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

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Contents

1 Time Integration of Reacting Flows

1.1 The Topic/Problem

The problem at hand involves the simulation of chemically reacting flows, the governing equations of which amount to the Navier-Stokes equations with (in our form):

- A source term added to the energy equation in the form of heat flux

- The addition of a governing equation for the rate of change of the mass fractions of each species in the chemical mechanism simulated

- The addition of governing equations specifying the rate of change of temperature and pressure, derived from a constant internal energy assumption (for the former) and the ideal gas law (for the latter).

These equations are given below, along with a brief explanation of the notation/nomenclature used.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j + P\delta_{ij} - \tau_{ij}) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}((\rho E + P)u_j + q_j - u_i\tau_{ij}) = 0 \tag{3}$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k u_j - \varphi_{ki}) = W_k\dot{\omega}_k \tag{4}$$

$$\frac{\partial T}{\partial t} + \frac{\sum_{k=1}^{N_{sp}} U_k(T)\frac{\partial \rho Y_k}{\partial t}\frac{1}{W_k}}{\sum_{k=1}^{N_{sp}} [C]_k C_{v,k}(T)} = 0 \tag{5}$$

$$\frac{\partial P}{\partial t} - \frac{R}{V}(T\frac{\partial n}{\partial t} + \frac{\partial T}{\partial t}n) = 0 \tag{6}$$

In these equations, ρ is the fluid density, u_i is the velocity in the i-th direction, and E is the total energy. δ_{ij} is the Kronecker delta, P is the pressure, T is the temperature, and Y_k is the mass fraction of species k. $[C]_k$ is the concentration of species k in the gas mixture, $C_{v,k}(T)$ is the specific heat at constant volume of species k at temperature T, and $U_k(T)$ is the internal energy of species k at temperature T. N_{sp} is the number of species in the chemical mechanism, W_k is the molecular weight of species k, n is the number of moles of the gas mixture, V is the volume of the gas, and $\dot{\omega}_k$ is the net production rate of species k. τ_{ij} is the viscous stress tensor, φ_{ki} are the diffusion fluxes, and q_j are the heat fluxes, defined by

$$q_j = -\frac{\partial(\lambda T)}{\partial x_j} + h_k\varphi_{kj}. \tag{7}$$

In this expression, λ is the thermal conductivity, and h_k is the enthalpy of species k. As for the diffusion fluxes, these are defined using a mixture-averaged approach - that is, φ_{ki}

is given by

$$\varphi_{ki} = \varphi_{ki}^* + \varphi_{ki}^c, \tag{8}$$

where φ_{ki}^* is the mixture-averaged approximation, and φ_{ki}^c is a correction term to ensure mass conservation. The mixture-averaged approximation is defined by

$$\varphi_{ki}^* = -\rho D_{k,m} \frac{W_k}{W} \frac{\partial X_k}{\partial x_i} \tag{9}$$

where $D_{k,m}$ is the mixture-averaged diffusivity of species k, W is the mean molecular weight, and X_k is the mole fraction of species k. Finally, the correction term is given by

$$\varphi_{ki}^c = -Y_k \sum_{n=1}^{N_{sp}} \varphi_{ni}^* \tag{10}$$

In this set of governing equations (1) - (6), the mass fraction source term on the right side of equation (4) is typically observed to be stiff relative to the surrounding equations governing the motion of the gas mixture and the change in its physical properties. This presents a time integration problem in that this term alone typically dictates either an oppressively low timestep or the need for an implicit approach, often using tools such as CVODE. In practice, fluid solvers also often decouple an explicit treatment of the Navier-Stokes equations (1) - (3) from the implicit treatment of the chemical kinetics, resulting in a splitting approach that is at best first order in time.

The topic of this section of the proposal, then, is to answer the following research question: **can we derive performance and/or temporal accuracy benefits from an application of multi-rate Adams integrators to this set of governing equations?**

1.2 Goals and Bounds

For outlining purposes, we will parse this section into a set of "must-haves", "nice-to-haves", and aspects of the problem described above that are deemed beyond the bounds of an eventual PhD thesis.

Must-Haves

The most obvious must-have is a demonstration of a novel time integration scheme driving a canonical or especially demonstrative reacting flow problem (ideally one that points directly to real-world impact) with improved efficacy identified by either superior accuracy/stability or faster performance. Also critical in this effort will be maintaining a solution that lies on the ideal gas constraint manifold (i.e. a physical solution) - this has been identified in early work as a potential sticking point when fully differential approaches to solving the governing equations (as opposed to differential-algebraic approaches that directly satisfy the constraints) are used. While the currently working method of solving the equations uses

a chemical kinetic Jacobian modified to include the algebraic constraints explicitly, fully differential approaches that use attenuation to force the solution towards the constraint manifold may also be employed to greater effect.

Nice-to-Haves

Perhaps most prominent among the nice-to-haves is a thorough investigation of the design space presented by the multi-rate framework we will use for time integration (see *The Plan*). The design choices inherent to this scheme include:

- Evaluation order ("fastest-first" vs. "slowest-first")

- Re-extrapolation

- Inclusion of additional history beyond order requirements (shown in [?] to provide real-axis stability improvement)

- Which solution components to include in error estimation for adaptive timestep control

- Whether error control is accomplished through timestep control or step ratio control

Another nice-to-have would amount to comparison of our scheme with CVODE as a proxy for the state of the art in time integration of chemically reacting flows, ideally achieving superiority in terms of observed temporal accuracy of the entire system, or in terms of performance (most accurately measurable by a reduction in the number of chemistry right-hand-side evaluations required to reach a given solution time).

Beyond Our Bounds

An aspect of the algorithms being implemented that has been identified early as beyond our bounds is the presence of multi-variable solves in a number of potential adaptive implicit integration scenarios, namely:

- Coupled implicit right-hand-sides

- Use of adaptive timestep controllers where the local error estimate of all solution components makes use of implicit and explicit state estimates.

1.3 The Plan

Numerics

The general path forward is to implement multi-rate Adams integrators (demonstrated in [?] as being a viable vehicle for performance improvement) with the added ability to not only integrate the chemistry right-hand side implicitly, but also to adapt the timestep of the resulting multi-rate integrator based on relative and/or absolute local error demands. This latter capability would serve to match a similar capability provided by CVODE while

also maintaining the coupling between the fluid and the chemistry (as well as the timestep flexibility) provided by the multi-rate framework.

In its current form, the timestep control algorithm used is that of ODE45, wherein a timestep multiplier r is calculated based on a local error estimate constructed from state estimates of two (differing) explicit orders:

$$r = \frac{\|s_{q+1} - s_q\|_2}{\text{ATOL} + \text{RTOL} \cdot \max(\|s_q\|_2, \|s_{q+1}\|_2)} \tag{11}$$

Here, s_q is the state estimate obtained using an order-q scheme, and ATOL and RTOL are absolute and relative error tolerances specified by the user. Once r is calculated, the timestep is *decreased* if $r >= 1$ via

$$\Delta t = 0.9 \Delta t (r)^{-1/q} \tag{12}$$

and *increased* if $r < 1$ via

$$\Delta t = 0.9 \Delta t (r)^{-1/(q+1)} \tag{13}$$

As mentioned in the previous section of this outline, this added capability alone presents a number of questions in terms of how best to accomplish this error control. In particular, step ratio adjustment in situ, rather than timestep adjustment, to meet error needs provides an implementation challenge in terms of code generation of these integrators, whereas the choice of which solution component(s) are involved in error estimation/timestep control also presents a design decision that could have notable effect on numerical performance.

Test Problem: Reacting Crossflow

With the plan for the numerical methods to be implemented in place, the dominant planning question then becomes: what is the test problem to which these new methods will be applied to establish their viability? The current plan is to use a reacting mixing layer problem with a hyperbolic tangent velocity profile for the baseflow (as used by [?] and [?]), with the San-Diego 9-species chemical mechanism employed for the chemical kinetics. By perturbing this baseflow with the mode having the highest growth rate to instability (based on the inviscid analyses of [?] and [?]), we can establish a fast-evolving solution component (the chemical kinetics/mass fractions of the species) and a slow-evolving solution component (the fluid), both possessing accessible means of rate modification (for the chemistry, we can accomplish this by scaling the pre-exponential factors in the Arrhenius reaction rates, and for the fluid, we can scale the magnitude of the initial crossflow).

In doing so, what should result is a problem with ample testbed capabilities for our new multi-rate integrators, and also a problem firmly rooted in physical utility in that it provides the simplest model for scramjet/ramjet combustion.
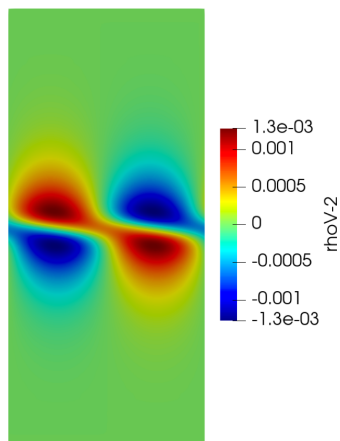
Figure 1: Perturbed vertical momentum of the hyperbolic tangent example - multispecies cold flow.

1.4 Impact

The proposed thesis has the potential to have a significant impact on the simulation of reacting flows, of which there are countless real-world applications including (but not limited to) subsonic and supersonic combustion for propulsion (gas turbines, ramjets/scramjets, rockets), furnaces and residential heating, and solution of problems relating to atmospheric sciences.

The proposed work would also serve to augment the capabilities of Leap and Dagrt, two Python packages for code generation of time integrators, by implementing the proposed integrators. While this work would focus the attention of those new integrators on reacting flows, additional useful application of implicit-explicit multi-rate with error-based step control amongst the software's user base is possible, if not probable.

Finally, the proposed work would also formally introduce new capabilities to another existing combustion software package, PyJac-V2. This software is responsible for code generation of callable source term and Jacobian functions for chemical kinetics, and our work (given its application to problems that often have large temperature ranges, not to mention a focus on high accuracy) would add a NASA9 polynomial representation of thermodynamic quantities to its codebase.

1.5 Risk Mitigation

An important question to ask amidst all of these promises is: textbfwhat if this doesn't work out? Assuming demonstration of improved performance or accuracy of the *multi-rate* integrators over the state-of-the-art is for reasons unforseen impossible, a "fallback" takeaway would be demonstration of improvement over the CVODE-fluid first-order splitting approach via Leap implementation of an existing IMEX Runge-Kutta based scheme that treats the chemistry implicitly via code-generated analytical Jacobians. Given the use of a coupled implicit-explicit scheme (for which high order has already been proven in other

circumstances), as well as a chemical Jacobian that is more accurately obtained than via finite differences (the method of CVODE), this outcome should be attainable at minimum.

1.6 Current Status

At present, implicit-explicit time integration of reacting flows using Runge-Kutta based methods in conjunction with code generation of source terms and Jacobians for the chemical mechanisms is implemented and undergoing testing with the fluid solver application. Implicit Adams methods (with single-rate Adams-Moulton being the baseline) for the purposes of chemistry integration are also being implemented, along with an application of the error-informed timestep control algorithm to both single-rate and multi-rate Adams methods. Construction of implicit-explicit multi-rate Adams methods with error-informed adaptivity are well underway, with testing of these new methods on small-scale Cantera reactor system problems in progress.

As for the reacting crossflow validation problem, an initial setup employing cold flow (no autoignition) with the perturbed baseflow applied to a nine-species (San Diego) gas mixture is complete, with validation via the growth rate of the unstable mode ongoing. Also implemented in the reacting flow solver is a one-dimensional laminar free flame problem, which may also be used as a first-pass validation (via comparison to the Cantera-estimated steady-state flame speed) for new integration methods for reacting flows as they become available.

2 Energy-Stable Hybrid Spatial Discretizations

2.1 The Topic/Problem

This section of the proposal targets a lack of high-order accurate and provably stable interface conditions between structured and unstructured meshes for computational fluid dynamic simulations. In particular, our aim is to create a provably stable and accurate interface between summation-by-parts finite difference discretizations (structured) and discontinuous Galerkin methods (unstructured). Achieving this would provide an option to create localized areas of unstructured meshing (with superior flexibility for discretizing complex boundaries/geometries) in existing simulations, providing an alternative to overset curvilinear meshes.

2.2 Goals and Bounds

(insert text here)
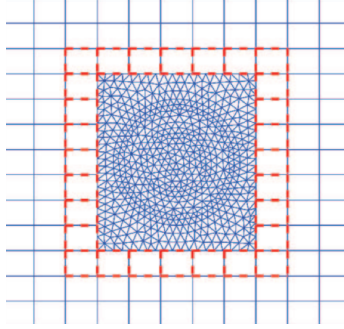
2.3 The Plan

(Insert text here)

Figure 2: An example of a discretization for which we hope to achieve a stable and accurate nonconforming interface. Image credit: *A Hybrid FETD-FDTD Method with Nonconforming Meshes*, B. Zhu, J. Chen, W. Zhong, Q. Liu. Commun. Computational Physics, Vol. 9, No. 3, pp. 828-842. March 2011.

2.4 Impact

(Insert text here)

2.5 Risk Mitigation

(Insert text here)

2.6 Current Status

(Insert text here)