An Overview of the GRINS Multiphysics Framework

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Acknowledgements

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University of Texas at Austin

Changing Definition of Prediction

Traditional Emphasis: Increasing model complexity

- Developing numerical formulations/schemes
- High Performance Computing, Algorithms
- Coupling PDEs
- Complex constitutive equations

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Shifting Emphasis: Incorporating Uncertainty

- Exascale resources enable UQ methodologies (not just the next DNS run)
- Several journals, conferences dedicated to UQ
- Need tools unifying research efforts in numerical methods for complex PDEs and methods for quantifying uncertainty

Forward Problem

“Complex” Problems

- Multiscale
- Multiphysics

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"Complex" Problems

- Multiscale
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"Modern" Algorithms

- Adaptive Mesh Refinement
  - Research activities over the past 30-40 years
  - **Still** not prominently used. Slowly changing.
  - **Vital** for efficient solutions, especially in UQ context

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- Adjoint-based Methods
  - QoI-based error estimations
    - Drive AMR for specified quantities to within tolerance
  - Gradients (sensitivities), Hessians
    - Local sensitivites analysis
    - Gradient/Hessian enhanced MCMC sampling methods

Forward Problem

Scalable and **Effective** Solvers

- Scalable Solvers: Multigrid
  - Algebraic: BoomerAMG, ML, MueLu, ...
  - Geometric: deal.ii/p4est — quad/octrees only, not simplices

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Scalable and **Effective** Solvers

- Scalable Solvers: Multigrid
  - Algebraic: BoomerAMG, ML, MueLu, ...
  - Geometric: deal.ii/p4est — quad/octrees only, not simplices
- Effective Solvers
  - For complex problems, **Do Not Know!**
  - **Must Experiment!**
  - $\Rightarrow$ "Composable Solvers" framework in PETSc*,**
    - Fieldsplit solvers
    - DM infrastructure $\Rightarrow$ Geometric Multigrid

* 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

Forward Problem

Software Abstractions for Multiphysics FEM

- **Runtime** decisions through input file and/or command line

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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 modeling kernels
- **Modular** framework for multiphysics simulation
  - Quantities of Interest (functionals)
  - Solvers (Steady, Unsteady, Continuation, etc...)
  - Boundary Conditions
  - Initial Conditions

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

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

*R. H. Stogner, "Parallel Adaptive C1 Macro-Elements for Nonlinear Thin Film and Non-Newtonian Flow Problems", 2008

libMesh FEMSystem Framework

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Problem Class: Second Order in Time

$$
\begin{aligned}
M(\boldsymbol{u})\ddot{\boldsymbol{u}} + C(\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} \\
\dot{\boldsymbol{u}}(\mathbf{x},0) &= \dot{\boldsymbol{u}}_0(\mathbf{x}) && \forall \mathbf{x} \in \overline{\Omega} \\
\boldsymbol{u}(t) &= \mathbf{g}(t), && \text{on } \Gamma_d \times (0,T) \\
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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 flexiblity in solver algorithms
    - Steady solvers only need $F(\boldsymbol{u})$, $G(\boldsymbol{u})$
    - First order systems additionally need $M(\boldsymbol{u})$
    - Second order systems additionaly (may) need $C(\boldsymbol{u})$
- Adheres to “strategy” pattern
    - Context object provides all neccessary 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*

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)

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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

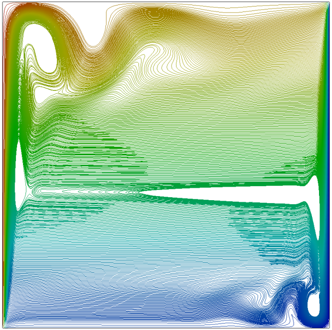
*J. Brown, M. G. Knepley, B. F. Smith, "Run-time extensibility and librarization of simulation software", arXiv:1407.2905

GRINS 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*



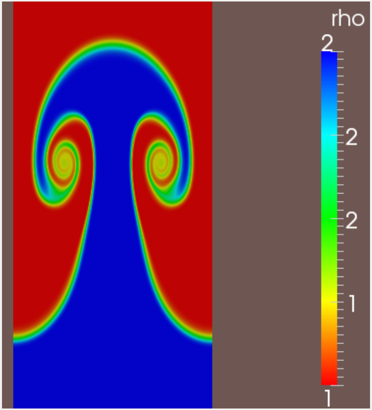
*P. Le Quéré et al, "Modelling Of Natural Convection Flows with Large Temperature Differences: A Benchmark Problem for Low Mach Number Solvers. Part 1. Reference Solutions", ESAIM: M2AN, 39(3), 2005

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

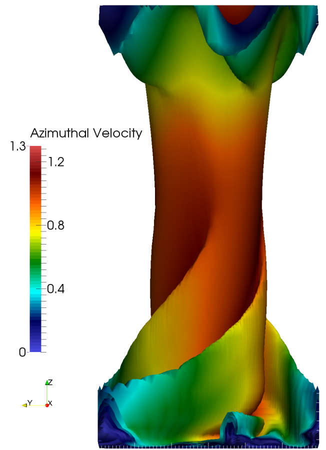


GRINS Example: Fluid Mechanics

Comments

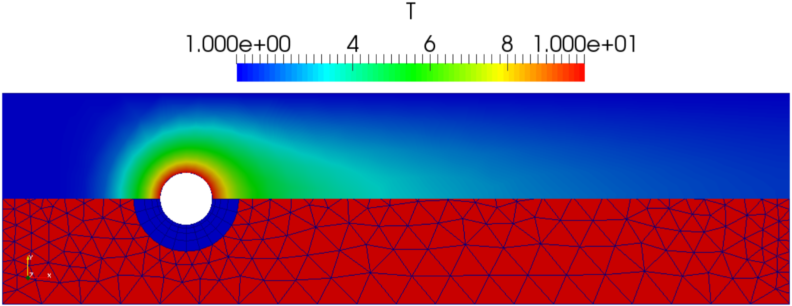
- Thermally driven vortex
- Georgia Tech project on alternative energy
- INS, heat transfer, boussinesq, “interesting” forcing functions
- All set at runtime

Thermally Driven Vortex*



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

GRINS Example: Conjugate Heat Transfer

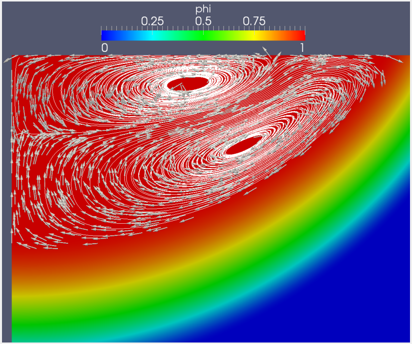


GRINS Example: MHD

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

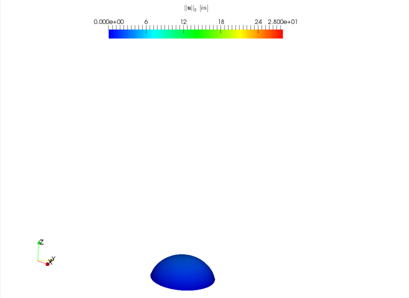


GRINS Example: Solid Mechanics on Manifolds

Comments

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

Inflating Membrane



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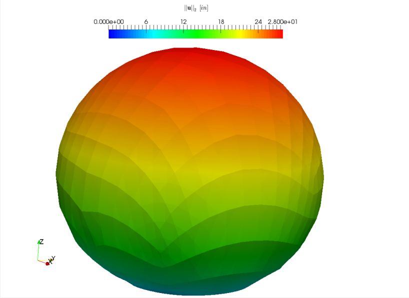
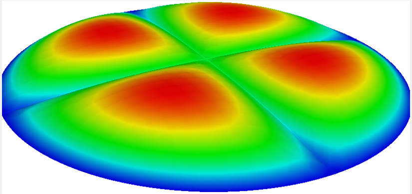


GRINS Example: Solid Mechanics on Manifolds

Comments

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

Inflating Membrane with Stiffener



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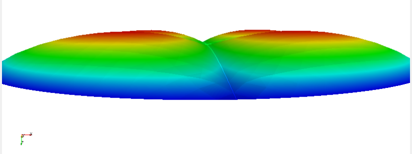
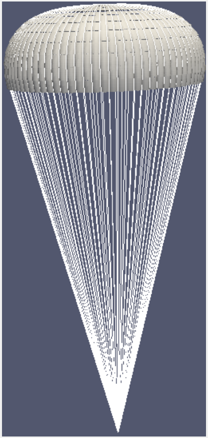


GRINS Example: Solid Mechanics on Manifolds

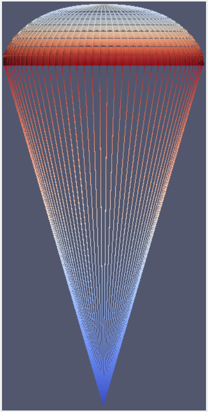
Comments

- Motivating application: parachute deployment
- Nylon membrane, Kevlar stiffeners

Mesh



Snapshot

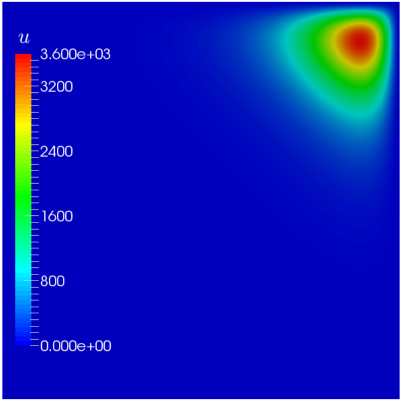


GRINS Example: Point QoIs AMR

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
- Point value code written, can be reused in any run

Point Value AMR*



*S. Prudhomme and J. T. Oden, “On goal-oriented error estimation for elliptic problems: application to the control of pointwise errors”, CMAME, 1999

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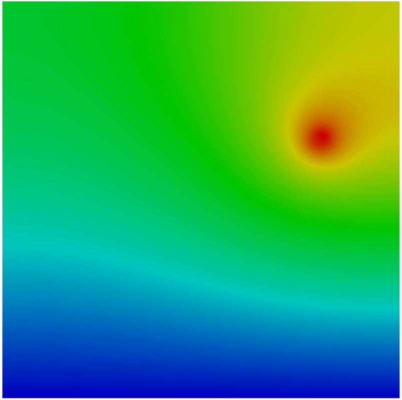

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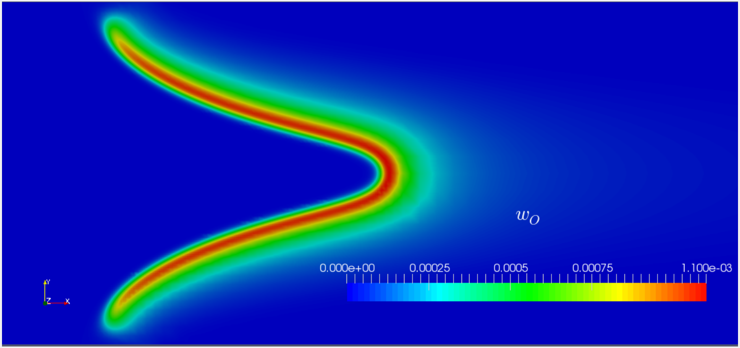
GRINS Example: Laminar Flame AMR

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

Ozone Flame



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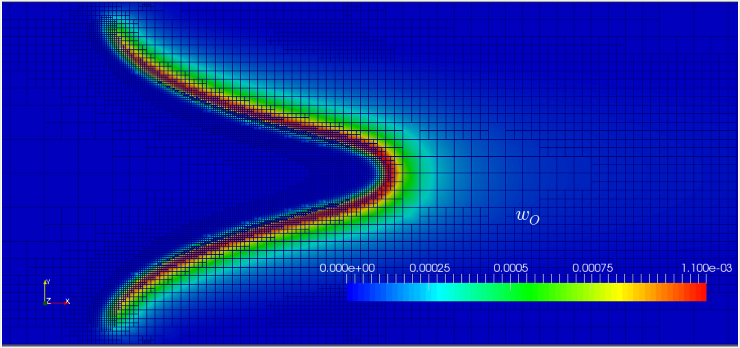


GRINS Applications at SIAM CSE

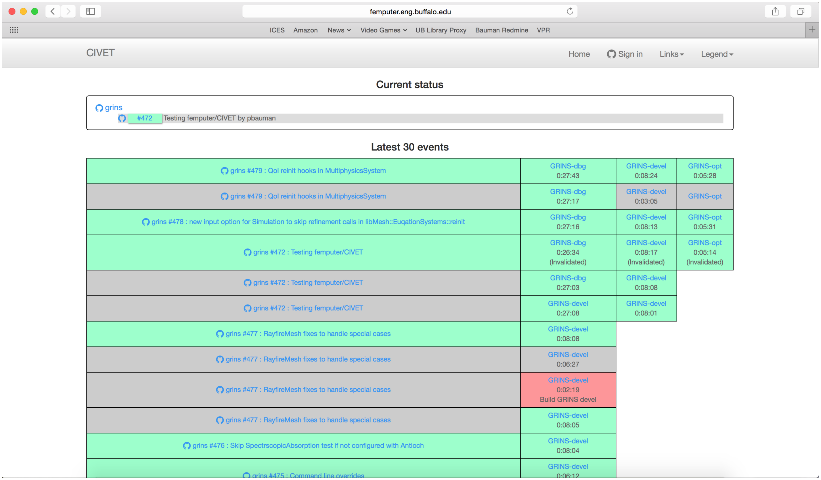
Variational IBM - Boris Boutkov

- Deploying FSI using IBM, reusing existing kernels as much as possible
- Updates required and challenges
- Friday March 3, 10 AM, MS 295, Room 301

Laser Attenuation in Reacting Flows - Tim Adowski

- Goal-oriented AMR for rayfire-based QoI
- Friday March 3, 12:35 PM, MS 315, Room 216

GRINS Continuous Integration: CIVET


femputer.eng.buffalo.edu

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CIVET Home Sign in Links Legend

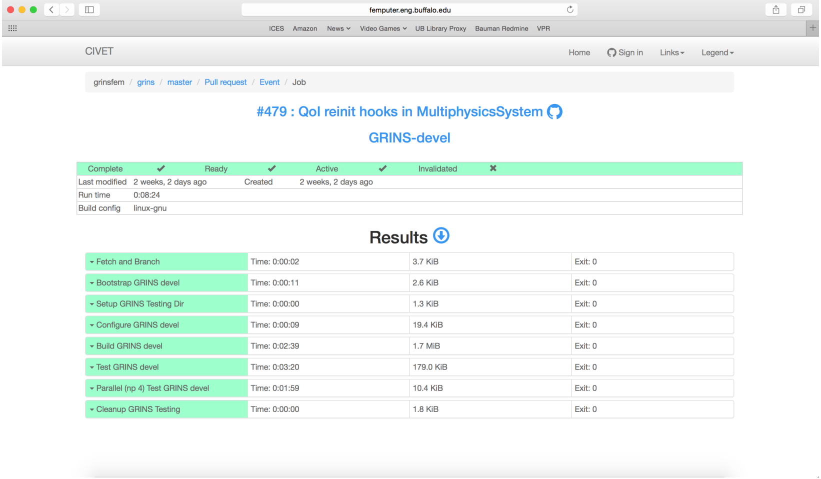
Current status

grins
#472 Testing femputer/CIVET by pbauman

Latest 30 events

grins #479 : QoI reinit hooks in MultiphysicsSystem	GRINS-dbg 0:27:43	GRINS-devel 0:08:24	GRINS-opt 0:05:28
grins #479 : QoI reinit hooks in MultiphysicsSystem	GRINS-dbg 0:27:17	GRINS-devel 0:03:05	GRINS-opt
grins #478 : new input option for Simulation to skip refinement calls in libMesh::EuqationSystems::reinit	GRINS-dbg 0:27:16	GRINS-devel 0:08:13	GRINS-opt 0:05:31
grins #472 : Testing femputer/CIVET	GRINS-dbg 0:26:34 (Invalidated)	GRINS-devel 0:08:17 (Invalidated)	GRINS-opt 0:05:14 (Invalidated)
grins #472 : Testing femputer/CIVET	GRINS-dbg 0:27:03	GRINS-devel 0:08:08	
grins #472 : Testing femputer/CIVET	GRINS-devel 0:27:08	GRINS-devel 0:08:01	
grins #477 : RayfireMesh fixes to handle special cases	GRINS-devel 0:08:08		
grins #477 : RayfireMesh fixes to handle special cases	GRINS-devel 0:06:27		
grins #477 : RayfireMesh fixes to handle special cases	GRINS-devel 0:02:19 Build GRINS devel		
grins #477 : RayfireMesh fixes to handle special cases	GRINS-devel 0:08:05		
grins #476 : Skip SpectrscopicAbsorption test if not configured with Antioch	GRINS-devel 0:08:04		
grins #475 : Command line overrides	GRINS-devel 0:06:12		

GRINS Continuous Integration: CIVET



Ongoing Work

Multiphysics

- Fluid-Structure Interaction
  - Investigating immersed boundary approaches
  - Future work: automate mesh motion equation in ALE

NSF SI2-SSE: libMesh Enhancements

- Geometric Multigrid
  - Leverage mesh hierarchy in libMesh
  - Provide restriction/interpolation to PETScDM infrastructure
- Generic Programming of Physics kernels
- Interaction with mesh geometry (AMR, Multigrid)

NSF CAREER: Inverse problems

- Runtime interaction with QUESO

Concluding Remarks

- Uncertainty becoming a critical aspect of predictions, enabled by “extreme-scale” computing
- 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