TIM 2023 Los Alamos Workshop on Time Integration for Multiphysics

August 8–August 11, 2023

Los Alamos, New Mexico

Los Alamos NATIONAL LABORATORY

The electronic version of this booklet can be found at:
`https://cnls.lanl.gov/tim2023/conference_program.pdf`

The open-source LaTeX template, AMCOS_booklet, used to generate this booklet is available at `https://github.com/maximelucas/AMCOS_booklet`

Contents

About

Los Alamos Workshop on Time Integration for Multiphysics

The "Los Alamos Workshop on Time Integration for Multiphysics" (T$\bar{\text{I}}$M2023) is a workshop hosted in Los Alamos, NM dedicated to time integration methods applied to multiphysics applications. The aim of this workshop is to bring researchers together to discuss current, state-of-the-art time integration techniques for numerical PDEs with applications in plasma physics, inertial confinement fusion, atmospheric/climate science, material science, high-explosives, and radiation-hydrodynamics. Invited presenters will deliver one-hour talks over the span of three days, followed by a collaboration day for discussions. A poster session will be held August 9 at Fuller Lodge.

The T$\bar{\text{I}}$M 2023 workshop is organized by researchers at Los Alamos National Laboratory (LANL) and at Texas A&M University (TAMU):

Organizing committee

Vitaliy Gyrya (T-5)
Christopher Newman (T-3)
Ben Southworth (T-5)
Eric Tovar (XCP-2 / CNLS)
Jean-Luc Guermond (TAMU / XCP-2)

Executive committee

Markus Berndt (HPC-DO)
Jimmy Fung (XCP-DO)
Marianne Francois (T-DO)

Timetable

IS: Invited Speaker, LT: LANL Talk

Tuesday, August 8; SALA Event Center

8:30–9:00	**Registration + Breakfast**		
9:00–9:15	**Welcome remarks**		
9:15–10:15	IS	**Adrian Sandu** Virgina Tech University	Multirate time integration: an overview
10:15–11:15	IS	**Dan Reynolds** Southern Methodist University	Implicit-Explicit Multirate Time Integration Methods
11:15–11:30	**Break**		
11:30–12:15	LT	**Luis Chacon** LANL	Challenges in multiphysics non-equilibrium simulations of Inertial Confinement Fusion experiments
12:15–1:30	**Lunch**		
1:30–2:30	IS	**Tommaso Buvoli** Tulane University	Runge-Kutta Methods for Nonlinearly Partitioned Systems, and Polynomial-Based Time Integrators
2:30–3:30	IS	**Zdzislaw Jackiewicz** Arizona State University	Strong Stability Preserving General Linear Methods
3:30–3:45	**Break**		
3:45–4:30	LT	**Brian Haines** LANL	Time Integration Challenges when Modeling Inertial Confinement Fusion and High Energy Density Physics Experiments

Wednesday, August 9; Fuller Lodge

8:00–9:00	**Registration + Breakfast + Social hour**		
9:00–10:00	IS	**Jean-Luc Guermond** Texas A&M University	Invariant-Domain preserving IMEX methods for nonlinear conservation equations
10:00–11:00	IS	**Delfim Soares Jr** Federal University of Juiz de Fora	Adaptive time integration procedures for solving PDEs
11-11:15	**Break**		
11:15–12:00	LT	**Ryosuke Park** LANL	Challenges in Thermal Radiative Transfer
12:00–1:00	**Lunch**		
1:00–2:00	IS	**Michael Minion** (Formerly) Lawrence Berkeley National Laboratory	Spectral Deferred Corrections
2:00–3:00	IS	**Chi-Wang Shu** Brown University	Stability of time discretizations for semi-discrete high order schemes for time-dependent PDEs
3:00–3:15	**Break**		
3:15–4:00	LT	**Rob Lowrie** LANL	Anomalous Behavior of Newtonian Hydrodynamics Coupled with Radiation Transport
4:00–5:00	**Poster session**		

Thursday, August 10; Fuller Lodge

8:00–9:00	**Breakfast + Social Hour**		
9:00–10:00	IS	**Steven Roberts** Lawrence Livermore National Laboratory	Overcoming First Order
10:00–11:00	IS	**Mark Carpenter** NASA Langley Research Center	Intrastep, Stage-Value Predictors for Diagonally-Implicit Runge–Kutta Methods
11:00-11:15	**Break**		
11:15–12:00	LT	**Phil Jones** LANL	Challenges in Simulating Future Climate
12:00–1:00	**Lunch**		
1:00–2:00	IS	**Raymond Spiteri** University of Saskatchewan	Fractional-Step Methods: Theory and Practice
2:00–3:00	IS	**Alexander Ostermann** University of Innsbruck	Splitting methods: basics, analysis, modifications, and applications
3:00–3:15	**Break**		
3:15–4:00	LT	**Eduardo Lozano** LANL	Implicit Fast Sweeping Methods for Conservation Laws
4:00–4:15	**Closing remarks**		

Friday, August 11; Oppenheimer Student Center

09:00–3:00	**Collaboration day – open schedule**

List of Abstracts – Talks

Tuesday, August 8

Multirate time integration: an overview

Adrian Sandu

Virginia Tech University

Computer simulations of evolutionary multiscale multiphysics partial differential equations are important in many areas of science and engineering. Algorithms for time integration of these systems face important challenges. Multiscale problems have components evolving at different rates. No single time step can solve all components efficiently (e.g., when an explicit discretization is used, and the spatial discretization uses both fine and coarse mesh patches). Multiphysics problems are driven by multiple simultaneous processes with different dynamic characteristics. No single time discretization method is best suited to solve all processes (e.g., when some are stiff and others non-stiff).

In order to address these challenges, multirate method have been proposed. Multirate schemes apply different time steps to different components of the system. We discuss several general aspects of mutirate methods for the integration for multiscale systems.

Implicit-Explicit Multirate Time Integration Methods

Daniel Reynolds

Southern Methodist University

In recent years computational simulations have rapidly evolved in complexity (high order discretizations, spatial adaptivity, wide arrays of physical processes), placing ever larger strains on the time integration methods on which they rely. High spatial order necessitates comparably high order time integration. Spatial adaptivity and multiphysics processes give rise to subsets of the solution that evolve at differing time scales, or to simulations that combine nonstiff/nonlinear processes with others that may be highly stiff but that are frequently linear. In this talk, I will discuss recent work on time integration methods that allow the flexibility to apply different techniques to distinct physical processes. While techniques for flexible time integration have existed for some time, including additive Runge–Kutta ImEx, multirate (a.k.a. multiple time stepping), and operator-splitting methods, there have been comparably few that combine these types of flexibility into a single family, while also supporting high orders of accuracy and temporal adaptivity. In this talk, I focus on the newly developed IMEX-MRI-GARK (Chinomona and R., 2022) and IMEX-MRI-SR (Fish, R. and Roberts, 2023) families of methods, along with novel techniques for time adaptivity in multirate infinitesimal time integration methods (Fish and R., 2023). While some of these methods are already available in the ARKODE time integration library within SUNDIALS, I will point out our release plans for the remainder.

Challenges in multiphysics non-equilibrium simulations of Inertial Confinement Fusion experiments

Luis Chacon

Los Alamos National Laboratory

Evidence that non-equilibrium (kinetic) plasma and radiation physics are important in (Inertial Confinement Fusion) ICF implosions is overwhelming. While kinetic descriptions of radiation (e.g., IMC) have been employed in rad-hydro simulations for a while, deployment of similar kinetic descriptions for the plasma has been lagging due to model complexity and spatial and temporal scale disparity. At LANL, we have been advancing the state of the art in ICF non-equilibrium simulation capabilities for both the capsule and its surrounding environment (the so-called hohlraum). Our algorithm portfolio to address scale disparity include both Eulerian and Lagrangian (PIC) descriptions, adaptivity in phase space, and a variety of implicit temporal schemes including fully implicit and IMEX. Implicit timestepping for high-dimensional kinetic PDEs is a highly nontrivial enterprise, and requires effective algorithmic acceleration. At LANL, we have pursued multi-fidelity algorithmic accelerators (so-called high-order/low-order, or HOLO), whereby a fluid description, closed by the evolving kinetic solution, is used to accelerate the kinetic solver. In this presentation, I will motivate our efforts, describe our algorithmic choices in our various simulation tools, and outline future directions.

Runge-Kutta Methods for Nonlinearly Partitioned Systems, and Polynomial-Based Time Integrators

Tommaso Buvoli

Tulane University

This talk will be divided in two parts. In the first half, I will introduce a framework that generalizes additive Runge-Kutta methods and can be used to solve nonlinearly partitioned equations. I will motivate the framework, discuss existing approaches, and present multiple new integrators including those that incorporate multirating ideas. In the second half of the talk, I will present a time integration framework that is based on continuous interpolating polynomials in time. I will show how this polynomial framework can be used to construct time integrators with desirable properties such as parallelism, high order of accuracy, and varying types of implicitness including fully-implicit, additive, and exponential.

Strong Stability Preserving General Linear Methods

Zdzisław Jackiewicz

We investigate the strong stability preserving (SSP) general linear methods (GLMs) with two external stages and s internal stages. Examples of SSP methods are derived of order $p = 2$, $p = 3$, and $p = 4$ with $2 \leq s \leq 10$ stages, which have larger effective Courant-Friedrichs-Levy coefficients than the class of two-step Runge-Kutta (TSRK) methods introduced by Jackiewicz and Tracogna, whose SSP properties were analyzes recently by Ketcheson, Gottlieb, and MacDonald, and the class of multistep multistage methods investigated by Constantinescu and Sandu. Numerical examples illustrate that the class of SSP methods discussed in this talk achieve the expected order of accuracy and do not produce spurious oscillations when applied to discretizations of hyperbolic conservation laws, when combined with appropriate discretizations in spatial variables. (This is a joint work with Giuseppe Izzo, University of Naples).

Time Integration Challenges when Modeling Inertial Confinement Fusion and High Energy Density Physics Experiments

Brian Haines

Los Alamos National Laboratory

State-of-the-art numerical simulation of inertial confinement fusion (ICF) and high energy density physics (HEDP) experiments provide unique challenges for time integration due to the use of disparate physics algorithms with high contrast, state-dependent coefficients. Nominally implicit methods for integrating single physics, such as heat conduction, can produce inaccurate solutions or fail to converge due to linearization of the specific heat and conductivity coefficients. Furthermore, time step restrictions imposed by one physics algorithm can decrease the accuracy of the solutions for other physics. For example, typically used hydrodynamics solvers becomes increasingly diffusive as the time step decreases away from the CFL condition. This can result in excessive shock dissipation or enhanced sensitivity to the mesh. In addition, highly nonlinear physics such as plasma transport can be important, yet these occur at much smaller time and spatial scales, requiring extreme resolutions and subcycling that can be prohibitively expensive. These and other issues related to time integration of multi-physics ICF and HEDP numerical simulations will be discussed.

Wednesday, August 9

Invariant-Domain preserving IMEX methods for nonlinear conservation equations

Jean-Luc Guermond

Texas A&M University

I will present implicit-explicit (IMEX) time stepping schemes for solving nonlinear conservation equations. The proposed method makes every implicit-explicit (IMEX) time stepping method invariant-domain preserving and mass conservative. One key idea is to write IMEX schemes in incremental form to make them maximally efficient. At each stage, one first combine a low-order and a high-order hyperbolic update using a limiting operator, then one combine a low-order and a high-order parabolic update using another limiting operator. The proposed technique, which is agnostic to the space discretization, allows to optimize the time step restrictions induced by the hyperbolic substep. To illustrate the proposed methodology, we derive four novel IMEX methods with optimal efficiency. All the implicit schemes are singly diagonal. One of them is A-stable and the other three are L-stable. The novel IMEX schemes are evaluated numerically on systems of stiff ordinary differential equations and nonlinear conservation equations.

Adaptive time integration procedures for solving PDEs

Delfim Soares Jr.

Federal University of Juiz de Fora

This talk aims to report and discuss some explicit, implicit, explicit/explicit, explicit/implicit, and semi-explicit/explicit time integration procedures to numerically analyse large scale problems that are governed by space-time partial differential equations. The referred time integration procedures are adaptively defined, locally adjusting themselves according to the physical properties of the model, to the adopted spatial discretization, to the adopted time-step value, and to the evolution of the computed responses. They are also entirely automated, automatically dividing the spatial domain of the model into different subdomains, at which different solution strategies are applied, as well as automatically computing the time-step values of the analyses for optimal computational performance. Applications considering wave propagation models are mainly focused to discuss the use of the referred adaptive time integration procedures and to illustrate their effectiveness solving space-time PDEs.

Challenges in Thermal Radiative Transfer

Ryosuke Park

Los Alamos National Laboratory

Accurate modeling of neutral particle transport behavior is of great importance in many science and engineering applications. In particular, Thermal Radiative Transfer (TRT) is a primary energy transfer mechanism in high-energy density physics applications. The Boltzmann transport equation describes the behavior of radiation through a host media. TRT is a multiscale problem spanning several orders of magnitude. Due to its high dimensionality and the multiscale nature of the problem, efficient TRT simulation is a challenging task. In this talk, we will discuss a brief overview of TRT system and current state-of-art solution methodology and challenges.

Spectral Deferred Corrections

Michael Minion

(Formerly) Lawrence Berkeley National Laboratory

Since its introduction in 2000, the iterative nature of Spectral Deferred Corrections has been often exploited to create higher-order time integration methods with features that are difficult to include in the most popular classical methods like Runge-Kutta or linear multi-step methods. I will present a summary of and motivation behind some of the more significant of these methods including semi- and multi-implicit methods, multi-rate methods, exponential integrators, iso-spectral methods, and methods for DAEs and 2nd-order differential equations. I will also summarize efforts to reduce the computational cost of SDC methods. Finally, I will describe some open or ongoing projects involving SDC.

Stability of time discretizations for semi-discrete high order schemes for time-dependent PDEs

Chi-Wang Shu

Brown University

In scientific and engineering computing, we encounter time-dependent partial differential equations (PDEs) frequently. When designing high order schemes for solving these time-dependent PDEs, we often first develop semi-discrete schemes paying attention only to spatial discretizations and leaving time t continuous. It is then important to have a high order time discretization to main the stability properties of the semi-discrete schemes. In this talk we discuss several classes of high order time discretization, including the strong stability preserving (SSP) time discretization, which preserves strong stability from a stable spatial discretization with Euler forward, the implicit-explicit (IMEX) Runge-Kutta or multi-step time marching, which treats the more stiff term (e.g. diffusion term in a convection-diffusion equation) implicitly and the less stiff term (e.g. the convection term in such an equation) explicitly, for which strong stability can be proved under the condition that the time step is upper-bounded by a constant under suitable conditions, the explicit-implicit-null (EIN) time marching, which adds a linear highest derivative term to both sides of the PDE and then uses IMEX time marching, and is particularly suitable for high order PDEs with leading nonlinear terms, and the explicit Runge-Kutta methods, for which strong stability can be proved in many cases for semi-negative linear semi-discrete schemes. Numerical examples will be given to demonstrate the performance of these schemes.

Anomalous Behavior of Newtonian Hydrodynamics Coupled with Radiation Transport

Rob Lowrie

Los Alamos National Laboratory

Dropping terms deemed small in multiscale physics models can lead to unexpected results. We show that Newtonian hydrodynamics coupled with radiation transport, using a wide range of methods for treating the material-motion corrections, results in anomalous behavior. In particular, the flow of infinite-medium equilibration will accelerate whenever viewed moving past an observer in the laboratory frame. The acceleration may cause the velocity to increase exponentially in time. The exact fully-relativistic solution has no acceleration, independent of the reference frame.

Current $\mathcal{O}(\beta)$-accurate radiation treatments, where β is the velocity magnitude divided by the speed of light, also predict acceleration. But the anomalous acceleration is not due to the radiation approximations, but rather from assuming that the hydrodynamics evolves on the fluid time scale, which leads to dropping terms from fully-relativistic hydrodynamics to give the Newtonian approximation. The addition of radiation energy and momentum sources to hydrodynamics introduces fast time scales, such as radiation equilibration. These fast time scales invalidate the use of Newtonian hydrodynamics for certain problems, even when β is small.

Thursday, August 10

Overcoming First Order

Steven Roberts

Lawrence Livermore National Laboratory

Many multiphysics simulations are first order accurate in time. Sometime this is simply because higher order methods have not been implemented, but sometimes this is because higher order methods fail to converge at their prescribed order. This talk will look at an example of these two situations and ways to break the order one barrier. The first part of this talk will focus on order reduction: a troublesome degradation in accuracy seen in many Runge-Kutta methods due to stiffness. Many remedies require expensive method structures or are limited to linear problems. To bridge this gap, I will show for the broad class of semilinear differential equations, it is possible to find practical Runge-Kutta methods devoid of order reduction. In the second part of this talk, I will discuss an ongoing project to upgrade the first order integrator in an ice-sheet modeling code called BISICLES. The underlying model pairs differential equations with algebraic constraints that are very expensive to solve. I will discuss how explicit Runge-Kutta methods from the SUNDIALS library can be applied to this problem and their benefits to the temporal accuracy.

Intrastep, Stage-Value Predictors for Diagonally-Implicit Runge–Kutta Methods

Mark Carpenter

To better identify the necessary attributes of good stage-value predictors (SVPs), numerous SVPs are designed for an existing: ESDIRK4(3)7L[2]SA (Kennedy2019) and a new: ESDIRK4(3)8L[2]SA (eight stages) scheme. Both are stiffly-accurate, stage-order two, explicit, singly-diagonally implicit Runge–Kutta (ESDIRK) schemes. Tradeoffs are studied in the parameter spaces enforcing the constraints on accuracy, linear stability, nonlinear stability and coefficient size to determine which objectives correlate with effective predictors. The SVPs are tested in challenging external aerodynamics simulations (10^7 DoFs) using the compressible Navier-Stokes equations (CNSE). An entropy stable spectral collocation formulation is used for discretizing the spatial terms in the equations. Simulations are performed at a wide variety of temporal error tolerances. At lax temporal error tolerances, the most efficient SVPs are those designed with second-order accuracy and the stability properties: A-stability, L-stability, rather than high accuracy constraints. Simulations requiring tight error tolerances are better suited for SVPs designed using high accuracy constraints. Designing SVPs with enhanced stability properties is tedious but worthwhile. Simulation times are reduced with optimal SVPs by as much as 100% on some stages, with combined stepwise improvements of between $50 - 100\%$ for both methods. A comparative study is performed with the two aforementioned methods as well as four other ESDIRKs. The newly designed ESDIRK4(3)8L[2]SA with $\gamma \approx 1/10$, proves to be the most efficient of the six tested ESDIRK schemes simulating the CNSE.

Challenges in Simulating Future Climate

Phil Jones

Los Alamos National Laboratory

Climate change is underway, and models are the primary tools we have for understanding and preparing for a rapidly warming world. The Energy Exascale Earth System Model is one example of such a model. We will describe this complex model and the challenges that remain for accurate simulation of climate change. Many of these challenges are associated with time integration.

Fractional-Step Methods: Theory and Practice

Raymond Spiteri

University of Saskatchewan

Fractional-step methods are a popular and powerful divide-and-conquer approach for the numerical solution of differential equations. The basic premise is that the right-hand side of the differential equation is split into terms that are integrated separately, often by specialized methods. Fractional-step methods arise from the practical need to solve problems that are beyond the reach of monolithic methods in terms of computational requirements such as memory or runtime. Although fractional-step methods have been well studied, there is still a lot to learn about their various aspects, in particular, how should one choose the coefficients of the splitting method, the individual sub-integrators, and the order in which they are applied — not to mention what makes for a good split of the right-hand side in the first place. In this presentation, we offer our experience with some observations in the literature about fractional-step methods in terms of these aspects.

Splitting methods: basics, analysis, modifications, and applications

Alexander Ostermann

University of Innsbruck

Splitting methods are a well-established tool for the numerical integration of time-dependent partial differential equations. The basic idea behind these methods is to split the vector field into disjoint components, integrate them separately with an appropriate time step, and combine the individual flows to obtain the desired numerical approximation. Splitting methods are also a fundamental part of dynamic low-rank integrators.

The merits and pitfalls of splitting methods will be discussed on the basis of several examples. These include reaction-diffusion equations, the cubic nonlinear Schrödinger equation, the Vlasov-Poisson equation (a kinetic model in plasma physics), the Korteweg-de Vries equation, and the Kadomtsev-Petviashvili equation. It is shown that splitting methods can have superior geometric properties (such as preservation of positivity and favorable long term behavior) compared to standard time integration schemes. Furthermore, it is often possible to overcome a CFL condition present in standard discretizations. Another advantage of splitting methods is that they can be implemented by making use of existing methods and codes for simpler problems, and that they often allow for parallelism in a straightforward way.

On the other hand, the use of splitting methods also requires a certain amount of care. The presence of (non-trivial) boundary conditions can lead to a strong order reduction and thus to computational inefficiency. Furthermore, non-smooth initial data pose a serious problem. For example, the traditional second-order Strang splitting requires four additional derivatives to solve the cubic nonlinear Schrödinger equation. To overcome all these problems, the integrators must be adapted accordingly as explained in the talk.

Implicit Fast Sweeping Methods for Conservation Laws

Eduardo Lozano[1], **Tariq D. Aslam**[1]

Los Alamos National Laboratory

Implicit time-accurate methods are often used to integrate stiff problems where explicit schemes impose severe time step restrictions. This talk discusses an efficient numerical framework based on the fast sweeping method (FSM) for solving linear and nonlinear hyperbolic systems of conservation laws. The solution at each discrete location is computed by sweeping the numerical domain in several predetermined directions that follow the causality of the characteristic families. The use of a fractional step strategy eliminates the need for a solution selection criterion while one-sided stencils limit the number of sweeps to at most 2^d for d space dimensions. The approach avoids the large computational and memory requirements associated with solving large block-diagonal systems of equations and preserves the nonlinear stability properties. We explore two separate implicit FSM methodologies: flux vector splitting and Godunov-type schemes. The former can be expressed in conservation form but it is generally limited to a flux that is a homogenous function of degree one—e.g., the Euler equations with a perfect gas equation of state. The latter can be used with exact or approximate Riemann solvers but the current formulation is only conservative for scalars. There is a need to extend both families of implicit FSM schemes in a conservative manner for general equations of state.

List of Abstracts – Posters

Wednesday Session

Finite Element Approximation of dispersive PDEs

Seth Gerberding

Texas A&M University

Dispersive PDEs provide a rich variety of dynamics. One special property of many dispersive equations is the ability to produce solitons– waves that travel with constant velocity without changing shape. However, these equations often involve a nonlinear hyperbolic term and a third-order term. A pressing problem, therefore, is how to discretize the problem in time. One possibility is an IMEX scheme–treat the non-linearity explicitly and the third order term implicitly. The work presented here address the second part: how to solve a third order problem using implicit methods.

Efficient Implicit Time Integration for Dynamic Low-Rank Representations of High-Dimensional PDEs

Hamad El Kahza

University of Delaware

We propose an efficient implicit time integration algorithm for a low-rank representation of high-dimensional PDEs. Starting from a solution ansatz expressed as a linear combination of basis vectors, our approach dynamically adapts the basis in time by employing a Krylov-like basis augmentation, thus avoiding the need to solve for evolution equations for the basis, resulting in significant efficiency gains vs. other approaches proposed in the literature [1]. Our algorithm begins by finding a suitable low-rank approximation space generated from extended Krylov subspaces [2], and solve for the coefficients governing the composition of the bases. An implicit timestep solve is performed on this reduced basis by solving a Sylvester equation. After each implicit update, we augment the basis for the new-time solution by extending the Krylov basis with a forward and inverse application of the system matrix, solve for the new set of coefficients, and truncate the basis before the next implicit timestep. Through a series of numerical experiments with diffusion-like problems, we demonstrate the efficiency of our low-rank algorithm, producing results identical to those of the classical full-rank integrator while resulting in significant acceleration in performance.

References

[1] A rank-adaptive robust integrator for dynamical low-rank approximation. Ceruti, G., Kusch, J. & Lubich, C. s.l. : Bit Numer Math 62, 1149–1174, 2022, Bit Numer Math 62, pp. 1149–1174.

[2] A new iterative method for solving large-scale Lyapunov matrix equations. Simoncini, Valeria. s.l. : SIAM Journal on Scientific Computing, 2007, Vol. 29.3, pp. 1268-1288.

CFL Optimized Forward-Backward Runge-Kutta Schemes for the Shallow Water Equations

Jeremy Lilly

Oregon State University

We present the formulation and optimization of a Runge-Kutta-type time-stepping scheme for solving the shallow water equations, aimed at substantially increasing the effective allowable time-step over that of comparable methods. This scheme, called FB-RK(3,2), uses weighted forward-backward averaging of thickness data to advance the momentum equation. The weights for this averaging are chosen with an optimization process that employs a von Neumann-type analysis, ensuring that the weights maximize the admittable Courant number. We show that an optimized FB-RK(3,2) can take time-steps up to 2.8 times as large as a popular three-stage, third-order strong stability preserving Runge-Kutta method in a quasi-linear test case. In fully nonlinear shallow water test cases relevant to oceanic and atmospheric flows, FB-RK(3,2) outperforms SSPRK3 in admittable time-step by factors between roughly between 1.6 and 2.2, making the scheme approximately twice as computationally efficient with little to no effect on solution quality.

An Implicit Approach to Phase Field Modeling of Solidification for Additively Manufactured Alloys

Chris Newman

Los Alamos National Laboratory

We develop a fully-coupled, fully-implicit approach to phase field modeling of solidification for additively manufactured alloys. Predictive simulation of solidification in additively manufactured metals remains a significant challenge in the field of materials science, as micro-structure formation during the solidification of the material plays an important role in the properties of the solid material. Our approach consists of a finite element spatial discretizatioon of the fully-coupled nonlinear system of partial differential equations at the microscale, which is treated implicitly in time with a preconditioned Jacobian-free Newton-Krylov (JFNK) method. The approach allows timesteps larger than those restricted by the traditional explicit CFL limit on structured and unstructured 2D and 3D meshes, is algorithmically scalable and efficient due to an effective preconditioning strategy. The computational tool leverages MPI, OpenMP, CUDA and ROCm; demonstrates parallel scalability and efficiency and is uniquely targeted toemerging exascale architectures.

Integration of extended Lagrangian Born-Oppenheimer molecular dynamics

Anders Niklasson

Los Alamos National Laboratory

The integration problem for the coupled nuclear and electronic equations of motion in extended Lagrangian Born-Oppenheimer molecular dynamics are presented and discussed.

Implicit-explicit Runge-Kutta for radiation hydrodynamics

Ben Southworth

Los Alamos National Laboratory

Radiation hydrodynamics are a challenging multiscale and multi- physics set of equations. To capture the relevant physics of interest, one typically must time step on the hydrodynamics timescale, making explicit integration the obvious choice. On the other hand, the cou- pled radiation equations have a scaling such that implicit integration is effectively necessary in non-relativistic regimes. A first-order Lie- Trotter-like operator split is the most common time integration scheme used in practice, alternating between an explicit hydrodynamics step and an implicit radiation solve and energy deposition step. However, such a scheme is limited to first-order accuracy, and nonlinear coupling between the radiation and hydrodynamics equations makes a more general additive partitioning of the equations non-trivial. Here, we develop a new formulation and partitioning of radiation hydrodynamics with gray diffusion that allows us to apply (linearly) implicit-explicit Runge-Kutta time integration schemes. We prove conservation of total energy in the new framework, and demonstrate 2nd-order convergence in time on multiple radiative shock problems, achieving error 3–5 orders of magnitude smaller than the first-order Lie-Trotter operator split at the hydrodynamic CFL, even when Lie-Trotter applies a 3rd-order TVD Runge-Kutta scheme to the hydrodynamics equations.

The Runge–Kutta discontinuous Galerkin method with compact stencils for hyperbolic conservation laws

Zheng Sun

The University of Alabama

In this poster, we present a new type of Runge–Kutta (RK) discontinuous Galerkin (DG) method for solving hyperbolic conservation laws. Compared with the original RKDG method, the new method features improved compactness and allows simple boundary treatment. The key idea is to hybridize two different spatial operators in an explicit RK scheme, utilizing local projected derivatives for inner RK stages and the usual DG spatial discretization for the final stage only. Limiters are applied only at the final stage for the control of spurious oscillations. We also explore the connections between our method and Lax–Wendroff DG schemes and ADER-DG schemes. Numerical examples are given to confirm that the new RKDG method is as accurate as the original RKDG method, while being more compact, for problems including two-dimensional Euler equations for compressible gas dynamics.

The effect of splitting strategy on qualitative property preservation

Siqi (Vicky) Wei

University of Saskatchewan

Mathematical models of physical systems often exhibit essential qualitative properties such as conservation of total population, positivity, and monotonicity. These models are often formulated as differential equations which can be solved using operator-splitting methods. Different splitting strategies impact the preservation of qualitative properties. We investigate the susceptible-infected-recovered (SIR) model from epidemiology with two splitting strategies. We noted the following

1. Solving the sub-system exactly improves qualitative property preservation.

2. Backward integration does not necessarily destroy monotonicity.

3. Qualitative property preservation does depend on the splitting strategy even if the sub-systems are integrated exactly.

We further extend our analysis to production-destruction systems where positivity and conservation property is possible by splitting into N ($N > 2$) sub-systems.

ML-based Surrogate Modeling for a collisional-radiative model

Xuping Xie

Los Alamos National Laboratory

Collisional-radiative (CR) models describe the atomic processes in a plasma by tracking the population density in ground and excited states for each charge state of the atom/ion. These models predict important plasma properties such as charge state distributions and radiative emissivity and opacity. Accurate descriptions of the CR balance of the plasma are essential in fusion whole device modeling, especially when significant impurities are introduced into the plasmas. In a coupled plasma and CR simulation, the CR model, which is a high-dimensional ODE, is solved on each grid point for the plasma solver, and can overwhelm the plasma simulation cost. In this work, we introduce a machine learning (ML) based method that discovers a latent space and learns its corresponding reduced order modeling (ROM) dynamics that can capture the essential physics to make accurate predictions of the quantities of interest, at much reduced online computational cost.

Sponsors

The TĪM2023 workshop is sponsored by the DDSTE Science Capability Investment & the Center For Nonlinear Studies (CNLS) at Los Alamos National Laboratory. External funding was provided by Texas A&M University.

Sponsors