Time Integration

Presented to
ATPESC 2017 Participants

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ATPESC Numerical Software Track

EXASCALE COMPUTING PROJECT

Outline

- Software
- Definition of ODEs and DAEs
- Stability and stability restrictions
- Implicit vs. explicit methods
- Stiffness
- Linear multistep methods
- Multistage methods and additive multistage methods
- Need for solvers
- Adaptive methods
- Rootfinding
- Data use
- SUNDIALS
- Summary

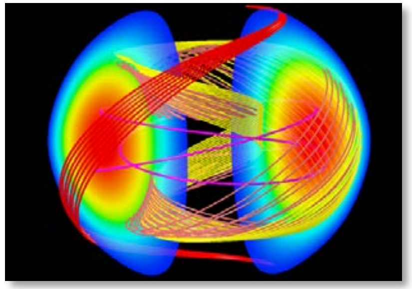
High performance time integration software is available in the DOE in different forms that meet different needs

- ***PETSc:*** TS package, includes DAE and ODE integrators based on variable step multistage methods and additive multistage methods, C
- ***Trilinos:*** Rythmos and Chronos, include ODE and DAE integrators, C++
- ***SUNDIALS:*** Variable step and variable order linear multistep methods, variable step multistage and additive multistage methods, C

While there are numerous integration packages, this talk will emphasize the way SUNDIALS handles each of presented topics

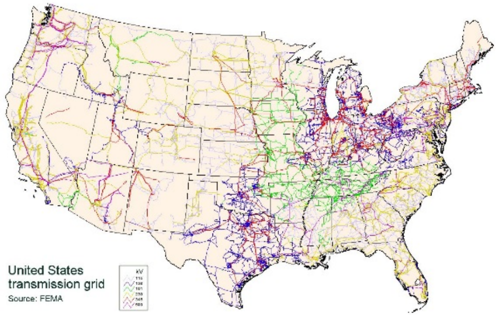
ODEs and DAEs arise in numerous application areas

- Ordinary Differential Equations (ODEs) $\dot{y} = f(t, y)$
  - Method of lines discretization of PDEs: *f* embeds all of the discrete spatial operations
  - Chemical reactions: *f* includes terms for each reaction



Magnetic reconnection

- Differential Algebraic Equations (DAEs) $F(t, y, \dot{y}) = 0, \quad y(0) = y_0$
  - Method of lines discretization of PDEs with algebraic constraints
  - Transmission power system models: *F* includes differential equations for power generators and a large network-based algebraic system constraining power flow
  - Circuit models
  - If $\partial F / \partial \dot{y}$ is invertible, we solve for $\dot{y}$ to obtain an ordinary differential equation (ODE), but this is not always the best approach
  - Else, the system is a differential algebraic equation (DAE)



US Transmission grid
(Wikimedia Commons)

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Stability is a key concept when discussing time integration

Dalquist test equation: $\dot{y} = \lambda y, \quad y_0 = 1$

Exact solution: $y(t_n) = y_0 e^{\lambda t_n}$

If Re(λ)<0, then $|y(t_n)|$ decays exponentially, and we cannot tolerate growth in y_n

Absolute stability requirement

$$|y_n| \leq |y_{n-1}|, \quad n = 1,2,\ldots$$

Region of absolute stability of an integrator: $S = \{z \in C; |R(z)| \leq 1\}$

where an integrator can be written as $y_n = R(z)y_{n-1}$, with time advance $z = h\lambda$

Forward and backward Euler show different stability restrictions

- Forward Euler: $y_n = y_{n-1} + h(\lambda y_{n-1}) \Rightarrow R(z) = 1 + h\lambda$

So, if λ < 0, FE has the step size restriction: $h \le \dfrac{2}{-\lambda}$

Forward Euler is an explicit method

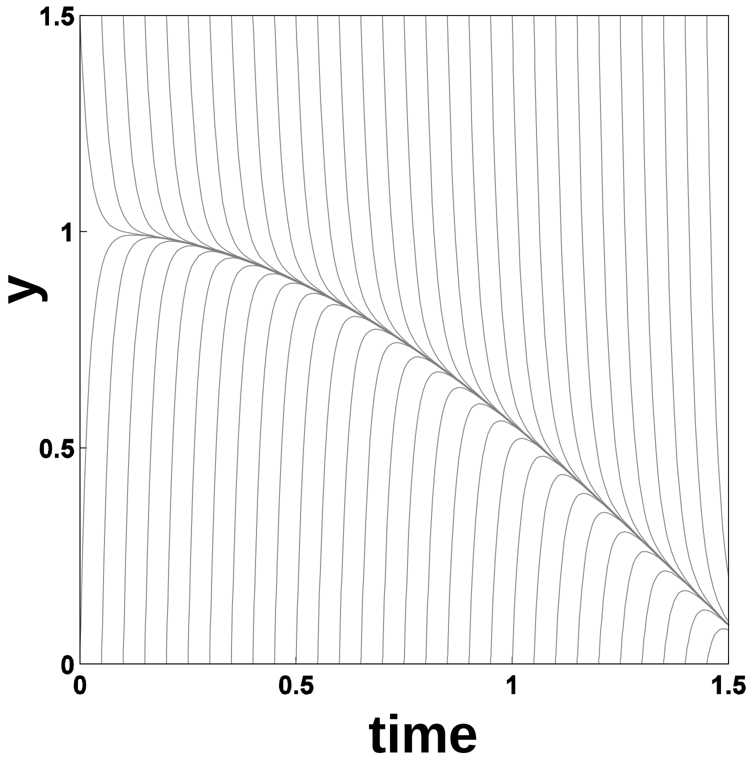
- Backward Euler: $y_n = y_{n-1} + h(\lambda y_n) \Rightarrow R(z) = \dfrac{1}{1 - h\lambda}$

So, if λ < 0, BE has the step size restriction: $h > 0$

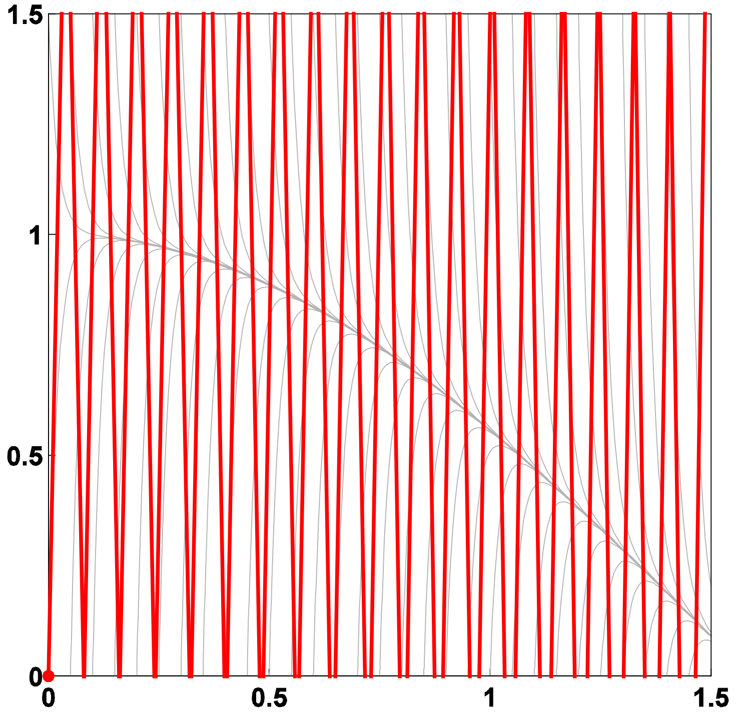
Backward Euler is an implicit method

Curtiss and Hirchfelder example demonstrates what can happen with failure to meet the stability step restriction

$$\dot{y} = -50(y - \cos(t)) \quad \lambda = -50$$



Solution curves



Forward Euler
h=2.01/50

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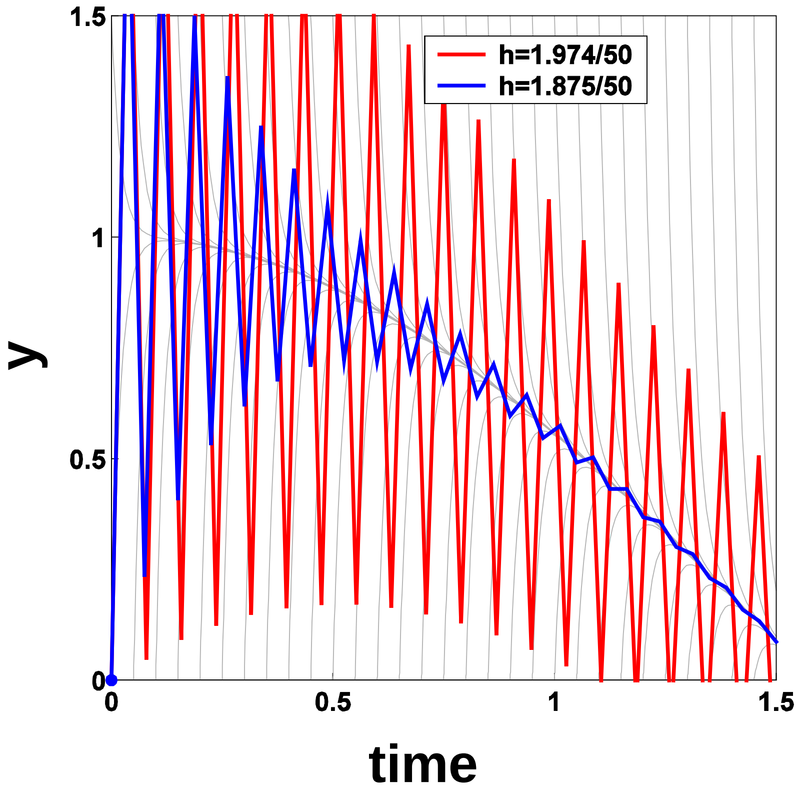
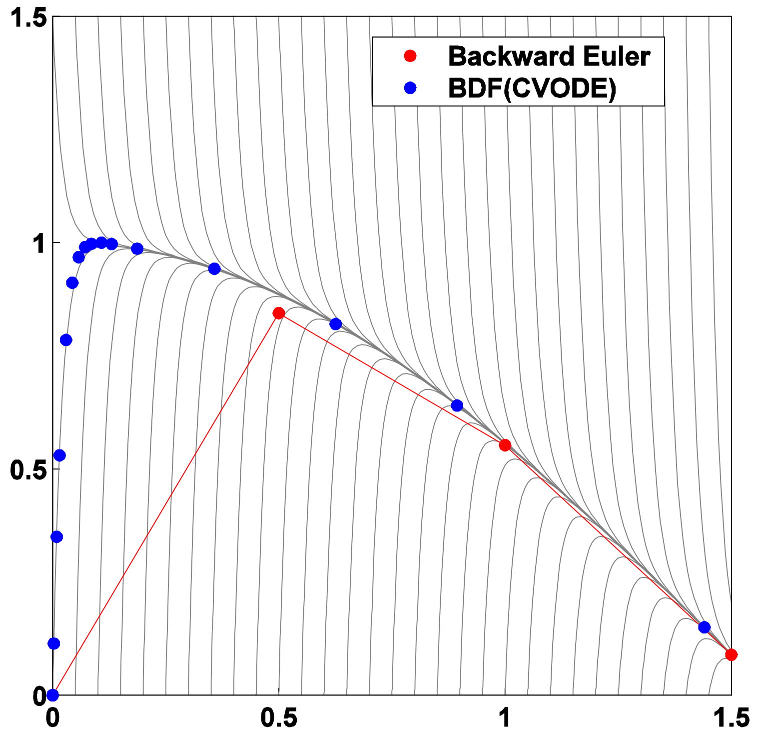
Meeting the restriction with an explicit method or using an implicit method makes a difference!

$$\dot{y} = -50\left(y - cos(t)\right) \quad \lambda = -50$$



Forward Euler



Implicit schemes
h=0.5 for BE

Explicit and implicit approaches should be selected based on needs of the problem

Explicit Methods

✓Easy to conceptualize

✓Easy to code

✓Do not require solvers

X Stability limits on step sizes

X Tracks fastest dynamics

Implicit Methods

✓Less or nonexistent stability limits

✓Steps over fastest dynamics

X Require linear and/or nonlinear solvers

X Solvers generally require coupling over all unknowns

X Code complexity higher

Implicit methods are most useful when fast dynamics of little interest are present, and accuracy requirements would dictate a much larger time step for resolution

For any time-dependent system, need to know if it is stiff before choosing a numerical solution approach

- (Ascher and Petzold, 1998): If the system has widely varying time scales, and the phenomena that change on fast scales are *stable*, then the problem is stiff
- Stiffness depends on
  - Jacobian eigenvalues, λ_j
  - System dimension
  - Accuracy requirements
  - Length of simulation
- In general a problem is stiff on $[t_0, t_1]$ if $(t_1 - t_0) \min_j \Re(\lambda_j) << -1$
- Due to stability requirements, stiff problems generally require implicit approaches

Implicit approaches for stiff problems often require a very robust nonlinear solver for each time step solution

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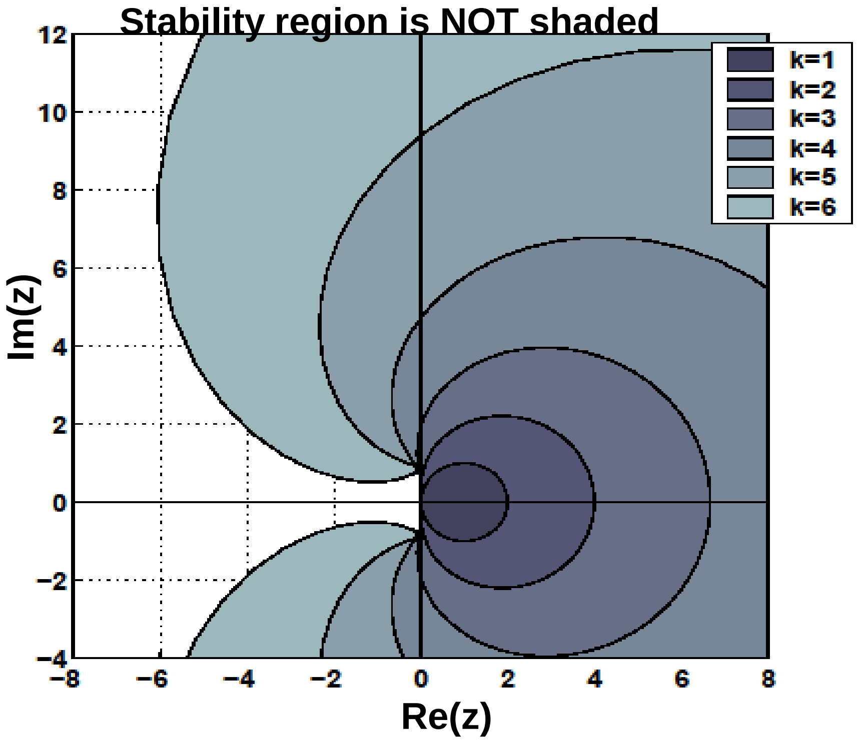
Linear multistep methods construct approximations based on prior states

- Linear Multistep Methods

$$\sum_{j=0}^{K_1} \alpha_{n,j} y_{n-j} + \Delta t_n \sum_{j=0}^{K_2} \beta_{n,j} \dot{y}_{n-j} = 0$$

- Nonstiff Implicit: Adams-Moulton
  - $K_1 = 1$, $K_2 = k$, $k = 1,\ldots,12$
- Stiff: Backward Differentiation Formulas [BDF]
  - $K_1 = k$, $K_2 = 0$, $k = 1,\ldots,5$
- Stiff integrators often use a predictor-corrector scheme:



Explicit predictor to give $y_{n(0)}$

$$y_{n(0)} = \sum_{j=1}^{q} \alpha_j^p y_{n-j} + \Delta t \beta_1^p \dot{y}_{n-1}$$

Implicit corrector with $y_{n(0)}$ as initial iterate

$$y_n = \sum_{j=1}^{q} \alpha_j y_{n-j} + \Delta t \beta_0 f_n(y_n)$$

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Multistage methods construct approximations based on estimates of derivatives at multiple points in a time step

- Multistage methods employ multiple stage solutions

$$\begin{aligned} \mathbf{z_i} &= \mathbf{y_{n-1}} + \mathbf{h_n} \sum_{\mathbf{j=1}}^{\mathbf{s}} \mathbf{a_{i,j} f(t_{n,j}, z_j)}, \quad \mathbf{i = 1, \ldots, s} \\ \mathbf{y_n} &= \mathbf{y_{n-1}} + \mathbf{h_n} \sum_{\mathbf{i=1}}^{\mathbf{s}} \mathbf{b_i f(t_{n,i}, z_i)} \end{aligned}$$

Butcher Tableau

$$\begin{array}{c|cccc} c_1 & a_{1,1} & a_{1,2} & \cdots & a_{1,s} \\ c_2 & a_{2,1} & a_{2,2} & \cdots & a_{2,s} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

- The a’s, b’s, c’s, and s define the method, its order of accuracy, and its stability
- Codes with adaptivity in spatial systems or models cannot easily use multi-step methods due to need to interpolate prior step information
- Runge-Kutta (RK) methods are multistage so do not require prior states
- RK methods require multiple nonlinear solves per time step
- Additive RK methods can apply explicit and implicit methods to a split system allowing consistent approximations while using different methods on each

Additive methods address systems with both stiff and nonstiff components

- Split system into stiff, f_I, and nonstiff, f_E, components $M\dot{y} = f_E(t,y) + f_I(t,y)$
- M may be the identity or any nonsingular mass matrix (e.g. FEM)
- Variable step size additive Runge-Kutta Methods combine explicit (ERK) and diagonally implicit (DIRK) RK methods to enable an ImEx integrator
- Let $t_{n,j} = t_{n-1} + c_j \Delta t_n$:

$$Mz_i = My_{n-1} + h_n \sum_{j=0}^{i-1} A^E_{i,j} f_E(t_{n-1} + c_j h_n, z_j) + h_n \sum_{j=0}^{i} A^I_{i,j} f_I(t_{n-1} + c_j h_n, z_j),$$

$$My_n = My_{n-1} + h_n \sum_{i=0}^{s} b_i \left(f_E(t_{n-1} + c_i h_n, z_i) + f_I(t_{n-1} + c_i h_n, z_i) \right),$$

- Solve for stage solutions, z_i, $i = 1, \ldots, s$, sequentially

Implicit solutions result in nonlinear systems at each time step or stage

- Use predicted value as the initial iterate for the nonlinear solver
- Nonstiff systems: Functional iteration or fixed point iteration

$$y_{n(m+1)} = \beta_0 \Delta t_n f(y_{n(m)}) + \sum_{i=1}^{q} \alpha_{n,i} y_{n-i}$$

- Stiff systems: Newton iteration

$$M\left(y_{n(m+1)} - y_{n(m)}\right) = -G\left(y_{n(m)}\right)$$

ODE $\quad \dot{y} = f(y)$

$M \approx I - \gamma \partial f / \partial y \qquad \gamma = \beta_0 \Delta t_n$

$$G(y_n) \equiv y_n - \beta_0 \Delta t_n f(t, y_n) - \sum_{i=1}^{k} \alpha_{n,i} y_{n-i} = 0$$

DAE $\quad F(\dot{y}, y) = 0$

$M \approx \partial F / \partial y + \gamma \partial F / \partial \dot{y} \qquad \gamma = 1/(\beta_0 \Delta t_n)$

$$G(y_n) \equiv F\left(t, (\beta_0 \Delta t_n)^{-1} \sum_{i=1}^{k} \alpha_{n,i} y_{n-i}, y_n\right) = 0$$

Adaptive methods choose time steps to minimize local truncation error and maximize efficiency

- User-defined tolerances:
  - Absolute tolerance on each solution component, $ATOL^i$
  - Relative tolerance for all solution components, RTOL
- Norm calculations are weighted by: $ewt^i = \frac{1}{RTOL|y^i| + ATOL^i}$
- Errors are measured with a weighted root-mean-square norm:

$$\|y\|_{WRMS} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(ewt^i \cdot y^i)^2}$$

- Choose time steps to bound an estimate of the local truncation error; can do with both multistep and multistage methods

The choice of tolerances is critical to accuracy and efficiency for these adaptive methods

- The relative tolerance controls error relative to the size of the solution
  - RTOL = 10^{-4} means that errors are controlled to 0.01%
  - We do not recommend an RTOL above 10^{-3} nor one close to unit roundoff, 10^{-15}
- The absolute tolerances control the absolute size of error when any solution component may be so small that pure relative error control is meaningless
  - Ex: solution starting at a nonzero value but decaying to a noise level, ATOL should be set to the noise level
  - If different components have different noise levels then want ATOL to be a vector
- In general, want to be a bit conservative with these tolerances
  - Rule of thumb: use tolerances 0.01 below desired limits to ensure global errors are below limit
- But not too conservative as the integrator will work harder to meet tight tolerances

To use these adaptive methods effectively, choose tolerances carefully!

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Rootfinding capabilities are critical in some applications

- Finds roots of solution-dependent user-defined functions, $g_i(t, y) = 0$ or $g_i(t, y, \dot{y}) = 0$
- Important in applications where problem definition may change based on a function of the solution
- Rootfinding is a critical feature for applications like power grid where solution-dependent system adaptations are common, e.g. voltage limit on a generator
- Roots are found by looking at sign changes, so only roots of odd multiplicity are found
- Checks each time interval for sign change
- When sign changes are found, apply a modified secant method with a tight tolerance to identify root

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Time integrator algorithms do not need to rely on specific data layouts

- All operations within the integrator can be conducted on vectors
- Packages define a vector API; users can use their structures coded to this API
- Within SUNDIALS, each vector implementation defines a content structure and all implemented vector operations, along with routines to clone vectors
- For an implicit method, data layouts are used in
  - Specific vector implementations (streaming and reduction)
  - Solvers (linear and/or nonlinear)
  - Problem-defining function evaluations, f and F, and Jacobian evaluations

Using a time integrator on a given machine requires an efficient implementation of the problem-defining functions, as these typically are the dominant cost

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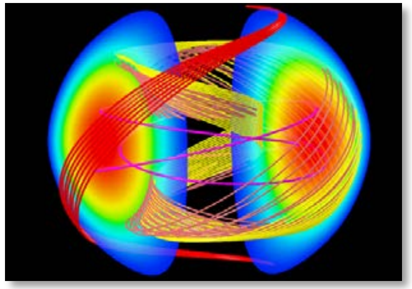
SUNDIALS: SUite of Nonlinear and DIfferential / ALgebraic equation Solvers

- *ODE integrators:*
  - (CVODE/CVODES) variable order and step stiff BDF and non-stiff Adams
  - (ARKode) variable step implicit, explicit, and additive IMEX Runge-Kutta
- *DAE integrators:* (IDA/IDAS) variable order and step stiff integrators
- CVODES and IDAS are equipped with forward and adjoint sensitivity analysis
- *Nonlinear Solver:* (KINSOL) Newton-Krylov, Picard, and accelerated fixed point
- Serial, MPI, openMP, and pthreads vectors; CUDA will be released this fall
- Written in C with interfaces to Fortran
- Designed to be easily incorporated into existing codes
- Modular design allows users to supply their own data structures
- CMAKE-based portable build system
- Freely available (BSD license); >11,000 downloads/year from around the world
- Active user community supported by *sundials-users* email list

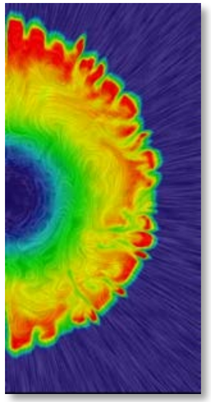
http://www.llnl.gov/CASC/sundials

SUNDIALS has been used worldwide in applications from research and industry

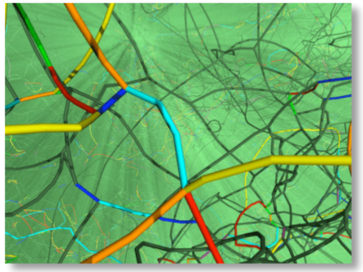
- Power grid modeling (RTE France, LLNL, ISU)
- Simulation of clutches and power train parts (LuK GmbH & Co.)
- Magnetism at the nanoscale (Magpar, Nmag)
- 3D parallel fusion (SMU, U. York, LLNL)
- Spacecraft trajectory simulations (NASA)
- Dislocation dynamics (LLNL)
- Combustion and reacting flows (Cantera)
- Large-scale subsurface flows (Mines, LLNL)
- 3D battery simulation (ORNL - AMPERE)
- Computational modeling of neurons (NEURON)
- Micromagnetic simulations (U. Southampton)
- Released in third party packages:
  - Red Hat Extra Packages for Enterprise Linux (EPEL
  - SciPy – python wrap of SUNDIALS
  - Cray Third Party Software Library (TPSL)



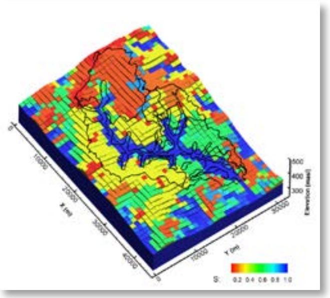
Magnetic reconnection



Core collapse supernova



Dislocation dynamics



Subsurface flow

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Summary

- When choosing a time integration method, need to understand
  - What the time scales in the system are
  - Whether the application requires resolving all time scales
  - Whether the system is stiff
  - Whether the system has adaptivity in the spatial or model components
  - What the accuracy requirements are
- The choice of tolerances can impact both accuracy and performance
- Multistep and multistage methods have different characteristics that may make each better suited to an application
- Implicit methods will need algebraic solvers (nonlinear and/or linear)
- Time integrators can be implemented in a data agnostic way allowing for use of application-specific data structures