Research Statement
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My research focuses on numerical methods for ODEs and PDEs. I developed novel constructions of Integral Deferred Correction (IDC) algorithms for problems with stiff and nonstiff terms in both ODE and PDE settings. IDC methods are motivated by defect correction methods [19, 11] and, more recently, Spectral Deferred Correction (SDC) methods [9]. By construction, they are accurate and efficient time integrators because they easily extend simple lower order methods to higher order schemes by correcting provisional solutions. Other related methods for problems containing stiff terms include semi-implicit SDC, multi-implicit SDC, and Krylov deferred correction [15, 14, 2, 12]. SDC methods, IDC methods, and their variants can be applied in areas such as chemical rate equations, hyperbolic conservation laws with or without relaxation, Vlasov equations in the plasma physics setting, and other similar (frequently multi-scale) problems [15, 14, 2, 12, 6, 4]. Additionally, recent developments allow parallelization of IDC algorithms, opening up new possibilities for increased computational speed [5]. I also investigated a dimensional splitting semi-Lagrangian method for PDEs that uses IDC for the time steps and WENO reconstruction in space [4].

With this background, I plan to investigate simulation and mathematical modeling of fuel cell systems. Although the basic premise of a fuel cell is quite simple (an electrical current is produced while hydrogen and oxygen ions meet through an electrolyte and combine to form water), the variety of materials and shapes of fuel cells, as well as the total system of preparing the fuel, managing the waste, and harnessing the resulting power, can be mathematically complicated [10, 17, 16]. Numerical methods for PDEs are essential in understanding complex systems such as these that are multiscale in both size and time.

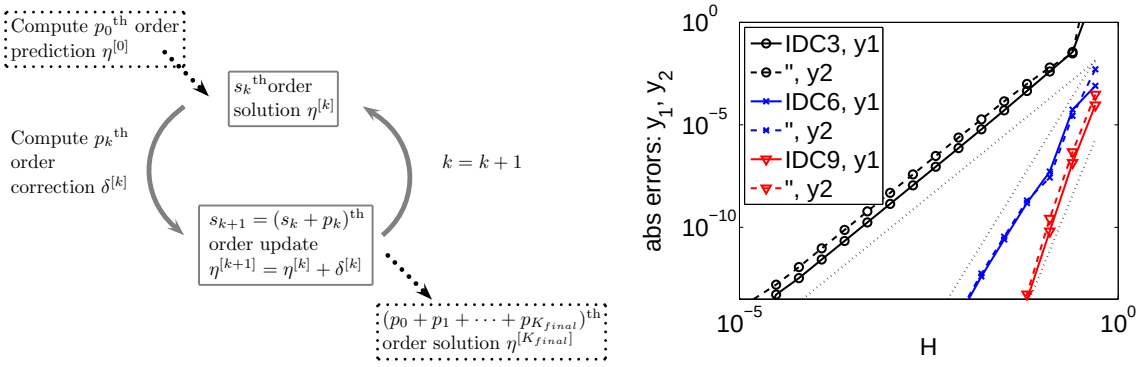
Semi-implicit integral deferred correction methods

Consider a method of lines semi-discretization of the PDE

$$\begin{aligned} U_t &= f(t,U,U_x,\dots) + g(t,U,U_x,\dots) \\ &\qquad \text{method} \downarrow \text{of lines} \\ u_t &= F(t,u) + G(t,u), \end{aligned} \tag{1}$$

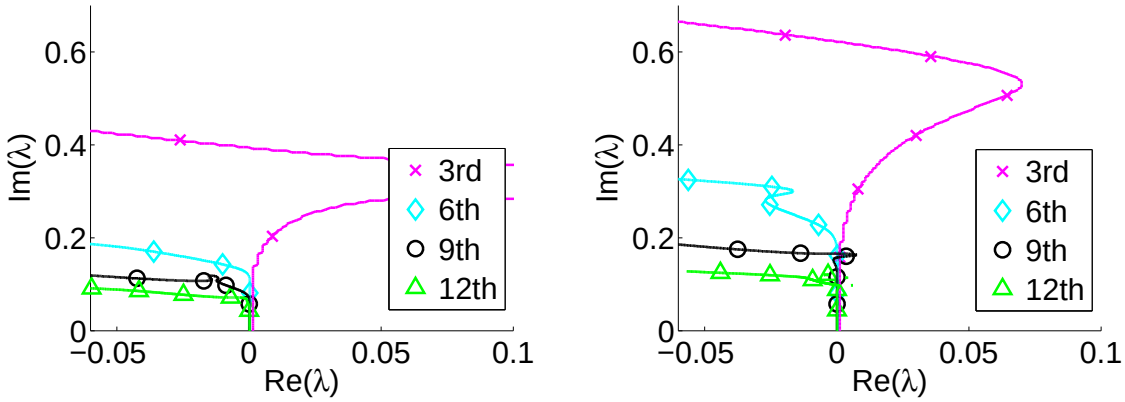
where F contains all the stiff terms and G contains only nonstiff terms. IDC methods compute a provisional solution (prediction), $\eta^{[0]}$, and correction iterations for (1) using a simple integrator to find an improved, higher order accurate numerical solution with each iteration (Figure 1a). If $F = 0$, explicit $p_k{}^{\text{th}}$ Runge-Kutta (RK) integrators may be used to compute the prediction and correction iterations so that these IDC-RK methods have order of accuracy $\mathcal{O}(\Delta t^{\sum_{k=0}^{K_{final}} p_k})$ [7]. I have extended the explicit IDC-RK construction and theoretical results to that of new arbitrary order semi-implicit IDC methods constructed with additive Runge-Kutta (ARK) integrators (IDC-ARK methods) and implemented supporting numerical examples [6]. For (1), within each IDC iteration, the semi-implicit ARK integrators use implicit and explicit RK methods applied to F and G, respectively. Order of accuracy results are similar to IDC-RK results (Figures 1a, 1b). Additionally, I have demonstrated that some IDC-ARK methods have larger stability regions than IDC methods constructed with backward and forward Euler integrators (IDC-FBE), and hence larger than the semi-implicit SDC methods in [15], which have similar stability regions to IDC-FBE methods (Figures 2a, 2b). To obtain very small errors, IDC-ARK methods at higher order are more efficient (require fewer function evaluations) than popular ARK methods and are constructed to higher order much more easily [6, 13]. I have applied IDC-ARK to a linear advection-diffusion equation,

$$u_t = -u_x + u_{xx},$$



(A) $k = 1, 2, \ldots, K_{final}$ (B) VdP, $\epsilon = 1$ (nonstiff), [6]

FIGURE 1. IDC algorithm (1a) and numerical convergence study (1b) [6] of absolute error at $T = 4$ vs timestep H, for 3rd, 6th, and 9th order IDC constructed using 3rd order ARK3KC with 0, 1, and 2 correction loops, resp. The order of accuracy is clear, as dotted reference lines (with slopes of 3, 6, 9) indicate.



(A) IDC-FBE, [6], compare to [15] (B) IDC-ARK3KC, [6]

FIGURE 2. Stability regions for 3rd, 6th, 9th, and 12th order IDC constructed using (2a) forward and backward Euler with 2, 5, 8, and 11 correction loops, resp., and (2b) 3rd order ARK3KC with 0, 1, 2, and 3 correction loops, resp. The stability regions are scaled by the number of implicit function evaluations.

where the stiff diffusion term is treated implicitly and the nonstiff term explicitly. The effective CFL was improved from $\mathcal{O}(\Delta x^2)$ to $\mathcal{O}(\Delta x)$.

IDC with Strang split hyperbolic solvers

In [8], conservative semi-Lagrangian WENO methods with dimensional Strang splitting are applied to the Vlasov–Poisson equations,

$$f_t + v \cdot \nabla_x f + E(t,x) \cdot \nabla_v f = 0,$$
$$E(t,x) = -\nabla_x \phi, \quad -\Delta_x \phi = \rho(t,x),$$

where $f(t,x,v)$ describes the probability of finding a particle with velocity v at position x at time t, E is the electric field, ϕ is the self-consistent electrostatic potential, and $\rho(t,x) = \int f(t,x,v)dv - 1$ is the

charge density. Here the CFL time step restriction is removed, and the higher order spatial methods have more effectively captured the physics which the Vlasov equations describe; e.g., for a two stream instability problem, the ninth order WENO clearly resolves the solution, while it is less clear for third order WENO. If resolved equally, the ninth order method is four times cheaper than the third order method [8]. While the spatial error is quite high order accurate, the error in time is limited to second order accuracy. Therefore I expanded their semi-Lagrangian Vlasov solver to the IDC framework [4]. I used IDC methods combined with WENO reconstruction to generate higher order solutions of Vlasov–Poisson equations. This novel method was applied to classic plasma problems, such as two stream instability and Landau damping. Both first order and second order temporal accuracy increases occurred at each IDC correction step using first order dimensional splitting and second order Strang splitting, respectively, and therefore the temporal error is significantly reduced. Conservation of mass is also proved. Unfortunately, although the semi-Lagrangian solver is not only higher order in space but also higher order in time, the correction steps of IDC introduce some CFL restrictions. The principles for split IDC methods [4] can be extended from the Vlasov–Poisson operators to other operators suitable for splitting methods, such as the Vlasov–Maxwell, BGK–Poisson, or BGK–Maxwell equations. Further applications are possible in solving split Schrödinger–Poisson equations, and IDC methods may also be applied in conjunction with nonsplit characteristic methods for Vlasov equations.

Fuel cell simulation and modeling

A fuel cell directly converts chemical energy from a fuel to electrical energy. The basic idea is that an electrical current is produced while hydrogen and oxygen ions meet through an electrolyte and combine to form water. Although this process is quite simple, the variety of materials and shapes of fuel cells, as well as the total system of preparing the fuel, managing the waste, and harnessing and distributing the resulting power, can be mathematically complicated [10, 17]. Multiple scales in both time and space occur in fuel cells, which results in stiff systems that present computational challenges. Many existing mathematical investigations of fuel cells focus on the structure of the fuel cell itself, effectiveness of certain materials, or water management, but for my future research, I am interested in modeling and computation for the process of harnessing the waste heat from a fuel cell to increase the efficiency of the system or a cycle of fuel cells whose byproducts can fuel another cell [17, 20, 3, 1, 18]. In particular, I plan to study numerical modeling for the fluid dynamics of such systems, which obey conservation laws [16]. Numerical methods for ODEs and PDEs are essential in understanding complex systems such as these.

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