Mokbel Karam

Research Statement

My Research Approach

Every day, new and sophisticated technologies are getting developed in different fields where the cost of experimenting on models is shooting up. Therefore, the need for faster and yet cheap simulation tools is pressing more than ever.

My research focuses on increasing the efficiency of numerical techniques for simulating reacting flows using the supercomputers. I am focused on producing and developing methods that help to reduce the the computational cost involved in these simulations. To achieve this goal, I am looking into two different disciplines: Numerical integration, and Machine learning. In the former, I am looking to modify existing techniques for solving the full equations at a lower cost by making use of previously stored data. With the letter, I am trying to design a machine learning model that could assist existing solvers. Generally speaking, my approaches to reducing cost is to look into existing techniques and find places for improvements.

Besides, I would like to highlight my interest in using modified equation analysis for looking into the behavior of numerical methods. For example, In some instances, the numerical solution could differ from the expected answer even though the implemented technique was correct which raises the question of what is the source of the problem. Also, I am interested in reverse engineering a problem and attempt to solve it from a machine learning perspective.

Background

After I earned a Mechanical engineering degree from Notre Dame University-Lebanon, I applied for the chemical engineering department at the University of Utah to continue my Ph.D. in computational physics and simulation sciences. During my undergraduate studies, I had the opportunity to develop my skills in using software to solve fluid and heat transfer problems numerically. For example, I used Matlab to create an hourly analysis program for computing the cooling load for one single room with different architectures. My passion for programming made my decision easy on what I want to focus on in my doctorate. During my first year as a graduate student at the University of Utah, I developed my skills in numerical methods especially time integration and modified equation analysis. Also, during the summer of the same year, I spend ten weeks at Lawrence Livermore National Laboratory under PSAAP II (Predictive Science Academic Alliance Program) working on Blastwave propagation using Machine Learning.

Papers and Work in progress

My first conference paper "An Explicit Variable-Density Projection Method for Low-Mach Reacting, Flows on Structured Uniform Grids" joint Tony Saad (first author), and James Sutherland, presents a method for solving Low-Mach flows without using the inefficient full gas dynamics equations.

Low-Mach flow lies in a category of flows where acoustic waves have a negligible effect on the thermodynamics of the stream. For example, if we consider a candle in a room with people talking near the flame, the density in the neighborhood of the flame doesn't depend on the pressure variation induced by the sound wave produced by people (e.g. acoustics). The inefficiency in solving the full gas dynamics equations is due to the small marching time step dictated by the acoustics. Here comes the newly developed method that aims at eliminating these acoustic timescales and allowing one to march in time at the much more attainable convective timescales. This new method was tested and formally verified against analytical and manufactured solutions of variable density flows with mixing and reactions. Also, I presented this work at the American Institute of Aeronautics and Astronautics conference in June 2018.

My first technical note in the Journal of Computational Physics (under review) "A Short Note on Deriving Modified Equations" joint Tony Saad, and James Sutherland aims at describing an alternative scheme for deriving the modified equation. The modified equation represents the actual physical processes that a computational method describes when it approximates a set of model equations. We use this type of analysis to study the effect of truncation errors induced by the numerical discretization scheme. These truncation errors could cause instability or unexpected behavior of the numerical solution. Based on previously reported work in the literature that has gone unnoticed we represent the method with clean notation, and we extend it to multiple dimensions. Additionally, we point out the existence of cross-derivative terms in the modified equation that can lead to an anisotropic behavior for diffusion and advection. In the end, we included a simple Python script that will illustrate how to use this method in practice. We will present this work at the American Institute of Aeronautics and Astronautics conference in June 2019.

In my second conference paper "A Framework for Analyzing the Temporal Accuracy of Pressure Projection Methods" joint Tony Saad, James Sutherland, and Michael Hansen we present a new framework for analyzing the temporal order of accuracy of pressure projection methods for incompressible flows. As a part of the algorithm for solving the equations of fluid dynamics (i.e. Navier-Stokes equations), pressure projection is used to decouple the velocity from the pressure and result in a Poisson equation that necessitates the use of a linear solver. From a parallel computing perspective, the use of a linear solve will increase the communication relative to the computation costs and reduce scalability. As a solution, we can use higher order time integrators such as Runge Kutta schemes to increase the arithmetic intensity (ratio of computation to data transfer). However, this requires the usage of a linear solver at every stage of the time integrator which defeats the intended purpose. The proposed framework in this paper will enable us to rationally reduce the number of Poisson solves while maintaining the formal temporal order of accuracy. For example, one linear solve is needed for second and third order Runge Kutta schemes which result in savings up to 50% in the global cost of one time-step. We will present part of this work at the SIAM Conference on Computational Science and Engineering in February 2019, and at the American Institute of Aeronautics and Astronautics conference in June 2019.

For ten weeks in the summer 2018, I did an internship at Lawrence Livermore National Laboratory (LLNL) under PSAAP II. The goal of this internship was to learn more about Machine Learning (ML) and how to apply it to a specific scientific problem. During these ten weeks, I worked on an assignment project where I had to use machine learning on the Sedov-von Neumann-Taylor Blastwave, under the supervision of Dr. Fady Najjar and Dr. Jiang Ming. The objective of our research was to develop a machine learning model able to predict the value of the initial energy and the time of the energy release given the value of the wave speed and maximum pressure at a certain distance from the source. I gave a seminar about this work at Lawrence Livermore National Laboratory, and at the Rocky Mountain Fluid Mechanics (RMFM) Research Symposium, CU Boulder. Also, we are going to present this work at the SIAM Conference on Computational Science and Engineering in February 2019.

Future Work

In the years to come, I plan to continue to work on the existing research projects I started in my first year and try to extend the analysis to more general cases.

• I aim to advance the study of the Low-Mach reacting flow to cover higher order time integrators such as Runge Kutta schemes.

• I aim to extend the scope of the "Framework for Analyzing the Temporal Accuracy of Pressure Projection Methods" that we developed to cover variable density cases.

• I aim to continue working on a project that we have started this year in the goal of using Machine Learning models to help to reduce the cost associated with existing linear solves for fluid flow problem.