Overview of PETSc Time Stepping Solvers

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PDEs, Optimization, and Eigenproblems with PETSc/TAO and SLEPc

EXASCALE COMPUTING PROJECT

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Importance of Numerical ODE/DAE Solvers

Needed for almost all time-dependent simulation

- Analytic solutions are rarely of practical use
- Different problems require fundamentally different solution techniques
- Large differences in efficiency depending on the method used

Two main HPC ODE/DAE Solver Packages

- SUNDIALS - Lawrence Livermore National Laboratory
- PETSc - Argonne National Laboratory
- Trilinos - Sandia National Laboratory - has some limited integrators

ODE/DAEs

$$M(t,u)u_t + A(t,u) = B(t,u)$$

$$u(0) = g$$

- $M(t,u)$ - mass matrix
- $A(t,u)$ - stiff portion of equation
- $B(t,u)$ - nonstiff portion

Linear example

$$u_t - Au = 0$$

PETSc TS API

PETSc abstraction

$$\underbrace{M(t,u)u_t + A(t,u)}_{G(t,u,u_t)} = \underbrace{B(t,u)}_{F(t,u)}$$

$$J_\alpha = \alpha G_{u_t} + G_u$$

- User provides
  - **FormRHSFunction**(ts, t, x, F, void *ctx);
  - **FormIFunction**(ts, t, x, xdot, G, void *ctx);
  - **FormIJacobian**(ts, t, x, xdot, alpha, J, Jp, void *ctx);
- The abstraction is general enough to support a wide range of problems
  - $M = \mathbf{I} \Rightarrow$ textbook ODE formulation $u_t = F(t,u)$ and $G_{u_t} = \mathbf{I}$
  - $M = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & 0 \end{pmatrix} \Rightarrow$ Differential Algebraic equation (DAE)
- The Jacobian matrix can be passed down to SNES without extra matrix assembly
- Single step interface so user can have own time loop
- Many holes in the step function for flexibility
  - **TSPreStage(), TSPostStage(), TSPreStep(), TSPostStep(), TSPostEvent()**

PETSc offers a large collection of time integrators

TS Name	Method	Class	Type	Order
euler	forward Euler	one-step	explicit	1
ssp	multistage SSP	Runge-Kutta	explicit	≤ 4
beuler	backward Euler	one-step	implicit	1
cn	Crank-Nicolson	one-step	implicit	2
theta	theta-method	one-step	implicit	≤ 2
alpha(2)	alpha-method	one-step	implicit	2
glle	general linear	general linear	implicit	≤ 3
eimex	extrapolated IMEX	one-step	≥ 1, adaptive	
arkimex	IMEX Runge-Kutta	IMEX Runge-Kutta	IMEX	$1-5$
rosw	Rosenbrock-W	Rosenbrock-W	linearly implicit	$1-4$
glee	method with global error estimation	general linear	explicit/implicit	$1-4$
bdf	standard BDF methods	multistep	implicit	$1-6$
sundials	standard BDF methods	multistep	implicit	variable
basicsymplectic	symplectic methods	one-step	explicit	$1-4$

High higher methods approximate the time derivative with higher order finite differences

- multistep - Use previous solutions (steps) to approximate the time derivatives
- multistage - Use new intermediate solutions (stages) to approximate the time derivatives

Implicit Explicit schemes

Treat the stiff portion of the equation implicitly and the rest explicitly

$$M(t,u^n)\frac{u^{n+1}-u^n}{\Delta t}+A(t,u^{n+1})=B(t,u^n)$$

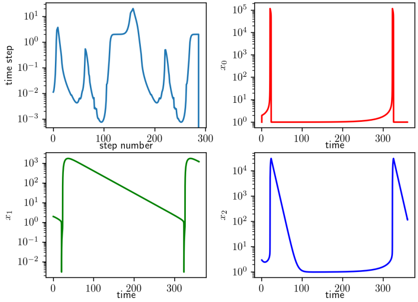
PETSc implements additive Runge-Kutta methods (ARKIMEX)

- Can have L-stable DIRK for stiff part G, SSP explicit part, etc.
- Orders 2 through 5, embedded error estimates
- Dense output, hot starts for Newton
- Extensible adaptive controllers, can change order within a family
- Easy to register new methods: TSARKIMEXRegister()

Rosenbrock schemes

Rosenbrock methods are linearly implicit versions of implicit Runge-Kutta methods. They use explicit function evaluations and implicit linear solves

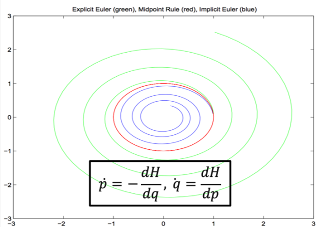
- Faster than the implicit RK because at each stage only a linear system needs to be solved
- Suitable for stiff problems and DAEs and PDAEs
- Approximated Jacobian leads to W-methods



Chemical reaction problem OREGO (TS ex8 OREGO)

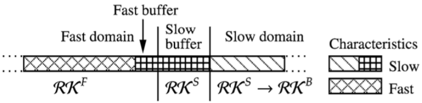
Other partitioned schemes

- Symplectic time integration methods



Separable Hamiltonian system

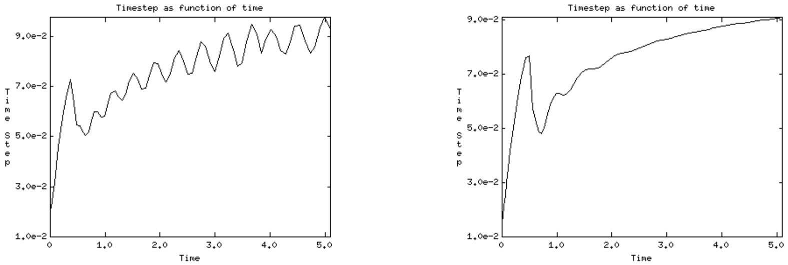
- Partitioned multi-rate Runge-Kutta methods



- Component-wise partitioning based on **TSRHSSplit** (similar to **FieldSplit**)
- Recent new additions, being actively developed

Adaptive Time Stepping

- Estimate the local truncation error induced by the finite differencing in time at each time step by integrating again with a higher order scheme
- Adjust the time-step to keep the local truncation error below a prescribed value
- May decrease or increase the time step
- Can lead to much more efficient (and accurate) computation of the solution
- **Usage** `-ts_adapt_type <basic> | <cfl> | <dsp> | <none>`



basic vs. **DSP** (TS ex11 advection equation)
[courtesy of Lisandro Dalcin]

TSEvent

- Support discontinuous dynamical systems
- Example 1

$$\begin{cases} x - x^{+} = 0, & \text{if } x \geq x^{+} \\ x - x^{-} = 0, & \text{if } x \leq x^{-} \\ \dot{x} = f(x), & \text{otherwise.} \end{cases}$$

- Example 2

$$\begin{cases} \dot{x} = f_1(x), & \text{if } g(t,x) < 0 \\ \dot{x} = f_2(x), & \text{if } g(t,x) \leq 0 \end{cases}$$

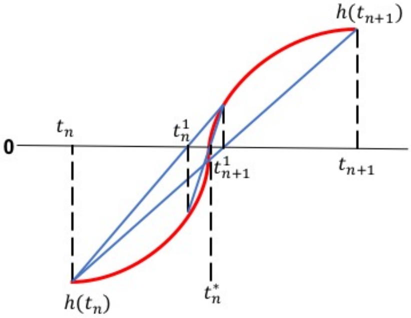
- TS performs integration along with finding “events” – zero crossings of a user-defined function

Event detection and location

- Event detection

$$sign(h(t_n)) \neq sign(h(t_{n+1}))$$

- Event location
  - use interpolation and successively shrink the time boundaries



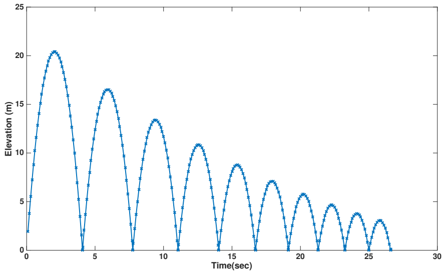
[courtesy of Shrirang Abhyankar]

Usage of TSEvent

```
TSSetEventHandler(TS ts,PetscInt nevents,PetscInt direction[],
  PetscBool terminate[],(*eventfun)(...),(*posteventfun)(...),void *ctx);
```

- nevents – total number of events (can handle multiple event within a timestep)
- direction – type of zero crossing detection
- terminate - terminate on event detection?
- eventmonitor – event monitoring function
- postevent – post-event handling routine

Bouncing ball example(TS ex40)



- Dynamics

$$\begin{cases} u_t = v \\ v_t = -9.8 \end{cases}$$

- Event function $u = 0$
- Post-event function $v = 0.9v$ ($\%10$ reduction in speed)

Takeaways

- PETSc provides a wide variety of high quality, scalable ODE/DAE integrators with different stability and conservation properties
- The TS API supports explicit, implicit and partitioned time integration methods and allows for easy switch between these at runtime
- Adaptive time-stepping provides an inexpensive way to to efficiently integrate ODEs/DAEs
- Event detection and handling enables simulation of hybrid dynamical systems