Time Integration of Reacting Flows and Energy-Stable Hybrid Spatial Discretizations

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Contents

1 Time Integration of Reacting Flows

1.1 Motivation & Background

1.1.1 Historical Context

Brief literature review on the time integration, specifically pertaining to both multi-rate integration and the state of time integration of reacting flows, the latter of which is likely to make specific mention of CVODE.

1.1.2 Goals, Bounds, and Impact

Primary goal: create a novel time integration scheme that makes use of the benefits of multi-rate integration while also handling the stiffness imposed by chemical kinetics in reacting flows, either via implicit integration or adaptivity (or both), exploring the design choices therein while verifying that this goal is met via comparison to CVODE as a state-of-the-art alternative.

Impact: augmentation of reacting flow simulation capability in terms of both accuracy and performance, allowing for improvement in modeling real-world applications for combustion (subsonic/supersonic propulsion via scramjets/ramjets, furnaces/heating, and atmospheric sciences).

1.2 Governing Equations

This subsection will describe in detail the Navier-Stokes equations with chemical reactions, discussing in detail how the chemical kinetics are incorporated via mixture-averaged mass diffusion, constant internal energy assumptions, and NASA9 thermodynamic polynomials.

1.3 Numerical Methods

1.3.1 Adams Methods

Discussing both explicit and implicit Adams methods, and how they are derived within Leap (similar to the JCP).

1.3.2 Multi-rate Adams Methods

Discussing how the Adams methods are extended into a multi-rate integration framework (similar to the JCP).

1.3.3 Timestep Control Algorithm

Discussing the timestep control algorithm, its formulation, and its potential weaknesses.

1.4 Verification

Discussing the test problems that will be used to verify our approach and show its efficacy, including the demonstrative reacting mixing layer problem as well as the Cantera two-reactor setup and the one-dimensional laminar free flame example, while also making specific mention of metrics by which we will gauge the success of the new time integration method(s).

1.5 Results

This subsection will focus on the results obtained thus far, including recreation of the mixing layer problem as described by Blumen and Michalke, and verification of the Leap-generated IMEX-RK scheme using PyJac via flame speed comparison in the free flame example.

1.6 Outlook

1.6.1 Current Status

This section will include a discussion of the current state of the project, including the fact that PyJac and Leap have been integrated into the fluid solver and are driving the free flame example, as well as discussion of the current state of the mixing layer problem construction (initial mode/growth rate verification with air), and the status of the multi-rate adaptive and explicit methods.

1.6.2 Risk Mitigation

This section will discuss the possibility of demonstrating improvement over CVODE in terms of accuracy using the existing IMEX-RK scheme with more accurate chemical Jacobians (and lack of a first-order splitting approach) as a "fallback" goal.

2 Energy-Stable Hybrid Spatial Discretizations

2.1 Motivation & Background

2.1.1 Historical Context

Brief literature review on the state of hybrid discretizations, and what existing formulations lack/possess.

2.1.2 Goals, Bounds, and Impact

Primary goal: create an interface for a hybrid SBP-DG discretization that is provably energy stable, meaning that the semi-discrete expression for the rate of change of total energy (energy across all subblocks) can be proven to be non-increasing. Initially, this will focus on/target the less complex interior stencils, with the hope of extending the lessons learned to the boundaries (is it fair to call the latter a "soft bound?").

Impact: provide a stable and accurate way to mesh complex geometries by allowing for the simplicity of finite differences away from physical boundaries, with the flexibility of DG near said boundaries.

2.2 Governing Equations

This subsection will lay out the target problem for the novel hybrid discretization, which for now is the acoustic wave equation in two dimensions.

2.3 Numerical Methods

This subsection will lay out the basics of the finite difference method (summation by parts), the basics of the DG method, and further discuss the approach for the interface, all in subsections.

2.3.1 Summation-by-Parts Operators

2.3.2 Discontinuous Galerkin Method

2.3.3 Interface Method

2.4 Validation

This section lays out the test problem we will use to determine whether or not our new method meets the goals laid out in the previous section(s), and also defines the success metrics we will use to measure this (namely, energy tracking - both to ensure that our semi-discrete energy relation is accurate to the actual numerical method at work, and to ensure that energy is non-increasing).

2.5 Results

This section will discuss the results obtained thus far, including the verification that Kozdon and Wilcox's projection operators (our starting point) do give an energy value that matches the semi-discrete relation used for the proof, and a demonstration showing the subpar nature of these operators as an ending point (this likely will be specific to the poor boundary behavior).

2.6 Outlook

2.6.1 Risk Mitigation

This section will discuss the potential fallback of extension of an existing interface method (Kozdon and Wilcox) to three dimensions, should our goal of a new interface method not come to fruition. Another fallback goal could involve determining whether this existing interface method imposes a timestep limitation and exposing this to multi-rate integration.

2.6.2 Current Status

This section will discuss the current status of the project, including the hunt for a unisolvent projection operator.