Time Integration (with hands-on examples using SUNDIALS)

Presented to

ATPESC 2025 Participants

David J. Gardner
Lawrence Livermore National Laboratory
SUNDIALS Developer

August 6, 2024

ATPESC Numerical Software Track

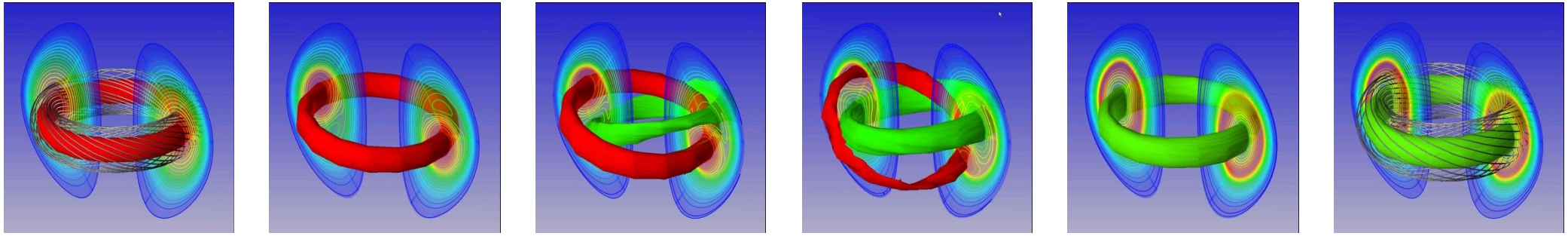
Time integrators in the HPC “landscape”

Most models of physical systems are formulated in terms of the *rate of change* of some variable, e.g. $\frac{\mathrm{d}u}{\mathrm{d}t}$

– Newton’s 2nd law: $\mathbf{f} = m\mathbf{a} \quad \Rightarrow \quad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{\mathbf{f}}{m}$

– Chemical rate equations: $A + B \rightarrow P \quad \Rightarrow \quad \frac{\mathrm{d}[P]}{\mathrm{d}t} = k(T)[A][B]$

- Time integrators are used to track changes in solutions as time proceeds, allowing studies of the ‘evolution’ of a model.



”Sawtooth” reconnection in a tokamak (NIMROD)

Time integrators in the HPC "landscape"

Unlike spatial discretization or visualization that live at the bottom/top of the software stack, respectively, time integrators typically live in the "middle." Consider some PDE systems,

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$
$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla p}{\rho} = \mathbf{g}$$
$$\partial_t e + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = 0$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} = -\nabla \left(\frac{p}{\rho_0} \right) + \mathbf{g}$$
$$\nabla \cdot \mathbf{u} = 0$$

- Using a "method of lines" approach, after spatial discretization, one considers the resulting ODE/DAE system:

$$\dot{y} = f(t, y), \quad y(t_0) = y_0 \qquad\qquad F(t, y, \dot{y}) = 0, \quad y(t_0) = y_0, \quad \dot{y}(t_0) = \dot{y}_0$$

  – y contains *all* discretized solution components; f or F encodes the physics & spatial discretization

LLNL-PRES-852979

Time integrator overview

- Let $y_n \approx y(t_n)$ and $t_{n+1} = t_n + \Delta t_n$, we only compute the solution at the finite set of times $\{t_n\}_{n=0\ldots N}$
- A "time marching" scheme computes these time-evolved solutions using a prescribed update formula:

$$y_{n+1} = \Phi(\Delta t_n, y_{n+1}, y_n, \cdots)$$

  e.g., explicit Euler, $y_{n+1} = y_n + \Delta t_n f(t_n, y_n)$ and implicit Euler, $y_{n+1} = y_n + \Delta t_n f(t_{n+1}, y_{n+1})$

- Time integrator types (explicit, implicit, IMEX):
  - If Φ depends on y_{n+1} then the method is *implicit*, and requires a nonlinear solve of the form

$$\boldsymbol{F}(y) \equiv y - \Phi(\Delta t_n, y, y_n, \cdots) = 0$$

  - If Φ does not depend on y_{n+1} then the method is *explicit,* in that the updated solution may be explicitly constructed using known data
  - Implicit-explicit (IMEX) methods arise when only some parts of Φ depend on y_{n+1}
  - *Multirate* methods use different time step sizes $\Delta t_n \gg \delta t_n$ to evolve separate problem components

LLNL-PRES-852979

Time integrator overview (continued)

- Time integration methods have multiple mechanisms for achieving increased accuracy:
  - "One-step" methods use multiple internal stages per step [Runge-Kutta, Rosenbrock]
    - More work per-step; amenable to problems with spatial adaptivity & hyperbolic effects
  - "Multistep" methods retain a longer history of previous solutions [Adams-Bashforth, BDF]
    - Less work per-step; amenable to problems with strong reaction and diffusion effects
- Linear stability: a method is numerically stable if for a desired Δt_n, roundoff error stays "controlled" throughout the simulation (vs growing out of control). For a brief refresher, see here
  - "A-stable": linearly stable no matter the Δt_n – this is only possible with implicit methods[1]
  - Otherwise, the method has a maximum stable step size Δt_n for any given problem (in PDEs, this is frequently given by the *CFL condition*, wherein $\Delta t_n \propto \Delta x$ or $\Delta t_n \propto \Delta x^2$)
  - *Stability ≠ accuracy* – just because a solution does not blow up, it is not necessarily accurate

[1]Exponential methods are explicit and may be A-stable, but require *significantly* more work per-step than traditional explicit methods.

Choosing between explicit and implicit methods

Explicit Methods	Implicit Methods
+ easy to conceptualize	+ less/nonexistent stability limits
+ easy to code	+ steps over fastest dynamics
+ no algebraic solvers required	− requires algebraic solvers
− stability limits on step sizes	− solvers generally couple all solution unknowns
− tracks fastest dynamics	− increased code complexity

- IMEX: a bit of both – one chooses the splitting to balance "cheaper" algebraic solvers and stability
- "Stiffness" helps us choose: "*The stepsize needed to maintain stability of the forward Euler method is much smaller than that required to represent the solution accurately.*" (Ascher and Petzold, 1998)
  - Depends on Jacobian eigenvalues, system dimension, accuracy requirements, length of simulation
  - For stability, stiff problems generally require implicit or IMEX methods, with robust implicit solvers
- DAEs nearly always require implicit methods to maintain stability due to the algebraic constraint
- Multirate methods may be preferable if the "slow" operator is much more costly than the "fast"

Adaptive time-step selection

- *Stability alone should never dictate the time steps used in an application*
- Given a maximum stable step, adaptive methods select Δt_n based on a desired accuracy:
  - At each internal step, computes both the solution and an estimate of the error introduced in that step
  - If that *local truncation error* is sufficiently small, the step is accepted; otherwise a new step size is chosen and the step is recomputed
  - Advanced "error controllers" adapt these step sizes to meet a variety of objectives:
    - minimize failed steps
    - maximize step sizes
    - maintain smooth transitions in the step sizes as integration proceeds
- Temporal adaptivity can lead to *much* more efficient (and accurate) results

LLNL-PRES-852979

"Solving" Initial-Value Problems with SUNDIALS

- SUNDIALS integrators consider initial-value problems (IVPs) of a variety of types:
  - Standard IVP [CVODE]: $y'(t) = f\big(t, y(t)\big), \qquad y(t_0) = y_0$
  - Linearly-implicit, split [ARKODE]: $M(t)\, y'(t) = f_E\big(t, y(t)\big) + f_I\big(t, y(t)\big), \qquad y(t_0) = y_0$
  - Multirate [ARKODE]: $y'(t) = f_F\big(t, y(t)\big) + f_S\big(t, y(t)\big), \qquad y(t_0) = y_0$
  - Differential-algebraic form [IDA]: $F\big(t, y(t), y'(t)\big) = 0, \qquad y(t_0) = y_0,\ y'(t_0) = y'_0$
- By "solve" we adapt time steps (and/or method order) to meet user-specified tolerances:

$$\left[\frac{1}{N}\sum_{k=1}^{N}\left(\frac{\text{error}_k}{\text{rtol}\,|y_k| + \text{atol}_k}\right)^2\right]^{1/2} < 1$$

  - $\text{error} \in \mathbb{R}^N$ is the estimated temporal error in the time step
  - $y \in \mathbb{R}^N$ is the previous time-step solution
  - $\text{rtol} \in \mathbb{R}$ encodes the desired relative solution accuracy (number of significant digits)
  - $\text{atol} \in \mathbb{R}^N$ is the "noise" level for any solution component (protects against $y_k = 0$)

LLNL-PRES-852979

Other DOE Time Integration Packages

- PETSc's *TS* module provides a unified interface for implicit, explicit, & IMEX ODEs and DAEs:

$$F(t, y, \dot{y}) = G(t, y), \quad y(t_0) = y_0$$

  - $F(t, y, \dot{y})$ – stiff portion; $G(t, y)$ – nonstiff portion

- Trilinos includes both an older *Rythmos* module for ODEs and DAEs:

$$F(t, y(t), \dot{y}(t)) = 0, \quad y(t_0) = y_0, \quad \dot{y}(t_0) = \dot{y}_0$$

  As well as a newer *Tempus* module for ODEs:

$$\begin{aligned} M(t, y)\, \dot{y}(t) &= G(t, y) + F(t, y), & y(t_0) &= y_0 \\ M\, \ddot{y}(t) + C\, \dot{y}(t) + K\, y(t) + F(t) &= 0, & y(t_0) &= y_0,\ \dot{y}(t_0) = \dot{y}_0 \end{aligned}$$

  - Top: $G(t, y)$ stiff, $F(t, y)$ nonstiff; Bottom: Newmark integrators for second-order ODEs

- All perform temporal adaptivity, and provide a range of algebraic solvers for implicit methods

LLNL-PRES-852979

Implicit methods require a nonlinear solver for $\boldsymbol{F}(y) = 0$

The PETSc team is presenting on nonlinear solvers in sessions parallel to this one, so I'll only give a high-level idea, leaving details for them

Nonlinear solvers must be iterative, since few nonlinear equations admit analytical solutions

The two largest classes of nonlinear solvers are *fixed-point* vs *Newton-based*

- FP typically use only $\boldsymbol{F}$ and converge linearly, but may have a large domain of convergence
- Newton uses both $\boldsymbol{F}$ and the Jacobian $J(y) \equiv \frac{\partial \boldsymbol{F}(y)}{\partial y}$ (or an approximation to it):
  - Each iteration requires a linear solve with the matrix J (see linear solver talks)
  - Typically converge quadratically (or super-linearly, depending on how well J is solved)
  - For most problems, Newton is algorithmically scalable – as the mesh is refined, the number of iterations remains fixed, so scalability hinges on the linear system solver

LLNL-PRES-852979

Why use a solver library (instead of “rolling your own”)

- Many applications (particularly early on) implement their own numerical methods to remove software dependencies. While functional, the methods may be overly simplistic (e.g., straight from “Numerical Recipes”) or buggy, may not leverage modern hardware, and/or omit advanced “expert” features.

- Solver libraries, on the other hand, are typically bug-free, heavily tested, and admit numerous benefits:
  - Time adaptivity – provide approximate solutions with requested accuracy and minimal work
  - Seamless integration with scalable algebraic solver libraries for implicit and IMEX problems
  - Native support for cutting-edge GPU hardware via CUDA, HIP, oneAPI, Kokkos, RAJA, …
  - Advanced options for later use: temporal root-finding, sensitivity analysis, solution constraints, …

- For more information:
  - SUNDIALS: https://computing.llnl.gov/projects/sundials
  - PETSc: https://www.mcs.anl.gov/petsc/
  - Trilinos: https://trilinos.github.io/

LLNL-PRES-852979

Hands-on lessons

Switch over to web-based hands-on lesson instructions – webpage

Agenda:

1. Explicit time integration (`HandsOn1.exe`)
2. Implicit / IMEX time integration (`HandsOn2.exe`)
3. Preconditioning (`HandsOn3.exe`)

Take Away Messages

- SUNDIALS, PETSc, and Trilinos provide a wide variety of high quality, scalable ODE/DAE integrators and nonlinear solvers
- PDEs can be converted to ODEs/DAEs via spatial semi-discretization, and then integrated using ODE/DAE libraries
- Stiffness is an important characteristic of ODEs, and helps dictate which methods are appropriate for any given problem
- Adaptive time-stepping provides an inexpensive means to combine algorithmic efficiency and solution quality
- Scalability of implicit and IMEX methods hinges on selection of robust and scalable algebraic solvers; while Newton methods can handle nonlinearities, robustness and scalability of the inner linear solver is critical (and often problem-dependent)

computing.llnl.gov/projects/sundials

github.com/LLNL/sundials

sundials.readthedocs.io

Linear Stability – A brief refresher

A fundamental question for any time integration method is how well it handles errors due to floating-point roundoff. To this end, we consider the simple "Dahlquist" test problem:

$$y'(t) = \lambda y(t), \quad y(0) = 1$$

- Here, y corresponds to the normalized floating-point error, and λ to the largest eigenvalue of the Jacobian of a prototypical ODE right-hand side function (assumed to satisfy $\Re(\lambda) < 0$).
- The true solution to this problem is just $y(t) = e^{\lambda t}$, which decays to zero as $t \to \infty$, indicating that roundoff errors should decay as the simulation proceeds.
- The numerical method, on the other hand, computes approximate solutions

  $$y_{n+1} = \Phi(\Delta t_n, y_{n+1}, y_n, \ldots)$$

  that may (or may not) similarly satisfy the similar requirement that $y_n \to 0 \text{ as } n \to \infty$.
- Generally, this decay in numerical roundoff error will only occur for specific values of $\Delta t \lambda = z \in \mathbb{C}$. We therefore define the *stability region* for a method as $S = \{z \in \mathbb{C} : \Phi_z(y_n) \to 0 \text{ as } n \to \infty\}$

LLNL-PRES-852979

Linear Stability Example – Explicit Euler

Consider the explicit Euler method: $y_{n+1} = y_n + \Delta t f(t_n, y_n)$

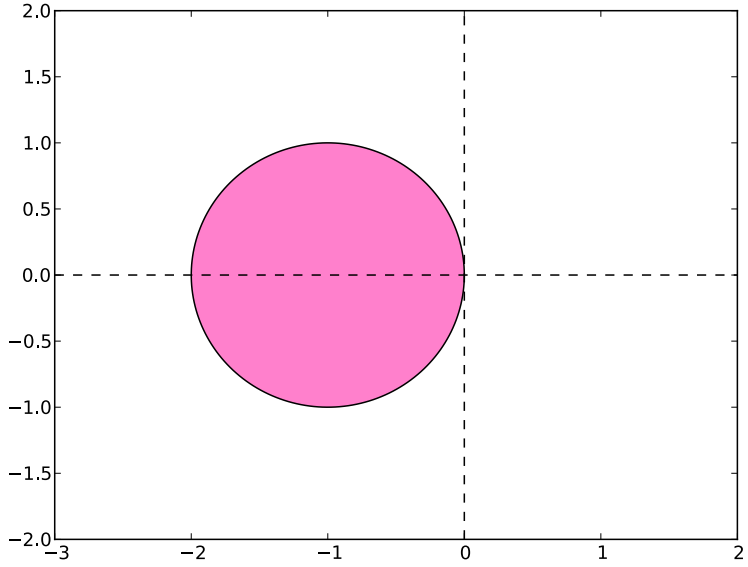
For the Dahlquist test problem, this becomes

$$y_{n+1} = y_n + \Delta t \lambda y_n = (1 + \Delta t \lambda) y_n = (1 + \Delta t \lambda)^2 y_{n-1} = \ldots = (1 + \Delta t \lambda)^{n+1} y_0 = (1 + \Delta t \lambda)^{n+1}$$

which only decays to zero if $|1 + \Delta t \lambda| < 1$.

Hence the explicit Euler linear stability region is

$$S = \{z \in \mathbb{C} \ : \ |1 + z| < 1\}$$



From https://en.wikipedia.org/wiki/Euler_method

Linear Stability Example – Implicit Euler

Consider the implicit Euler method: $y_{n+1} = y_n + \Delta t f(t_{n+1}, y_{n+1})$

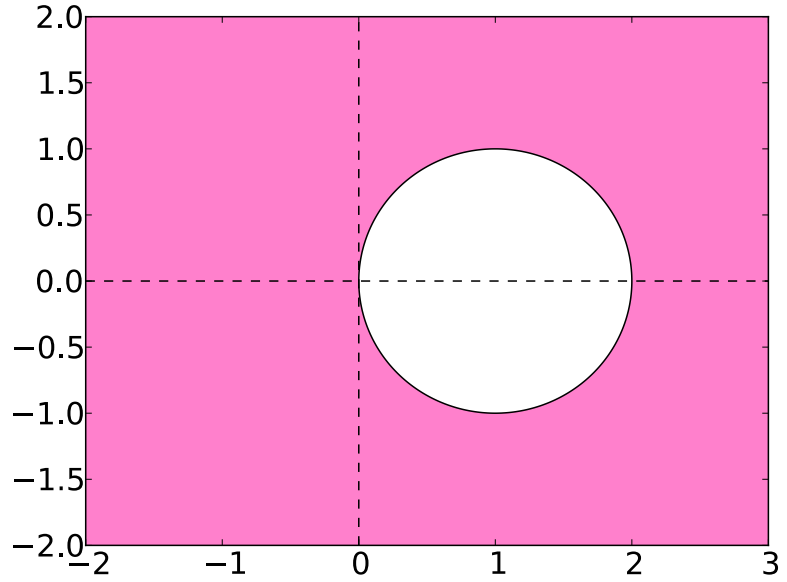
For the Dahlquist test problem, this becomes

$$y_{n+1} = y_n + \Delta t \lambda y_{n+1} \quad \Leftrightarrow \quad y_{n+1} = (1 - \Delta t\lambda)^{-1} y_n = \ldots = (1 - \Delta t\lambda)^{-(n+1)}$$

which only decays to zero if $|1 - \Delta t\lambda| > 1$.

Hence the explicit Euler linear stability region is

$$S = \{z \in \mathbb{C} \ : \ |1 - z| > 1\}$$



From https://en.wikipedia.org/wiki/Backward_Euler_method

LLNL-PRES-852979