Lawrence Livermore National Laboratory

SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers

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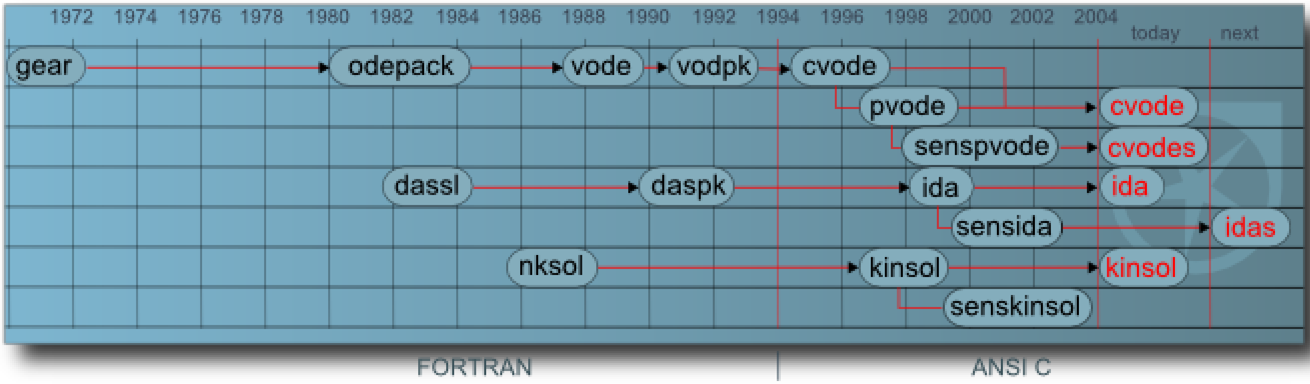
Outline

- SUNDIALS Overview
- ODE and DAE integration
  - Initial value problems
  - Implicit integration methods
- Nonlinear Systems
  - Newton’s method and inexact Newton’s method
  - Preconditioning
- SUNDIALS: usage, applications, and availability
- Upcoming additions

LLNL has a long history of R&D in ODE/DAE methods and software

- Fortran solvers written at LLNL:
  - VODE: stiff/nonstiff ODE systems, with direct linear solvers
  - VODPK: with Krylov linear solver (GMRES)
  - NKSOL: Newton-Krylov solver - nonlinear algebraic systems
  - DASPK: DAE system solver (from DASSL)
- Recent focus has been on sensitivity analysis
- Organized into a single suite, SUNDIALS, written in C and including CVODE and CVODES, IDA, IDAS, and KINSOL



May 2009

Push to solve large, parallel systems motivated rewrites in C

- CVODE: rewrite of VODE/VODPK [Cohen, Hindmarsh, 94]
- PVODE: parallel CVODE [Byrne and Hindmarsh, 98]
- KINSOL: rewrite of NKSOL [Taylor and Hindmarsh, 98]
- IDA: rewrite of DASPK [Hindmarsh and Taylor, 99]
- Sensitivity variants: SensPVODE, SensIDA, SensKINSOL [Brown, Grant, Hindmarsh, Lee, 00-01]
- New sensitivity-capable solvers:
  - CVODES [Hindmarsh and Serban, 02]
  - IDAS [Serban, Petra, and Hindmarsh, 09]

- Organized into a single suite, SUNDIALS, including CVODE and CVODES, IDA, IDAS, and KINSOL

The SUNDIALS package offers Newton solvers, time integration, and sensitivity solvers

- **CVODE: implicit ODE solver, y' = f(y, t)**
  - **Variable-order, variable step BDF (stiff) or implicit Adams (nonstiff)**
  - **Nonlinear systems solved by Newton or functional iteration**
  - **Linear systems by direct (dense or band) or iterative solvers**
- **IDA: implicit DAE solver, F(t, y, y') = 0**
  - **Variable-order, variable step BDF**
  - **Nonlinear system solved by Newton iteration**
  - **Linear systems by direct (dense or band) or iterative solvers**
- **KINSOL: Newton solver, F(u) = 0**
  - **Inexact and Modified (with dense solve) Newton**
  - **Linear systems by iterative or dense direct solvers**
- **CVODES: sensitivity-capable (forward & adjoint) CVODE**
- **IDAS: sensitivity-capable (forward & adjoint) IDA**
- **Iterative linear Krylov solvers: GMRES, BiCGStab, TFQMR**

SUNDIALS was designed to easily interface with legacy codes

- **Philosophy: *Keep codes simple to use***
- **Written in C**
  - **Fortran interfaces: FCVODE, FIDA, and FKINSOL**
  - **Matlab interfaces: sundialsTB (CVODES, IDA, & KINSOL)**
- **Written in a data structure neutral manner**
  - **No specific assumptions about data**
  - **Application-specific data representations can be used**
- **Modular implementation**
  - **Vector modules**
  - **Linear solver modules**
- **Require minimal problem information, but offer user control over most parameters**

Initial value problems (IVPs) come in the form of ODEs and DAEs

- The general form of an IVP is given by

$$F(t, \dot{x}, x) = 0$$
$$x(t_0) = x_0$$

- **If $\partial F / \partial \dot{x}$ is invertible, we solve for $\dot{x}$ to obtain an ordinary differential equation (ODE), but this is not always the best approach**
- **Else, the IVP is a differential algebraic equation (DAE)**

- **A DAE has differentiation index *i* if *i* is the minimal number of analytical differentiations needed to extract an explicit ODE**

Stiffness of an equation can significantly impact whether implicit methods are needed

- (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

$$\boxed{(t_1 - t_0)\min_j \Re(\lambda_j) << -1}$$

Dalquist test problem shows impact of stability on step sizes for explicit and implicit methods

Dalquist test equation: $\dot{y} = \lambda y, \; y(0) = y_0$

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

Absolute stability requirement

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

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

Region of absolute stability of an integrator written as:

$y_n = R(z)y_{n-1}$, with time step $z = h\lambda$

$$S = \{z \in C; |R(z)| \le 1\}$$

Forward and backward Euler show different stability restrictions

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

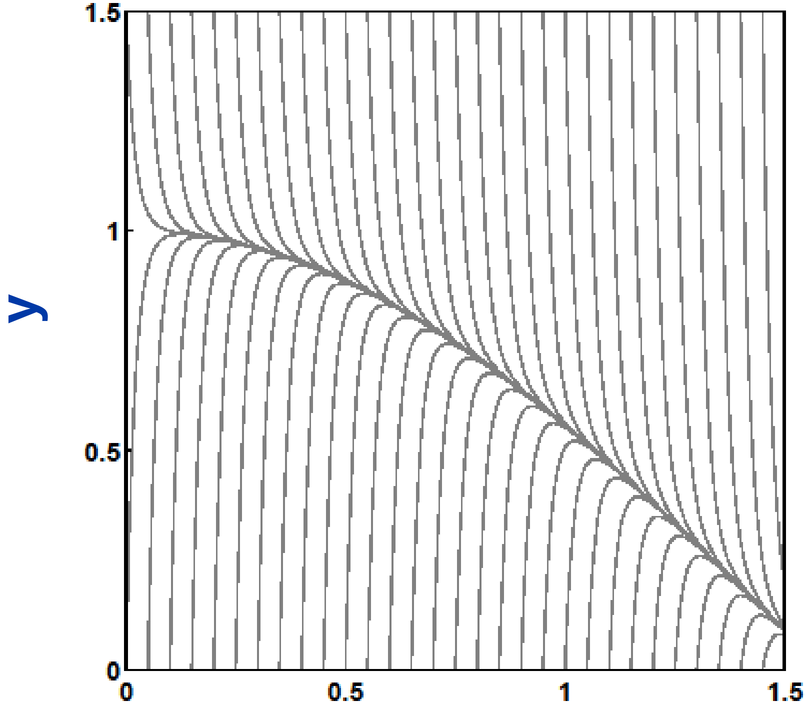
So, if λ < 0, FE has the step size restriction: $\boldsymbol{h \le \frac{2}{|\lambda|}}$

- Backward Euler: $\boldsymbol{y_n = y_{n-1} + h(\lambda y_n) \Rightarrow R(z) = \left|\frac{1}{1 - h\lambda}\right|}$

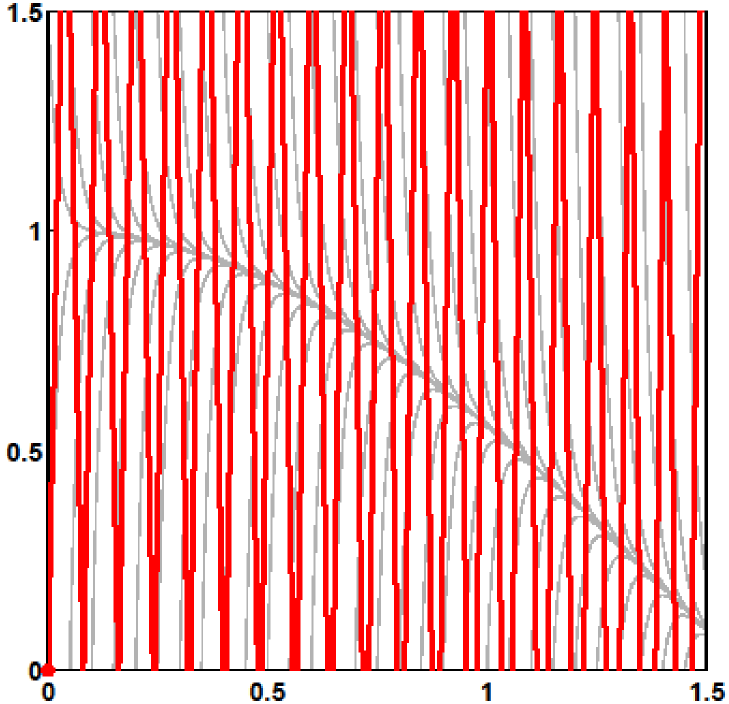
So, if λ < 0, BE has the step size restriction: $\boldsymbol{h > 0}$

Curtiss and Hirchfelder example

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



Solution curves

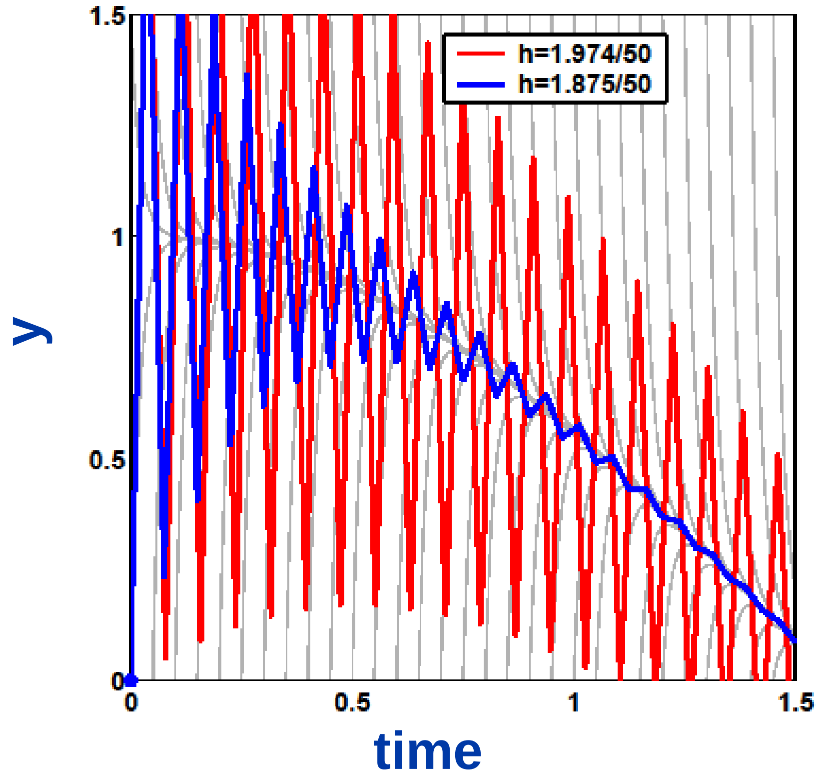


Forward Euler

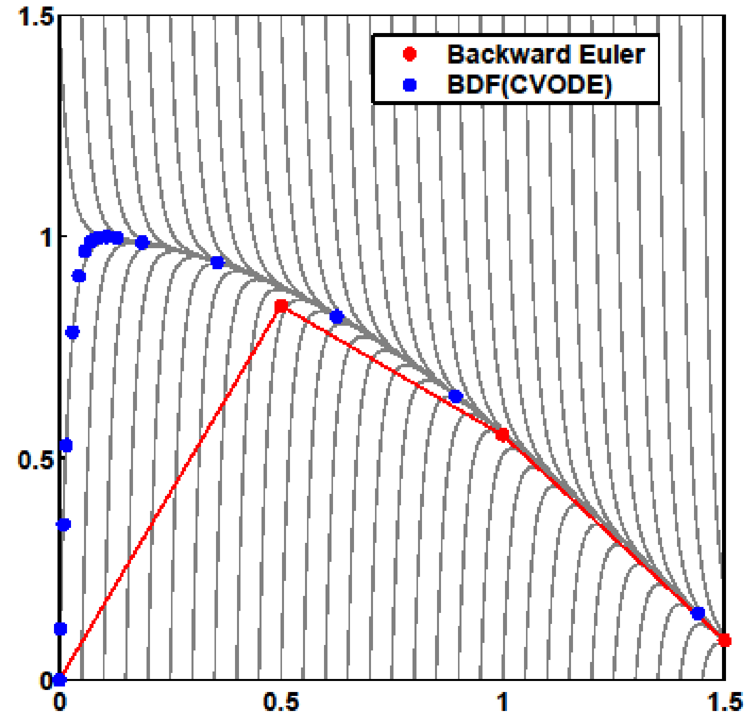
h=2.01/50

Curtiss and Hirchfelder example

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



Forward Euler



Implicit schemes

h=0.5 for BE

SUNDIALS has implementations of Linear Multistep Methods (LMM)

General form of LMM: $$\sum_{i=0}^{K_1} \alpha_{n,i} y_{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} \dot{y}_{n-i} = 0$$

- Two methods:
  - Adams-Moulton (nonstiff); $K_1 = 1$, $K_2 = k$, $k = 1,\ldots,12$
  - BDF (stiff); $K_1 = k$, $K_2 = 0$, $k = 1,\ldots,5$

- Nonlinear systems (BDF)
  - ODE:

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

  - DAE:

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

Stability is very restricted for higher orders of BDF methods

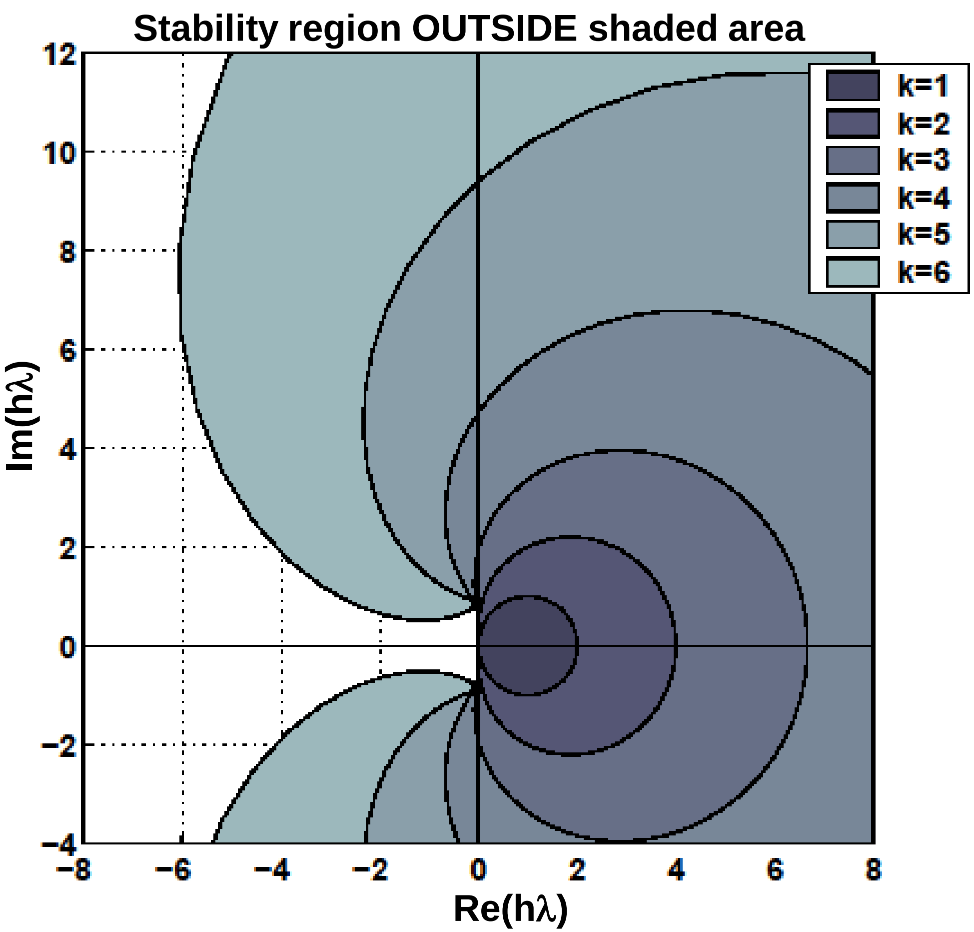
$$y_n - \beta_0 h_n \dot{y}_n = \sum_{i=1}^{k} \alpha_{n,i} y_{n-i}$$

Regions of instability grow with the order

CVODE and IDA allow up to order 5

CVODE includes an optional stability limit detection algorithm:

- **Based on linear analysis**
- **Limits step if it detects a potential stability problem**



CVODE solves $\dot{y} = f(t, y)$

- Variable order and variable step size methods:
  - BDF (backward differentiation formulas) for stiff systems
  - Implicit Adams for nonstiff systems
- (Stiff case) Solves time step for the system $\dot{y} = f(t, y)$
  - applies an explicit predictor to give $y_{n(0)}$

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

  - applies an implicit corrector with $y_{n(0)}$ as the initial guess

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

Time steps and order are chosen to minimize the local truncation error

- Time steps are chosen by:
  - Estimate the error: $E(\Delta t) = C(y_n - y_{n(0)})$
    - Accept step if $||E(\Delta t)||_{WRMS} < 1$
    - Reject step otherwise
  - Estimate error at the next step, $\Delta t'$, as

$$E(\Delta t') \approx (\Delta t' / \Delta t)^{q+1} E(\Delta t)$$

  - Choose next step so that $||E(\Delta t')||_{WRMS} < 1$
- Choose method order by:
  - Estimate error for next higher and lower orders
  - Choose the order that gives the largest time step meeting the error condition

Computations weighted so no component disproportionally impacts convergence

- An absolute tolerance is specified for each solution component, ATOL^i
- A relative tolerance is specified for all solution components, RTOL
- Norm calculations are weighted by:

$$\mathbf{ewt}^{i} = \frac{1}{\mathbf{RTOL}\cdot\left|\mathbf{y}^{i}\right| + \mathbf{ATOL}^{i}} \qquad \|\mathbf{y}\|_{\mathbf{WRMS}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{ewt}^{i}\cdot\mathbf{y}^{i}\right)^{2}}$$

- Bound time integration error with:

$$\left\|\mathbf{y}_{n} - y_{n(0)}\right\| < \tfrac{1}{6}$$

The 1/6 factor tries to account for estimation errors

Nonlinear system will require nonlinear solves

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

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

- Stiff systems: Newton iteration

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

  - ODE: $M \approx I - \gamma\,\partial f/\partial y, \quad \gamma = \beta_0 h_n$
  - DAE: $M \approx \partial F/\partial y + \gamma\,\partial F/\partial \dot{y}, \quad \gamma = 1/\left(\beta_0 h_n\right)$

SUNDIALS provides many options for linear solvers

- Iterative linear solvers
  - Result in inexact Newton solver
  - Scaled preconditioned solvers: GMRES, Bi-CGStab, TFQMR
  - Only require matrix-vector products
  - Require preconditioner for the Newton matrix, *M*
- Jacobian information (matrix or matrix-vector product) can be supplied by the user or estimated with finite difference quotients
- Two options require serial environments and some pre-defined structure to the data
  - Direct dense
  - Direct band

An inexact Newton-Krylov method can be used to solve the implicit systems

- Krylov iterative methods find the linear system solution in a Krylov subspace: $K(J,r) = \{r, \quad Jr, \quad J^2 r, \quad \ldots\}$
- Only require matrix-vector products
- Difference approximations to the matrix-vector product are used,

$$J(x)v \approx \frac{F(x + \theta v) - F(x)}{\theta}$$

- Matrix entries need never be formed, and memory savings can be used for a better preconditioner

IDA solves $F(t, y, y') = 0$

- C rewrite of DASPK [Brown, Hindmarsh, Petzold]
- Variable order / variable coefficient form of BDF
- Targets: implicit ODEs, index-1 DAEs, and Hessenberg index-2 DAEs
- Optional routine solves for consistent values of y_0 and y_0'
  - Semi-explicit index-1 DAEs, differential components known, algebraic unknown OR all of y_0' specified, y_0 unknown
- Nonlinear systems solved by Newton-Krylov method

- Optional constraints: $y^i > 0$, $y^i < 0$, $y^i \geq 0$, $y^i \leq 0$

KINSOL solves $F(u) = 0$

- C rewrite of Fortran NKSOL (Brown and Saad)
- Inexact Newton solver: solves $J\,\Delta u^n = -F(u^n)$ approximately
- Modified Newton option (with direct solves) – this freezes the Newton matrix over a number of iterations
- Krylov solver: scaled preconditioned GMRES, TFQMR, Bi-CGStab
  - Optional restarts for GMRES
  - Preconditioning on the right: $(J\,P^{-1})(Ps) = -F$
- Direct solvers: dense and band (serial & special structure)
- Optional constraints: $u_i > 0$, $u_i < 0$, $u_i \geq 0$ or $u_i \leq 0$
- Can scale equations and/or unknowns
- Dynamic linear tolerance selection

An inexact Newton's method is used to solve the nonlinear problem

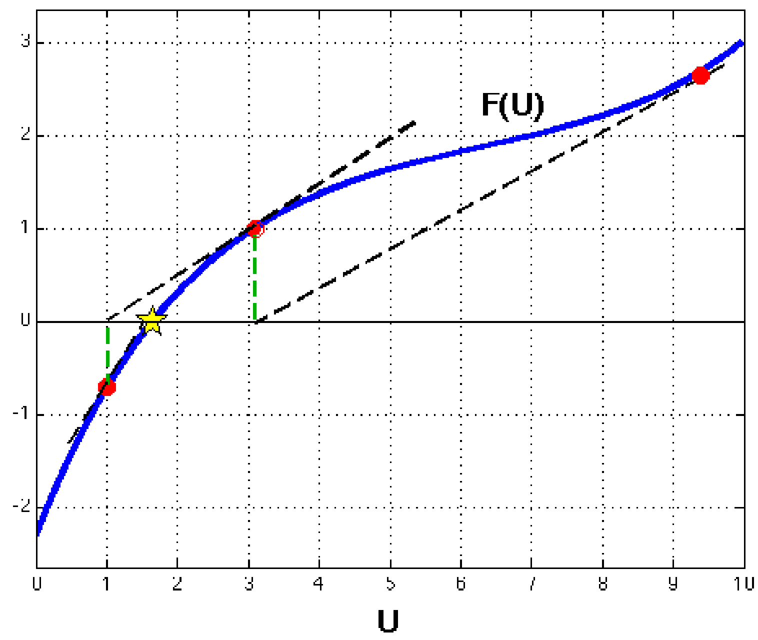
1. Starting with x^0, want x^* such that $F(x^*) = 0$

2. Repeat for each k until $\left\| \mathbf{F}(\mathbf{x}^{k+1}) \right\| \leq \mathbf{tol}$

   a. Solve (approximately)

   $$\mathbf{J}(\mathbf{x}^k)\mathbf{s}^k = -\mathbf{F}(\mathbf{x}^k)$$

   b. Update, $x^{k+1} = x^k + \lambda s^k$



courtesy of D. Reynolds (SMU)

- tol may be chosen adaptively based on accuracy requirements
- λ is a search parameter
- $\|.\|$ is a weighted L-2 norm

Linear stopping tolerances must be chosen to prevent "oversolves"

The linear system is solved to a given tolerance:

$$\left\| \mathbf{F}(\mathbf{x}^{k}) + \mathbf{J}(\mathbf{x}^{k})\mathbf{s}^{k+1} \right\| \leq \eta^{k} \left\| \mathbf{F}(\mathbf{x}^{k}) \right\|$$

- Newton method assumes a linear model
  - Bad approximation far from solution, loose tol.
  - Good approximation close to solution, tight tol.
- Eisenstat and Walker (SISC 96)
  - Choice 1 $\eta^{k} = \left| \left\| F^{k} \right\| - \left\| F^{k-1} - J^{k-1} s^{k-1} \right\| \right| \Big/ \left\| F^{k-1} \right\|$
  - Choice 2 $\eta^{k} = 0.9 \left(\left\| \mathbf{F}^{(k)} \right\| \Big/ \left\| \mathbf{F}^{(k-1)} \right\| \right)^{2}$
- ODE literature $\eta^{k} = 0.05$

Inexact methods maintain the fast rate of convergence of Newton's method

- Convergence of Newton's method is *q-quadratic* locally, for some constant C

$$\left\| \mathbf{x}^{k+1} - \mathbf{x}^{*} \right\| \le \mathbf{C} \left\| \mathbf{x}^{k} - \mathbf{x}^{*} \right\|^{2}$$

- Convergence of an inexact Newton method is
  - *q-linear* if η^{k} is constant in *k*
  - *q-super-linear* if $\lim_{k \to \infty} \eta^{k} = 0$
  - *q-quadratic* if for some constant C

$$\left\| \mathbf{F}(\mathbf{x}^{k}) + \mathbf{J}(\mathbf{x}^{k}) \mathbf{s}^{k+1} \right\| \le \mathbf{C} \left\| \mathbf{F}(\mathbf{x}^{k}) \right\|^{2}$$

- Eisenstat and Walker methods are *q-quadratic*

Line-search globalization for Newton's method can enhance robustness

- User can select:
  - Inexact Newton
  - Inexact Newton with line search
- Line searches can provide more flexibility in the initial guess (larger time steps)
- Take, $x^{k+1} = x^k + \lambda s^{k+1}$, for λ chosen appropriately (to satisfy the Goldstein-Armijo conditions):
  - sufficient decrease in F relative to the step length
  - minimum step length relative to the initial rate of decrease
  - full Newton step when close to the solution

Preconditioning is essential for large problems as Krylov methods can stagnate

- Preconditioner P must approximate Newton matrix, yet be reasonably efficient to evaluate and solve.
- Typical P (for time-dep. ODE problem) is $I - \gamma \tilde{J}, \quad \tilde{J} \approx J$
- The user must supply two routines for treatment of P:
  - Setup: evaluate and preprocess P (infrequently)
  - Solve: solve systems Px=b (frequently)
- User can save and reuse approximation to J, as directed by the solver
- SUNDIALS offers hooks for user-supplied preconditioning
- Band and block-banded preconditioners are supplied for use with the supplied vector structure

Sensitivity Analysis

- Sensitivity Analysis (SA) is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation in inputs.
- Applications:
  - Model evaluation (most and/or least influential parameters), Model reduction, Data assimilation, Uncertainty quantification, Optimization (parameter estimation, design optimization, optimal control, …)
- Approaches:
  - Forward sensitivity analysis
  - Adjoint sensitivity analysis

The SUNDIALS vector module is generic

- Data vector structures can be user-supplied
- The generic NVECTOR module defines:
  - A `content` structure (void *)
  - An `ops` structure – pointers to actual vector operations supplied by a vector definition
- Each implementation of NVECTOR defines:
  - Content structure specifying the actual vector data and any information needed to make new vectors (problem or grid data)
  - Implemented vector operations
  - Routines to clone vectors
- Note that all parallel communication resides in reduction operations: dot products, norms, mins, etc.

SUNDIALS provides serial and parallel NVECTOR implementations

- *Use is optional*

- Vectors are laid out as an array of doubles (or floats)
- Appropriate lengths (local, global) are specified
- Operations are fast since stride is always 1
- All vector operations are provided for both serial and parallel cases
- For the parallel vector, MPI is used for global reductions

- These serve as good templates for creating a user-supplied vector structure around a user's own existing structures

SUNDIALS provides Fortran interfaces

- CVODE, IDA, and KINSOL
- Cross-language calls go in both directions:
- Fortran user code ←→ interfaces ←→ CVODE/KINSOL/IDA

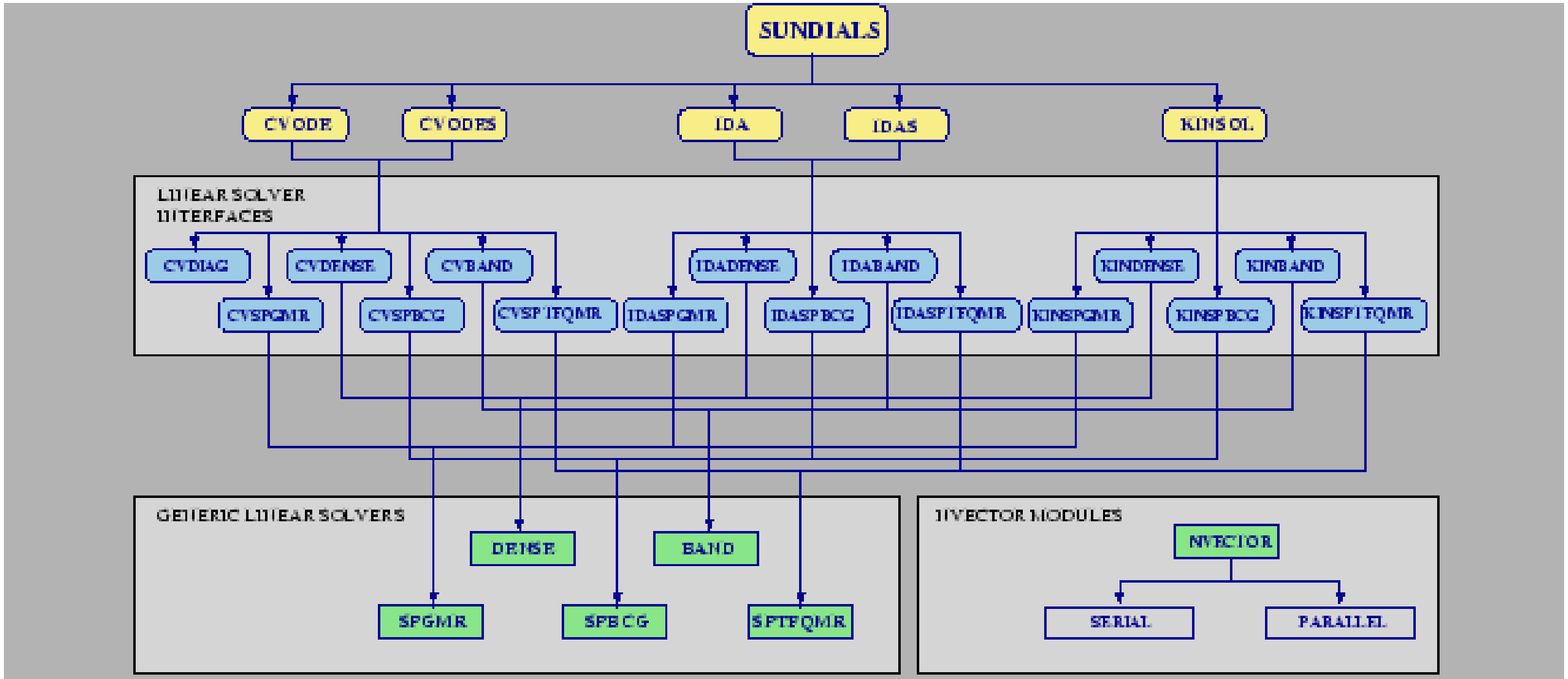
- Fortran main → interfaces to solver routines
- Solver routines → interface to user's problem-defining routine and preconditioning routines

- For portability, all user routines have fixed names
- Examples are provided

SUNDIALS provides Matlab interfaces

- CVODES, KINSOL, and IDAS
- The core of each interface is a single MEX file which interfaces to solver-specific user-callable functions
- Guiding design philosophy: make interfaces equally familiar to both SUNDIALS and Matlab users
  - all user-provided functions are Matlab m-files
  - all user-callable functions have the same names as the corresponding C functions
  - unlike the Matlab ODE solvers, we provide the more flexible SUNDIALS approach in which the 'Solve' function only returns the solution at the next requested output time.
- Includes complete documentation (including through the Matlab help system) and several examples

Structure of SUNDIALS



High-level diagram (note that none of the Lapack-based linear solver modules are represented.)

SUNDIALS code usage is similar across the suite

- Have a series of Set/Get routines to set options
- For CVODE with parallel vector implementation:

```
#include “cvode.h”
#include “cvode_spgmr.h”
#include “nvector_*.h”

y = N_VNew_*(n,…);
cvmem = CVodeCreate(CV_BDF,CV_NEWTON);
flag = CVodeSet*(…);
flag = CVodeInit(cvmem,rhs,t0,y,…);
flag = CVSpgmr(cvmem,…);
for(tout = …) {
   flag = CVode(cvmem, …,y,…);  }

NV_Destroy(y);
CVodeFree(&cvmem);
```

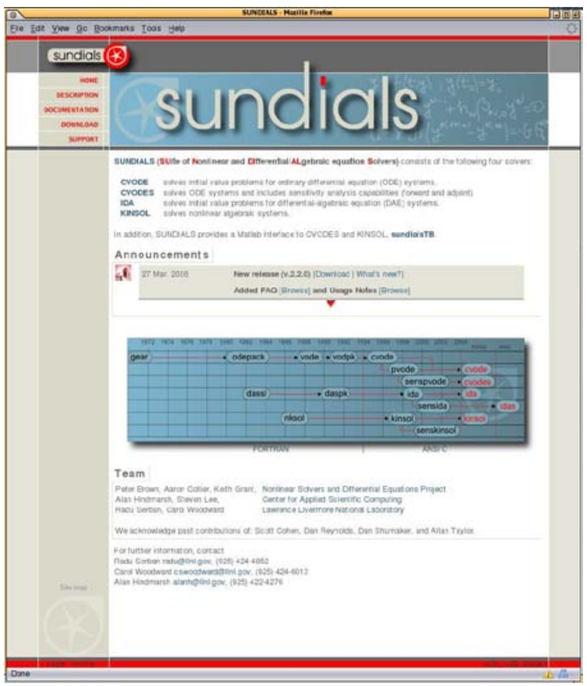
Availability

Open source BSD license

https://computation.llnl.gov/casc/sundials

Publications

https://computation.llnl.gov/casc/sundials/documentation/documentation.html



Web site:

Individual codes download

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User manuals

User group email list

The SUNDIALS Team:

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