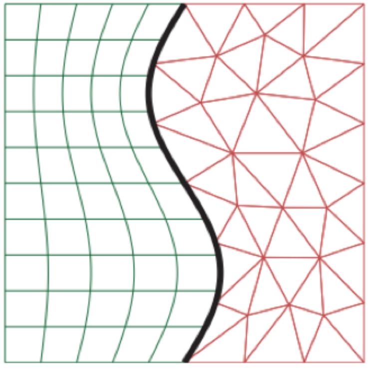
Preliminary Exam – Proposal Outline (December 2020)



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Time Integration of Reacting Flows

The Topic/Problem

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

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

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

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

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

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

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

- In these equations:
- ρ = density
- u_i = velocity in ith direction
- δ_{ij} = Kronecker delta
- τ_{ij} = fluid stress tensor
- E = total energy
- T = temperature
- P = pressure
- q = heat flux
- W_k = molecular weight of kth species
- $\dot{\omega}_k$ = production rate of kth species
- R = gas constant
- n = number of moles of gas
- $[C]_k$ = concentration of kth species
- $C_{v,k}$ = specific heat at constant volume of kth species
- $U_k(T)$ = internal energy of kth species at temperature T
- Y_k = mass fraction of kth species
- φ_{ki} = diffusion flux of kth species

The Topic/Problem

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

Cons. of mass

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

Cons. of momentum

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

Cons. of energy

Navier-Stokes

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

Species mass fraction equation

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

Derived from constant internal energy assumption

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

Time derivative of ideal gas law

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

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

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

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

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

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

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
- **Research Question:** Can we derive performance benefit from using multi-rate Adams integrators?

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
  - Current candidate problem: **reacting mixing layer**
  - See planning slides for more detail on this problem
- Must-have: monitor and maintain presence of solution on constraint manifold (ideal gas law)
  - Fully differential approach to satisfying constant volume/constant internal energy assumptions can produce nonphysical solutions
  - Potential mitigation approaches: modified Jacobian to incorporate algebraic constraints, kinetic RHS attenuation (DAEs)

Goals and Bounds (cont'd)

- Nice-to-have: report on and/or optimize time integration within design space provided by multi-rate framework
  - Adaptivity choices (see next slide)
  - Evaluation order (”fastest-first” vs. ”slowest-first”, etc.)
  - Re-extrapolation?
  - Inclusion of additional history (shown in [1] to improve stability/timestep restrictions)
- Nice-to-have: demonstrate tangible improvement over CVODE (state of the art) in at least one metric
  - Temporal order of accuracy, specifically when coupled with fluid solver
  - Number of chemistry RHS calls required to reach end time – proxy for performance improvement beyond simple walltime measurement
- 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

$$\boxed{r = \frac{\|s_{q+1} - s_q\|_2}{\mathrm{ATOL} + \mathrm{RTOL} \cdot max(\|s_q\|_2, \|s_{q+1}\|_2)}}$$

r >= 1

$$\Delta t = 0.9(\Delta t)(r)^{\frac{-1}{q}}$$

r < 1

$$\Delta t = 0.9(\Delta t)(r)^{\frac{-1}{q+1}}$$

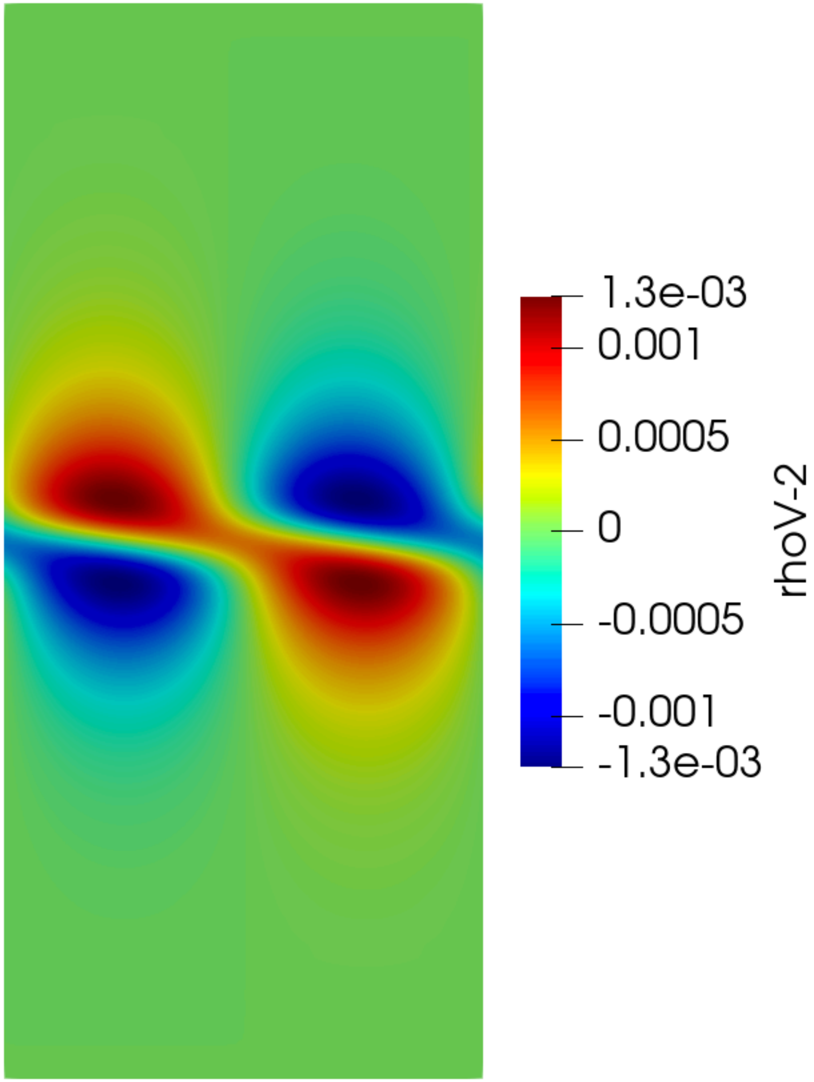
- q = order
- s_q = state estimate obtained via explicit scheme of order q

The Plan (cont'd)

- Adding adaptivity based on error estimates also introduces a number of design choices to be explored
- Timestep adaptivity versus step ratio adaptivity
  - Incurs long-standing software research question of generating variable step-ratio multi-rate code
  - Step ratio adaptivity would make constant-timestep runs with error control possible, provided the fast component dominates overall error
  - Error control mechanism based on step ratio alteration may prove to be more efficient
- Track local error/make adaptivity decisions based on subset of solution components?
  - Fast-evolving solution component (species mass fractions) may dominate local error
  - Confirming this would allow us to reduce overhead in terms of both memory and cost by refraining from tracking the slow component

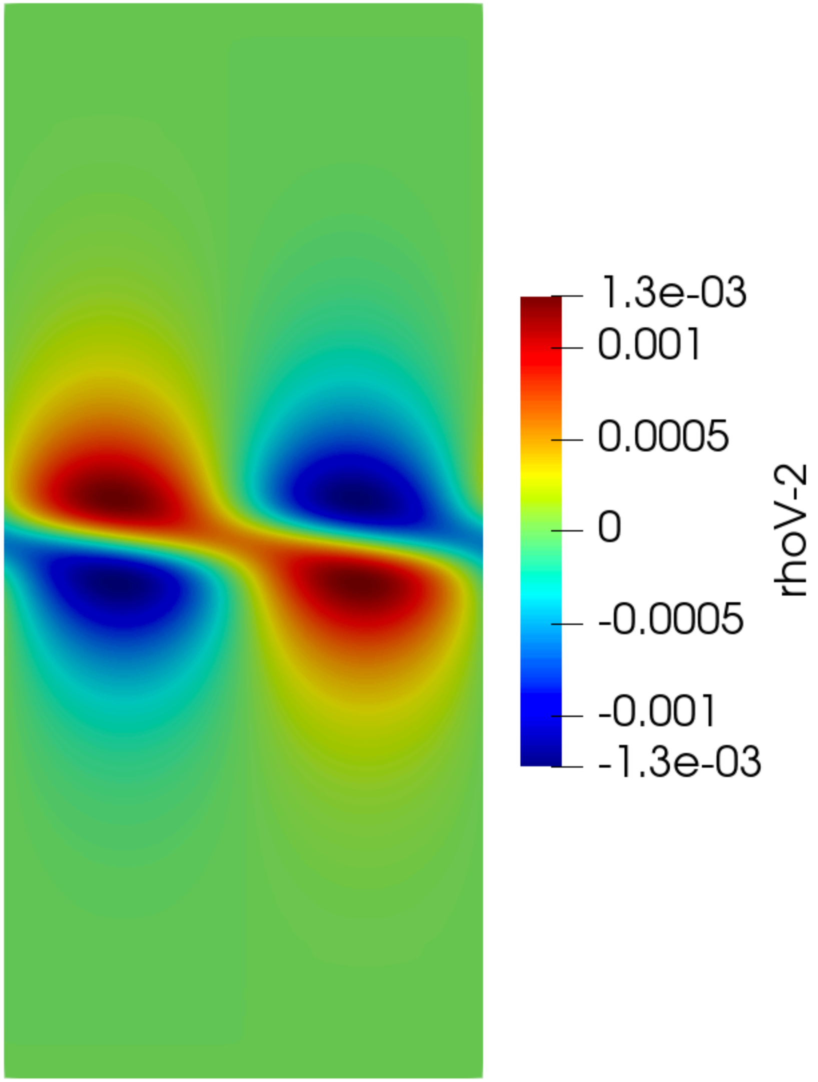
The Plan (cont'd)

- **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
- This problem is *suitable* for our uses in that it provides multiple turnable "knobs" for changing the rates of the fluid vs. the chemical kinetics, and vice versa
  - Scale magnitude of hyperbolic tangent velocity profile
  - Scale species production rates by altering reaction Arrhenius rates



The Plan (cont'd)

- **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
- This problem is *interesting* and physically useful in that it provides the simplest relevant model of combustion in a scramjet/ramjet



Impact

- **Software:** development of additional integration schemes within Leap/Dagrt framework, additional PyJac-V2 development
  - NASA9 thermodynamic polynomial descriptions already implemented in PyJac-V2 as added feature
- **Broader Impact:** improved time-to-solution at high order for reacting flow problems
  - Subsonic/supersonic combustion for propulsion: gas turbines, scramjets/ramjets, rockets
  - Furnaces/residential heating
  - Atmospheric sciences

Risk Mitigation

- Important question: **what if this doesn’t work out?**
  - Reinforces CVODE as state-of-the-art for implicit treatment of chemical kinetics
  - However, a ”fallback” of sorts would be demonstrating a higher degree of temporal accuracy in the coupled fluid problem using a Leap-generated IMEX approach with PyJac-generated Jacobians
  - Given that these Jacobians are not finite difference, and given that this eliminates the splitting scheme currently employed (at best first-order), I’m much more confident in this as a preliminary outcome
- Is this ”fallback” outcome interesting enough?
  - If so, should proving this (showing first order in splitting approach and higher-order with Leap RK approach on a demonstrative problem) be the initial goal?
  - If not, what is left?

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
  - Working its way through code review
- Error-informed timestep adaptivity incorporated into single-rate and multi-rate Adams integrators
  - Local error estimate formed using explicit methods of differing orders
  - Multi-rate implementation needs to be tested w/stiff problem

Current Status (cont’d)

- Implicit-explicit multi-rate w/adaptivity in development
- Fluid solver requires incorporation of mass diffusion terms in governing equations
- Reacting mixing layer in development (demonstrative case)
  - Currently struggling to stand up simulation
  - As of 12/28, cold flow case with unstable mode as initial condition is running
  - This is functioning to eyeball norm, but growth rate/physics need to be verified before introducing temperature variation/ignition
  - Whether the unstable mode still provides a good initial condition in the reacting case is unclear and needs to be determined
- One-dimensional premixed laminar flame
  - Functioning as a baseline case to compare reacting fluid solver’s estimated laminar flame speed with steady-state analysis (Cantera)

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
  - Most approaches to this present in literature appear to have at most second-order accuracy
  - Few approaches provide any claims about stability

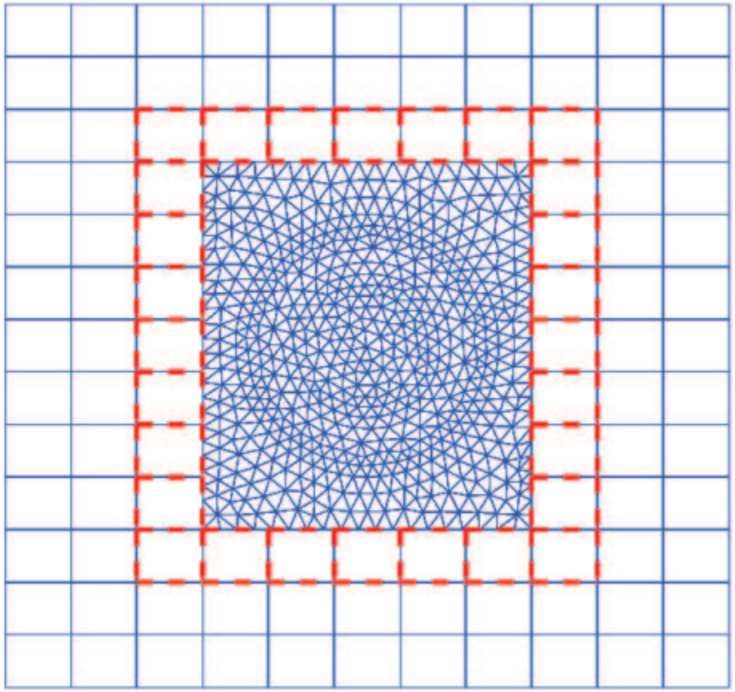


Image credit: “A hybrid FETD-FDTD method with nonconforming meshes”, Zhu et. al

The Topic/Problem

- 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

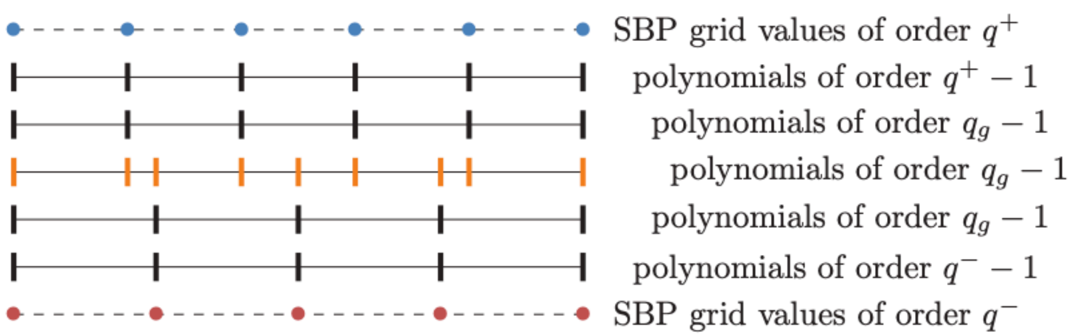


Illustration of glue-grid method in traversing nonconforming SBP-to-SBP boundaries.

The Topic/Problem/Impact

- **Research Question:** can we make stability guarantees in a manner similar to this work while avoiding ad-hoc/optimization-based approach to operator construction?
- **Draft theorem to prove:** *If a function defined on a finite-difference mesh is coupled to an unstructured mesh via a nonconforming interface, the coupling is stable and accurate to order q provided the projection operators from finite-difference to unstructured (and vice versa) satisfy condition X.*
- **Broader Impact:** improved flexibility in modeling fluid problems with complex geometries
  - Provide alternative to overset/multiblock curvilinear meshing for such problems
  - Locally introduce shock-handling benefits of DG into previously finite-difference-only simulations with relative ease

Goals and Bounds

- Must-have: stable, accurate, and *unisolvent* approach to interior projection from structured (SBP) to unstructured (DG) meshes in 2D
  - Unisolvent: same number of unknowns (DOFs) as constraint equations
  - Seek one-to-one projection: round trip across interface does not result in data loss
  - 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

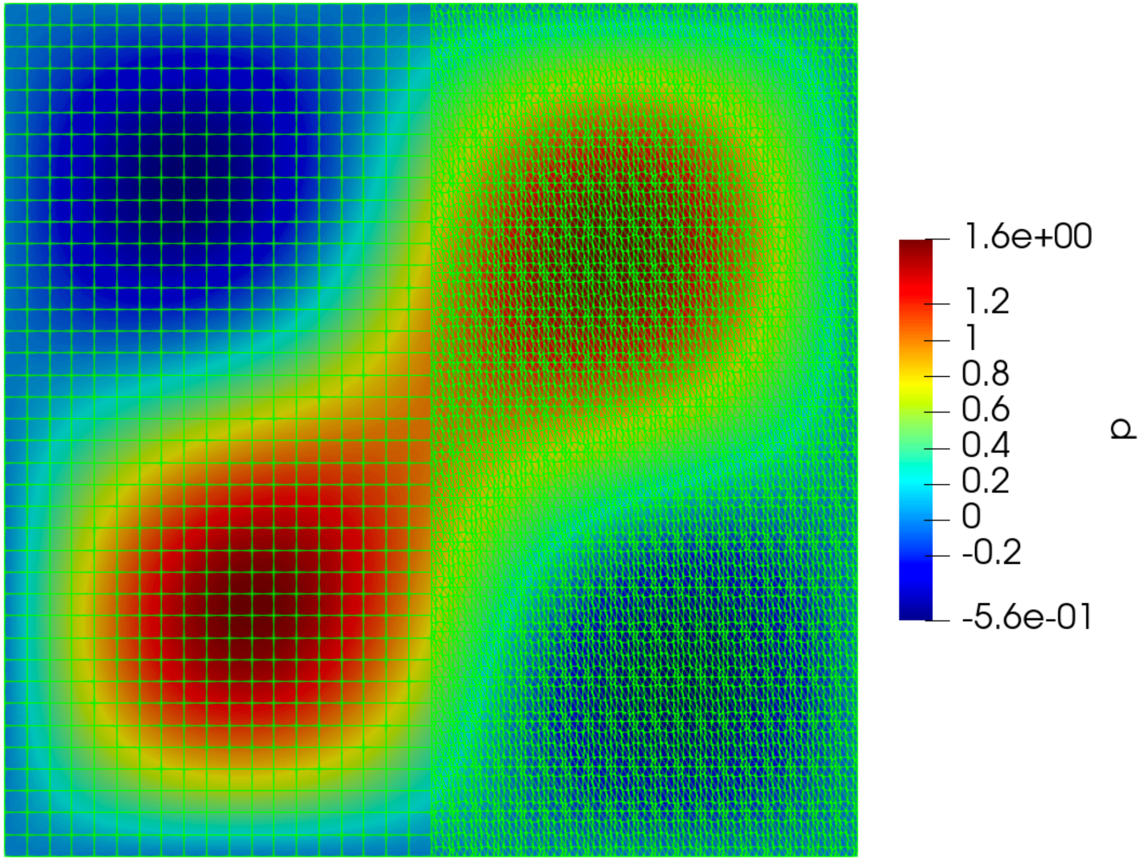
- Starting point: remove more complicated boundary treatment from setup, construct interior-only periodic projection operators
  - Be able to write down *time-continuous* proof of stability (via energy) - this may result in a different operator condition than K+W’s compatibility, and may require a more 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)

The Plan (cont’d)

- Prove the efficacy of these projection operators in 2D
  - Demonstrate code that solves set of constraint equations for set of unknowns to produce projection operators (and provide as electronic supplement)
  - Practically demonstrate order of accuracy of projection across interface using L2 error
  - Numerically demonstrate non-increasing energy on demonstrative problem, and compare numerically observed energy rate-of-change to that derived by the energy stability proof
- Apply lessons learned to boundary treatment

The Plan (cont'd)

- **Application:** 2D acoustic wave equation on split domain



Risk Mitigation

- Important question: **what if this doesn’t work out?**
  - Can try to establish more concretely why Kozdon and Wilcox’s underdetermined result is truly the best one for our purposes while highlighting suspect error behavior at boundary
  - Can attempt to extend this method to 3D (not done in their paper/unclear what challenges this could potentially pose)
  - Can also determine whether there is a timestep limitation imposed by Kozdon and Wilcox’s method, and – if so – attempt to expose the coupling to multi-rate for performance improvement
- Is this ”fallback” outcome interesting enough?
  - If not, what is left?

Current Status

- Python-based testing setup created which implements split-domain 2D acoustic wave problem described on the previous slide
  - SBP-side boundary fluxes incorporated into DG software package
  - Energy stability verified with Kozdon and Wilcox's operators via comparison of numerically observed energy rate-of-change and that used in their energy stability proof
- 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)
  - Needed: experimentation with alternatives to compatibility condition – how to find out whether any other suitable operator conditions exist?

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.

Changelog (v1 – v2)

- **Time Integration of Reacting Flows:**
  - Removes initial (useless) outline slide
  - Made significant attempt to clarify/explain governing equations and notation (Topic/Problem)
  - Poses usage of multi-rate to improve performance as a question rather than a given (Topic/Problem)
  - Expands “Goals and Bounds” into two slides in order to include more detail on these goals, in particular the initial must-have (stating the current candidate problem) and expounding upon adaptivity choices and potential success metrics
  - Expands the first plan slide into multiple slides, both in an attempt to flesh out the mathematical model behind the error control scheme, and to further elaborate on adaptivity choices as worth exploring
  - Removes software tool discussion from the Plan (instead adding this in brief to the impact slide, as directed), and further fleshes out the usefulness/appropriateness of the reacting mixing layer as a demonstrative problem
  - Adds an Impact slide (software + broader impact)
  - Adds a Risk Mitigation slide (“what if this doesn’t work out?”)
  - Expands Current Status slide into two slides, largely in an effort to increase frankness

Changelog (v1 – v2) (cont'd)

- **Energy-Stable Hybrid Spatial Discretizations:**
  - Adds to the Topic/Problem slides to hash out why the problem is interesting based on existing work, and what the primary research question is, as well as a neat picture
  - Adds broader impact as well as draft theorem to prove to final Topic/Problem slide
  - Elaborate in Goals and Bounds on what exactly unisolvency is/what our ideal projection operator would look like
  - Removed any mention of software, as my software impact on this side of things will likely prove minimal
  - Elaborate in the Plan section on what "efficacy" of projection operators implies
  - Adds Risk Mitigation slide similar to Time Integration section
  - Adds to Current Status slide to better document where we left off with the 2D acoustic wave simulation