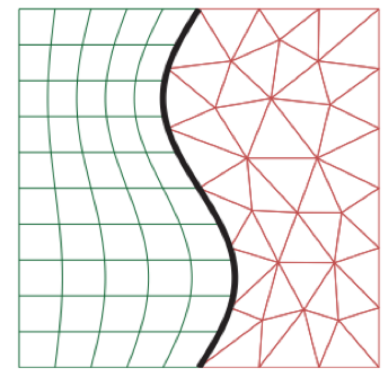
Preliminary Exam – Proposal Outline (December 2020)



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Goals for This Outline

- Describe the two focus topics for the prelim proposal

- Establish both the goals and the bounds of the problem(s)
  - “Must-haves” and “nice-to-haves”

- Lay out a plan for accomplishing these goals, for now in minimal detail

- State the current status of each project

Time Integration of Reacting Flows

The Topic/Problem

- The mission statement: develop stable, accurate, and efficient multi-rate time integration schemes for reacting flows

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j + P\delta_{ij} - \tau_{ij}) = 0$$

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}((\rho E + P)u_j + q_j - u_i\tau_{ij}) = 0$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k u_j - \varphi_{ki}) = \boxed{W_k \dot{\omega}_k}$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} + \frac{\sum_{k=1}^{N_{sp}} U_k(T) \frac{\partial(\rho Y_k)}{\partial t} \frac{1}{W_k}}{\sum_{k=1}^{N_{sp}} [C]_k C_{v,k}} = 0$$

$$\frac{\mathrm{d}P}{\mathrm{d}t} - \frac{R}{V}\left(T\frac{\mathrm{d}n}{\mathrm{d}t} + \frac{\mathrm{d}T}{\mathrm{d}t}n\right) = 0$$

Species production rates (stiff)

- Chemical source terms in governing equations tend to be stiff, setting the limiting timestep to be oppressively low relative to the fluid motion or requiring implicit treatment
- As with disparate overset mesh sizes, this presents an opportunity for multi-rate to save the day

Goals and Bounds

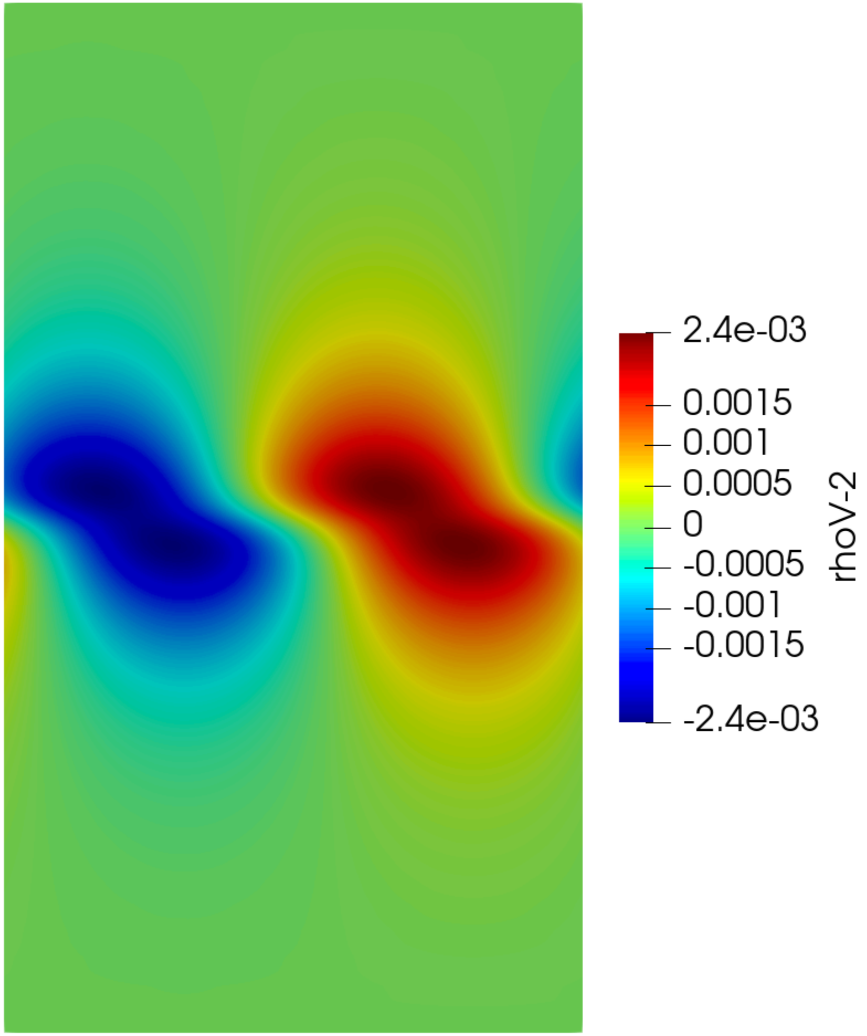
- Must-have: demonstrate a novel scheme (adaptive implicit-explicit multi-rate) driving a canonical or demonstrative reacting flow problem (more) correctly and (more) efficiently
  - Monitor and maintain presence of solution on constraint manifold (ideal gas law)
- Nice-to-have: report on and/or optimize time integration within design space presented by adaptivity choices (see next slide)
- Nice-to-have: demonstrate tangible improvement over CVODE (state of the art) in at least one metric
- Beyond our bounds: multivariable solves incurred by certain situations (multiple coupled implicit RHSs, IMEX LTE)

The Plan

- Implement multi-rate Adams integrators (established as a viable vehicle for performance improvement by [1])
  - Add ability to integrate chemistry implicitly, and at a different timestep than that of the fluid motion
  - Coupling the chemistry with the fluid RHS will elevate temporal accuracy beyond that of the previous splitting approach (first order)
  - Timestep adaptivity also identified as critical need in early testing – add this capability to multi-rate Adams integration using local error estimates as with ODE45/CVODE
- This latter capability also introduces a number of design choices worth exploring
  - Timestep adaptivity versus step ratio adaptivity
  - Track local error/make adaptivity decisions based on subset of solution components?

The Plan (cont'd)

- **Software:** PlasCom2 (fluid solver), Leap/Dagrt (code generation for integrators), PyJac-V2 (code generation for chemical kinetic Jacobians)
- **Application:** demonstrative reacting mixing layer problem
  - Hyperbolic tangent velocity profile as baseflow ([2], [3])
  - San Diego 9-species chemical mechanism
  - Initial condition: introduce temperature variation to localize autoignition to the mixing layer



Current Status

- Leap RK IMEX integration built into PlasCom2, using PyJac-generated chemical Jacobian for implicit solve
  - PyJac modified to include NASA9 thermodynamic polynomials (useful/required for maintaining accuracy for ignition problems with large temperature ranges)
- Adams-Moulton integrators implemented as baseline for implicit treatment of chemistry in multi-rate Adams
- Error-informed timestep adaptivity incorporated into single-rate and multi-rate Adams integrators
  - Local error estimate formed using explicit methods of differing orders
- Implicit-explicit multi-rate w/adaptivity in development
- Test problem(s) in development
  - Mixing layer (demonstrative case)
  - One-dimensional laminar flame (baseline case?)

Energy-Stable Hybrid Spatial Discretizations

The Topic/Problem

- The mission statement: create a stable and accurate interface between structured (SBP) and unstructured (DG) spatial discretizations
  - Introducing localized regions of unstructured meshing allows for superior meshing of complex geometries
- Starting point: nonconforming interface method of Kozdon and Wilcox ([4])
  - Boundary between spatial schemes traversed via projection of solution into “glue grid” polynomial space
  - Choice of polynomial space in glue grid/structure of projection operators can allow for proof of energy stability
  - However, resulting projection stencils give an underdetermined system, with optimization used to produce final projection operators

Goals and Bounds

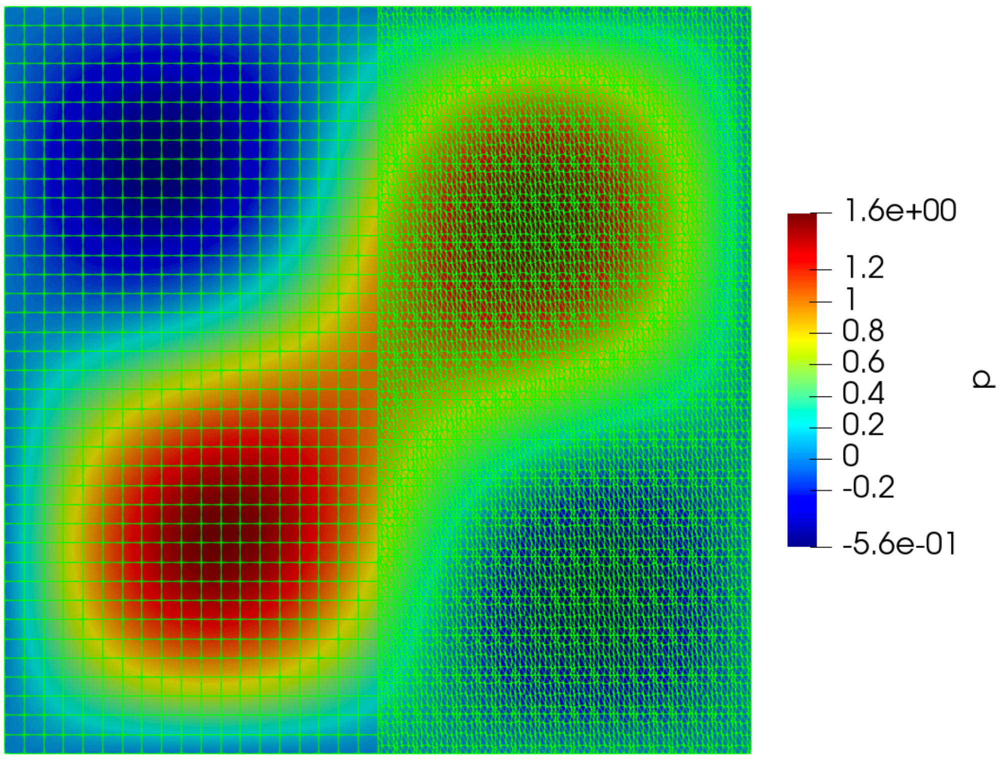
- Must-have: stable, accurate, and *unisolvent* approach to interior projection from structured (SBP) to unstructured (DG) meshes in 2D
  - Apply this to a periodic problem as a baseline proof-of-concept
- Nice-to-have: application to 3D problems
- Nice-to-have but based on our current experience will be tricky: stable, accurate, and unisolvent boundary projection
  - Boundary stencils are currently what make the whole-operator solves of Kozdon and Wilcox underdetermined

The Plan

- Starting point: remove more complicated boundary treatment from setup, construct interior-only periodic projection operators
  - Be able to write down proof of stability (via energy) - this may result in a different operator condition than K+W’s compatibility, and may require a more thorough search for all possible operator conditions than has yet been performed
  - Establish a sensible set of DOFs
  - Solve for these operators from a square system based on accuracy conditions for projection in *both* directions (grid-to-glue, glue-to-grid), in addition to any constraints we need to impose to ensure stability (based on conditions mentioned above)
- Prove the efficacy of these projection operators in 2D
- Apply lessons learned to boundary treatment

The Plan (cont'd)

- **Software:** Grudge (w/meshmode and other tools, for DG discretization), Leap/Dagrt (for time integration)
- **Application:** 2D acoustic wave equation on split domain



Current Status

- Python-based testing setup created which implements split-domain 2D acoustic wave problem described on the previous slide
- Matlab and Maxima codes written with the goal of experimenting with different DOF/constraint setups to produce a unisolvent and stable interior projection operator
  - Needed: firmer understanding of how compatibility condition of K+W fulfills interior projection operator accuracy constraints in both directions (pencil and paper)

References

- [1] Mikida, Cory, Andreas Klöckner, and Daniel Bodony. "Multi-rate time integration on overset meshes." *Journal of Computational Physics* 396 (2019): 325-346.
- [2] Michalke, Alfons. "On the inviscid instability of the hyperbolictangent velocity profile." *Journal of Fluid Mechanics* 19.4 (1964): 543-556.
- [3] Blumen, William. "Shear layer instability of an inviscid compressible fluid." *Journal of Fluid Mechanics* 40.4 (1970): 769-781.
- [4] Kozdon, Jeremy E., and Lucas C. Wilcox. "Stable coupling of nonconforming, high-order finite difference methods." *SIAM Journal on Scientific Computing* 38.2 (2016): A923-A952.