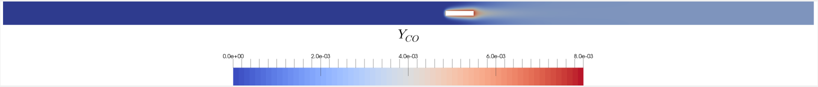
http://media.americanlaboratory.com/m/20/article/129080-fig1.jpg

Flow Field



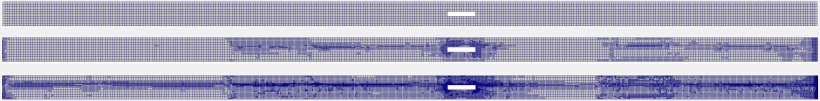

$T\,[K]$


$||\mathbf{u}||\ [m/s]$

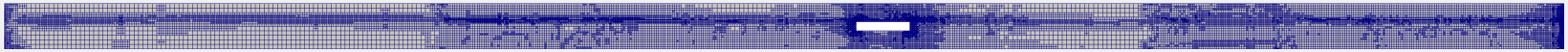

Y_{CO}

Adaptive Refinements

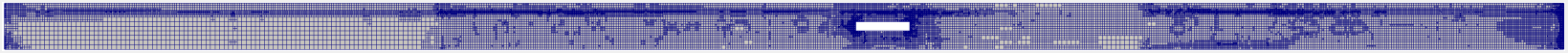
Base Case



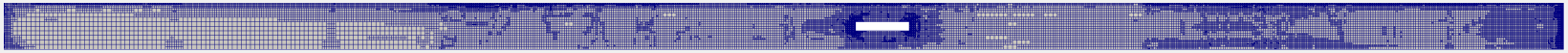
Offset Case



Offset of $1mm$



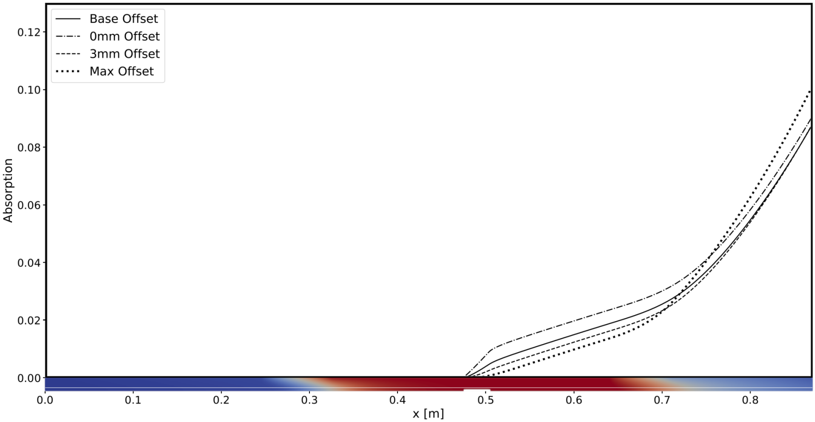
Offset of $5mm$



Offset of $10mm$

Angled Case

GRINS Example: TDLAS in Reacting Flow

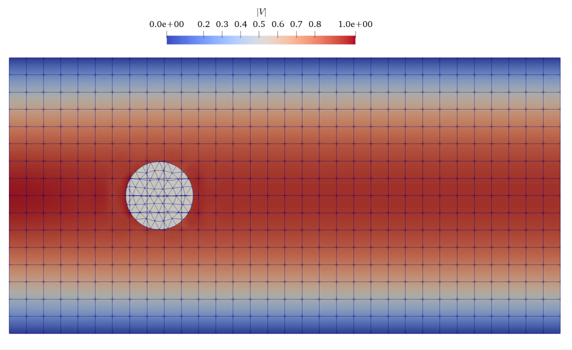


Ongoing Work

Multiphysics

- Fluid-Structure Interaction
  - Investigating immersed boundary approaches

Convecting Solid Cylinder



Ongoing Work

NSF SI2-SSE: libMesh Enhancements

- Geometric Multigrid
    - Full Approximation Scheme
    - Extend to include Hdiv, HCurl conforming projections
- Interaction with mesh geometry (AMR, Multigrid)
- Generic Programming of Physics kernels

NSF CAREER: Inverse problems

- Runtime interaction with QUESO
- Facilitate experimental design

Concluding Remarks

- Runtime experimentation of models, algorithms, formulations will facilitate rapid scientific and engineering developments
  - Already demonstrated at the solver level in the PETSc composable solvers framework
- Especially true for statistical inverse problems
  - Vary prior models, surrogate models, evaluate model plausibilities
- Enabled by reusability, flexibility, and using good software abstractions
- GRINS+libMesh, QUESO, other supporting packages provide a unifying framework for computational science research and facilitating predictions with uncertainty