# An Introduction to Multirate Methods for Multiphysics Applications

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# Multiphysics Scientific Simulations

In recent decades computation has rapidly assumed its role as the third pillar of the scientific method [Vardi, *Commun. ACM*, 53(9):5, 2010]:

- Simulation complexity has evolved from simplistic calculations of only 1 or 2 basic equations, to massive models that combine vast arrays of processes.
- Early algorithms could be analyzed using standard techniques, but mathematics has not kept up with the fast pace of scientific simulation development.
- Presently, many numerical analysts construct elegant solvers for models of limited practical use, while computational scientists "solve" highly-realistic systems using *ad hoc* methods with questionable reliability.

The purpose of this mini-symposium is to discuss recent advances in numerical methods that aim to bridge this gap between mathematical theory and computing practice.

In the next few slides, I'll present a few of the mutiphysics applications that I have worked on in recent years, in order to illustrate some of the challenges they present for numerical methods.

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# Climate – Nonhydrostatic Atmospheric Models

- Increased computational power enables spatial resolutions beyond the hydrostatic limit.
- Nonhydrostatic models consider the 3D compressible Navier Stokes equations; these support acoustic (sound) waves.
- Acoustic waves have a negligible effect on climate, but travel much faster than convection (343 m/s vs 100 m/s horizontal and 1 m/s vertical), leading to overly-restrictive explicit stability restrictions.
- To overcome this stiffness, nonhydrostatic models traditionally utilize split-explicit, implicit-explicit, or fully implicit time integration.
- Additionally, climate "dycores" are coupled to myriad other processes (ocean, land/sea ice, . . . ), each evolving on significantly different time scales.

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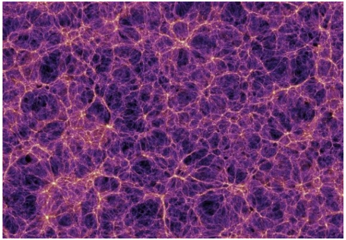
# Cosmic Reionization – The Origins of the Universe

- After the Big Bang, primordial matter (96% dark matter, 2.92% H, 1% He) was strewn throughout the universe.
- Gravitational attraction condensed this into the "cosmic web," the large-scale structure that connects/creates galaxies.
- When pressure is sufficient, stars 'ignite' and emit radiation.
- When stars collapse, supernovae spread heavier species.



[http://svs.gsfc.nasa.gov/cgi-bin/details.cgi?aid=10118]

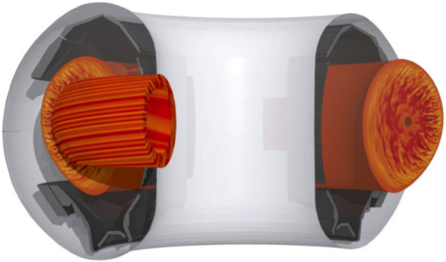
Modern cosmological models combine a myriad of physical processes:

- Models for cosmological expansion of the universe.
- Particle motion for cold dark matter.
- Compressible Euler equations for hydrodynamic motion.
- Multi-frequency radiation transport.
- Multi-species chemical ionization.

# Fusion Plasma Simulations

Large-scale, nonlinear simulation of fusion plasmas is critical for the design of next-generation confinement devices.

- Fusion easy to achieve but difficult to *stabilize*, as needed to increase yield and protect device.
- Linear modes present in fluid models are typically well-controlled.
- Most current work focuses on disruptions due to nonlinear instabilities and kinetic effects.
- Turbulence in the sharp edge disrupts the core, but is difficult to simulate:
  - must accurately couple ions and electrons in high dimensions: $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{v} \in \mathbb{R}^d$, $t \in \mathbb{R}$; $d = \{2, 3\}$
  - mass/velocity differences result in $100\times$ spatial/temporal scale separation.



GENE gyrokinetic simulation of core turbulence

# Multiphysics Challenges

Multiphysics problems exhibit key characteristics that challenge traditional numerical methods:

- "Multirate" structure: different processes evolve on distinct time scales, but these are too close to analytically reformulate (e.g., via steady-state approximation).
- The existence of stiff components prohibits fully explicit methods.
- Nonlinearity and insufficient differentiability challenge fully implicit methods.
- "Multiscale" structure: some spatial regions may be well-modeled via coarse meshes, while others require high resolution.
- Extreme parallel scalability demands optimal algorithms. While robust and scalable algebraic solvers exist for some pieces (e.g., FMM for particles, multigrid for diffusion), none are optimal for the full problem.

# "Classical" Time Integrators (and their deficiencies)

Historically, IVP research has focused on two simple problem types:

$$y'(t) = f(t, y(t)), \qquad y(t_0) = y_0 \qquad \text{[ODE]}$$

$$0 = F(t, y(t), y'(t)), \qquad y(t_0) = y_0, \qquad y'(t_0) = y_0' \qquad \text{[DAE]}$$

Corresponding solvers thus enforced overly-rigid standards:

- Treat all components implicitly or explicitly, without IMEX flexibility.
  - Fully explicit: "stiff" components require overly-small time steps for stability.
  - Fully implicit: scalable/robust algebraic solvers difficult for highly nonlinear or nonsmooth terms.
- Treat all components using the same time step size, without multirate flexibility.
  - If time step is set by 'fastest' process, 'slow' operators may be called too frequently (inefficient).
  - If time step is set by 'slowest' process, then 'fast' operators must be implicit to remain stable, but their accuracy can be lost.

# *Ad Hoc* Algorithms Pervade Scientific Computing Applications

On the other hand, practitioners frequently "split" their problems apart based on the physical operators under consideration, e.g.,

$$y'(t) \;=\; f_1(t,y) \;+\; \cdots \;+\; f_m(t,y), \quad y(t_0) = y_0.$$

The simplest approaches may then apply a basic "Lie-Trotter" splitting:

$$\begin{aligned}
y_1'(t) &= f_1\left(t, y_1\right), & t_0 < t < t_0 + h, & \quad y_1(t_0) = y_0, \\
y_2'(t) &= f_2\left(t, y_2\right), & t_0 < t < t_0 + h, & \quad y_2(t_0) = y_1(t_0 + h), \\
& & \vdots & \\
y_m'(t) &= f_m\left(t, y_m\right), & t_0 < t < t_0 + h, & \quad y_m(t_0) = y_{m-1}(t_0 + h),
\end{aligned}$$

and the time-evolved solution is taken to be $y(t_0+h) = y_m(t_0+h)$.

Here, each component may be tackled independently (or even subcycled) using, e.g., something from "Numerical Recipes."

# *Ad Hoc* Algorithms II

Some applications attempt to achieve higher order by instead applying a "Strang-Marchuk" splitting:

$$\begin{aligned}
y_1'(t) &= f_1\left(t, y_1\right), & t_0 < t < t_0 + \tfrac{h}{2}, && y_1(t_0) &= y_0, \\
&\vdots \\
y_{m-1}'(t) &= f_{m-1}\left(t, y_{m-1}\right), & t_0 < t < t_0 + \tfrac{h}{2}, && y_{m-1}(t_0) &= y_{m-2}(t_0 + \tfrac{h}{2}), \\
y_m'(t) &= f_m\left(t, y_m\right), & t_0 < t < t_0 + h, && y_m(t_0) &= y_{m-1}(t_0 + \tfrac{h}{2}), \\
y_{m+1}'(t) &= f_{m-1}\left(t, y_{m+1}\right), & t_0 + \tfrac{h}{2} < t < t_0 + h, && y_{m+1}(t_0 + \tfrac{h}{2}) &= y_m(t_0 + h), \\
&\vdots \\
y_{2m}'(t) &= f_1\left(t, y_{2m}\right), & t_0 + \tfrac{h}{2} < t < t_0 + h, && y_{2m}(t_0 + \tfrac{h}{2}) &= y_{2m-1}(t_0 + h),
\end{aligned}$$

Unfortunately, both approaches suffer from:

- Low accuracy – Lie-Trotter is $\mathcal{O}(h)$ and Strang-Marchuk is $\mathcal{O}(h^2)$; extrapolation can improve this but at significant cost [Ropp, Shadid & Ober 2005].
- Poor/unknown stability – even when each part utilizes a 'stable' step size, the combined problem may admit unstable modes [Estep et al., 2007].

# Filling this 'Disconnect' between Mathematical Theory and Multiphysics Practice

In recent years, many researchers have worked to construct *flexible* time integration methods to improve temporal integration of multiphysics systems.

Goals include:

- Stability/accuracy for each component, as well as inter-physics couplings.
- Custom/flexible time step sizes for distinct components.
- Robust temporal error estimation & adaptivity of step size(s).
- Built-in support for spatial adaptivity.
- Ability to apply optimally efficient and scalable solver algorithms.
- Support for experimentation and testing between methods and solution algorithms.

# IMEX Methods – Matching Stiff Solvers With Stiff Operators

IMEX methods allow us to treat only the stiff terms using implicit methods. For example, temporally-adaptive, single-rate, Additive Runge–Kutta methods [Ascher et al. 1997; Araújo et al. 1997; Kennedy & Carpenter 2003; . . . ] are formulated for split problems:

$$y'(t) = f^E(t,y) + f^I(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0,$$

where $f^E(t,y)$ contains the nonstiff terms and $f^I(t,y)$ contains the stiff terms.

These combine two $s$-stage RK methods; denoting $h_n = t_{n+1} - t_n$, $t^E_{n,j} = t_n + c^E_j h_n$, $t^I_{n,j} = t_n + c^I_j h_n$:

$$z_i = y_n + h_n \sum_{j=1}^{i-1} a^E_{i,j} f^E(t^E_{n,j}, z_j) + h_n \sum_{j=1}^{i} a^I_{i,j} f^I(t^I_{n,j}, z_j), \quad i = 1, \dots, s,$$

$$y_{n+1} = y_n + h_n \sum_{j=1}^{s} \left[ b^E_j f^E(t^E_{n,j}, z_j) + b^I_j f^I(t^I_{n,j}, z_j) \right] \quad \text{(solution)}$$

$$\tilde{y}_{n+1} = y_n + h_n \sum_{j=1}^{s} \left[ \tilde{b}^E_j f^E(t^E_{n,j}, z_j) + \tilde{b}^I_j f^I(t^I_{n,j}, z_j) \right] \quad \text{(embedding)}$$

# Exponential Methods

Exponential integrators analytically solve a subset of the physics. For example, exponential Rosenbrock methods [Hochbruch et al., 2009; Luan & Ostermann, 2014; ...] consider a specific additive splitting:

$$y'(t) = f(y) = \mathcal{J}(y)y + \mathcal{N}(y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0,$$

$\mathcal{J}(y) \equiv \frac{\partial f(y)}{\partial y}$ is assumed stiff, and $\mathcal{N}(y) \equiv f(y) - \mathcal{J}(y)y$ contains any remaining nonlinearities [assumed nonstiff]. Using the variation-of-constants formula we may analytically solve over $t \in [t_n, t_n + h]$:

$$y(t) = \mathrm{e}^{(t-t_n)\mathcal{J}(y_n)} y(t_n) + \int_0^t \mathrm{e}^{(t-\tau)\mathcal{J}(y_n)} \mathcal{N}(u(t_n + \tau)) \mathrm{d}\tau.$$

By approximating the integral via quadrature, an $s$-stage ExpRB method may be written:

$$z_i = y_n + c_i h\, \varphi_1(c_i h \mathcal{J}(y_n)) f(y_n) + h \sum_{j=2}^{i-1} a_{ij}(h\mathcal{J}(y_n)) (\mathcal{N}(z_j) - \mathcal{N}(y_n)),$$

$$y_{n+1} = y_n + h\, \varphi_1(h\mathcal{J}(y_n)) f(y_n) + h \sum_{i=2}^{s} b_i(h\mathcal{J}(y_n)) (\mathcal{N}(z_i) - \mathcal{N}(y_n))$$

where $z_1 = y_n$. Efficiency/scalability hinge on evaluation of matrix $\varphi_k$ functions, that comprise $a_{ij}$ and $b_i$.

# 'Infinitesimal' Multirate Methods (MIS, MRI, . . . ) [Schlegel et al. 2009; Sandu 2019; Bauer & Knoth 2019; . . . ]

The 'infinitesimal' family of multirate methods allow a higher-order approach to subcycling, through more tightly coupling the 'fast' and 'slow' operators. Consider the splitting

$$y'(t) = f^S(t,y) + f^F(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0.$$

- $f^S(t,y)$ contains the "slow" dynamics, integrated with time step $H$.
- $f^F(t,y)$ contains the "fast" dynamics, integrated with time step $h \ll H$
- The slow component is integrated using an "outer" RK method, while the fast component is advanced between slow stages by solving a modified ODE with a subcycled "inner" RK method:

$$v'(t) = f^F(t,v) + \sum_{j=1}^{i} \alpha(t) f^S(t_{n,j}, z_j), \quad t_{n,i-1} < t < t_{n,i}, \quad v(t_{n,i-1}) := z_{i-1}^{\{slow\}}, \quad z_i^{\{slow\}} := v(t_{n,i}).$$

- Historically limited to $\mathcal{O}(h^3)$ accuracy, but recent work has resulted in *significant* improvements.
- Highly efficient – many require only a single traversal of $[t_n, t_{n+1}]$ to achieve high order.

# MS 316 – Friday, March 5, 8:30-10:10 am

- Daniel R. Reynolds: *An Introduction to Multirate Methods for Multiphysics Applications*
- Oswald Knoth: *How to Obtain Order Conditions for Multirate Infinitesimal Methods (MIS)*
- Steven Roberts: *A New Multirate Time-Stepping Strategy for ODE Systems Equipped with a Surrogate Model*
- Rujeko Chinomona: *High-Order Implicit-Explicit Multirate Infinitesimal Methods for Multiphysics Applications*
- Tobias Bauer: *Multirate Runge-Kutta Methods for Idealized Coupled Atmosphere-Ocean Simulations*

# MS 347 – Friday, March 5, 10:20 am - 12:00 pm

- Vu Thai Luan: *Multirate Exponential Rosenbrock Methods*
- David J. Gardner: *Multirate Time Integrators in Sundials*
- Valentin Dallerit: *High-Order Numerical Solutions to the Nonlinear Shallow-Water Equations on the Rotated Cubed-Sphere Grid*
- David Shirokoff: *Semi-Implicit (ImEx) Schemes for the Dispersive Shallow Water Equations*
- Giacomo Rosilho De Souza: *Multirate Stabilized Explicit Methods based on a Modified Equation for Problems with Multiple Scales*