SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers

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Outline

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- ODE integration
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  - ARKode
- DAE integration
  - IDA
- Sensitivity Analysis
- Nonlinear Systems
  - KINSOL
  - Fixed point solver
- SUNDIALS: usage, applications, and availability

SUite of Nonlinear and DIfferential-ALgebraic Solvers

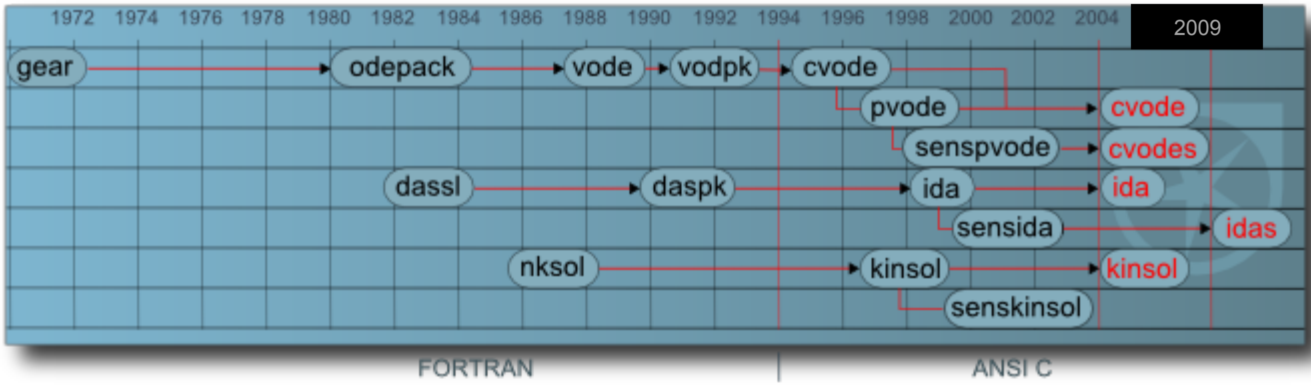
- Suite of time integrators and nonlinear solvers
  - ODE and DAE time integrators with forward and adjoint sensitivity capabilities, Newton-Krylov nonlinear solver
  - Written in C with interfaces to Fortran and Matlab
  - Designed to be incorporated into existing codes
  - Modular implementation: users can supply own data structures
    - Linear solvers / preconditioners
    - Vector structures – core data structure for all the codes
    - Supplied with serial and MPI parallel structures
- Freely available, released under BSD license

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

LLNL has a strong history of nonlinear solver and time integration research

SUNDIALS package evolved from innovation in methods and software

- Newton solvers evolved from the first Newton-Krylov method and code for PDEs
- ODE codes from odepack (> 200K downloads)
- DAE codes from DASSL



SUNDIALS 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
- CVODES and IDAS: sensitivity-capable (forward & adjoint)
- Adaptive time step and order selection minimize local truncation error
- KINSOL: Newton solver, F(u) = 0
  - Inexact and Modified (with dense solve) Newton
  - Linear systems by iterative or dense direct solvers
- Iterative linear Krylov solvers: GMRES, BiCGStab, TFQMR

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

- Variable order and variable step size Linear Multistep Methods

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

- Adams-Moulton (nonstiff); K_1 = 1, K_2 = k, k = 1,…,12
- Backward Differentiation Formulas [BDF] (stiff); K_1 = k, K_2 = 0, k = 1,…,5
- Rootfinding capability - finds roots of user-defined functions, $g_i(t,y)$
- The stiff solvers execute 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

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

Convergence and errors are measured against user-specified tolerances

- 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:

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

- Bound time integration error with:

$$\|y_n - y_{n(0)}\| < \frac{1}{6}$$

The 1/6 factor tries to account for estimation errors

Time steps 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, Δt’, 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

Nonlinear systems at each time step will require nonlinear solves

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

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

- Stiff systems: Newton iteration

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

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

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

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

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

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

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

CVODE offers Newton, Newton-Krylov and function iteration as nonlinear solvers

- Non-stiff systems can use function iteration, or a fixed point solver
- Stiff systems generally require a Newton nonlinear solver
  - SUNDIALS provides dense solvers or hooks to LAPACK
    - Can reuse Jacobian over multiple steps -> modified Newton
  - Newton-Krylov solvers only require matrix-vector products
    - Approximations to the matrix-vector product are used,

$$J(y)v \approx \frac{G(y+\epsilon v) - G(y)}{\epsilon}$$

    - Matrix entries need never be formed

We are adding Runge-Kutta (RK) ODE time integrators to SUNDIALS via ARKode

- RK methods are multistage: allow high order accuracy without long step history (enabling spatial adaptivity)
- Implicit RK methods require multiple nonlinear solves per time step
- Additive RK methods apply a pair of explicit (ERK) and implicit (DIRK) methods to a split system, allowing accurate and stable approximations for multi-rate problems.
- Can decompose the system into “fast” and “slow” components to be treated with DIRK and ERK solvers
- ARKode provides 3rd to 5th order ARK, 2nd to 5th order DIRK and 2nd to 6th order ERK methods; also supports user-supplied methods.
- Applies advanced error estimators, adaptive time stepping, Newton and fixed-point iterative solvers
- ARKode will be released with SUNDIALS later this year

http://faculty.smu.edu/reynolds/arkode

ARKode solves $M\dot{y} = f_E(t,y) + f_I(t,y)$

- Variable step size additive Runge-Kutta Methods:

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

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

$$M\tilde{y}_n = My_{n-1} + h_n \sum_{i=0}^{s} \tilde{b}_i \left(f_E(t_{n-1} + c_i h_n, z_i) + f_I(t_{n-1} + c_i h_n, z_i)\right).$$

- ERK methods use $A^I=0$; DIRK methods use $A^E=0$,
- z_i, $i = 1,\ldots,s$ are the inner stage solutions,
- y_n is the time-evolved solution, and
- $\tilde{y}_n$ is the embedded solution (used for error estimation),
- M may be the identity (ODEs) or a non-singular mass matrix (FEM).

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

- The general form of an IVP is given by

$$\boxed{\begin{aligned} F(t,\dot{x},x) &= 0 \\ x(t_0) &= x_0 \end{aligned}}$$

- 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

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
- Rootfinding capability - finds roots of user-defined functions, $g_i(t,y,y')$
- Nonlinear systems solved by Newton-Krylov method

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

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

Sensitivity Analysis Approaches

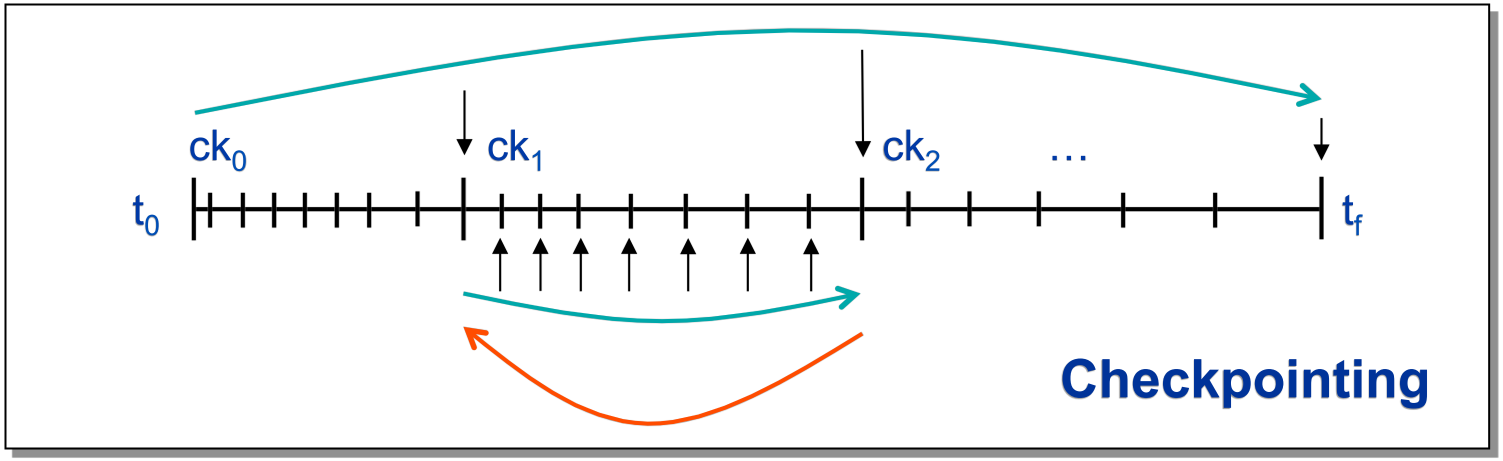
Parameter dependent system

$$\begin{cases} F(x,\dot{x},t,p) = 0 \\ x(0) = x_0(p) \end{cases}$$

FSA	**ASA**
$\begin{cases} F_{\dot{x}}\dot{s}_i + F_x s_i + F_{p_i} = 0 \\ s_i(0) = dx_0 / dp_i \end{cases}, \quad i = 1,\ldots,N_p$	$\begin{cases} (\lambda^* F_{\dot{x}})' - \lambda^* F_x = -g_x \\ \lambda^* F_{\dot{x}} x_p = \ldots \quad \text{at } t = T \end{cases}$
$g(t,x,p)$ $\dfrac{dg}{dp} = g_x s + g_p$	$G(x,p) = \int_0^T g(t,x,p)dt$ $\dfrac{dG}{dp} = \int_0^T (g_p - \lambda^* F_p)dt - \left(\lambda^* F_{\dot{x}} x_p\right)\Big\|_0^T$
Computational cost: $(1+N_p)N_x$ increases with N_p	Computational cost: $(1+N_g)N_x$ increases with N_g

Adjoint Sensitivity Analysis Implementation

- Solution of the forward problem is required for the adjoint problem → need predictable and compact storage of solution values for the solution of the adjoint system



- Cubic Hermite or variable-degree polynomial interpolation
- Simulations are reproducible from each checkpoint
- Force Jacobian evaluation at checkpoints to avoid storing it
- Store solution and first derivative
- Computational cost: 2 forward and 1 backward integrations

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
- Backtracking and line search options for robustness
- Dynamic linear tolerance selection

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

Fixed point and Picard iteration will be added to KINSOL in the next release

- Define an iterative scheme to solve F(h) = h - G(h) = 0 as,

```
Initialize $h^0$.
For $k = 0,1,\ldots,$ until $\|F(h^k)\| < \tau$
    Set $h^{k+1} = G(h^k)$.
end
```

- Picard iteration is a fixed point method formed from writing F as the difference of a linear, Lu, and a nonlinear, N(u), operator

$$F(u) = Lu - N(u); \quad L^{-1}N(u) = u - L^{-1}F(u) \equiv G(u)$$

$$u^{k+1} \approx u^k - L^{-1}F(u^k) = G(u^k)$$

Like Newton with L approximating J

- Fixed point iteration has a global but linear convergence theory
- Requires G to be a contraction $\|G(x) - G(y)\| \le \gamma \|x - y\|, \quad \gamma < 1$

KINSOL will have both Picard and fixed point iterations *with acceleration*

SUNDIALS provides many options for linear solvers

- Iterative Krylov 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*
- Two options require serial environments and some pre-defined structure to the data
  - Direct dense
  - Direct band
- Jacobian information (matrix or matrix-vector product) can be supplied by the user or estimated with finite difference quotients

We are developing a SUNDIALS interface to sparse direct solvers

- Requires serial vector kernel now – only for transfer of RHS information for Jacobian systems
- Will generalize to more generic vector interface in the future
- Matrix information is passed via new SUNDIALS sparse_matrix structure which utilizes a compressed sparse column format
- First instantiation is an interface to SuperLU_MT (multi-threaded version of SuperLU)
- Will also develop interfaces to KLU (serial) and possibly PARDISO (threaded)

Preconditioning is essential for large problems as Krylov methods can stagnate

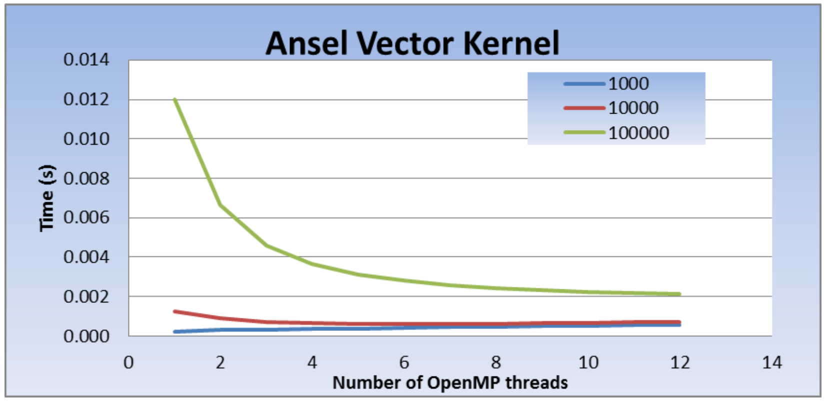
- Preconditioner P must approximate Newton matrix, yet be reasonably efficient to evaluate and solve.
- Typical P (for time-dep. ODE problem) is $I - \gamma\tilde{J}, \quad \tilde{J} \approx J$
- The user must supply two routines for treatment of P:
  - Setup: evaluate and preprocess P (infrequently)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

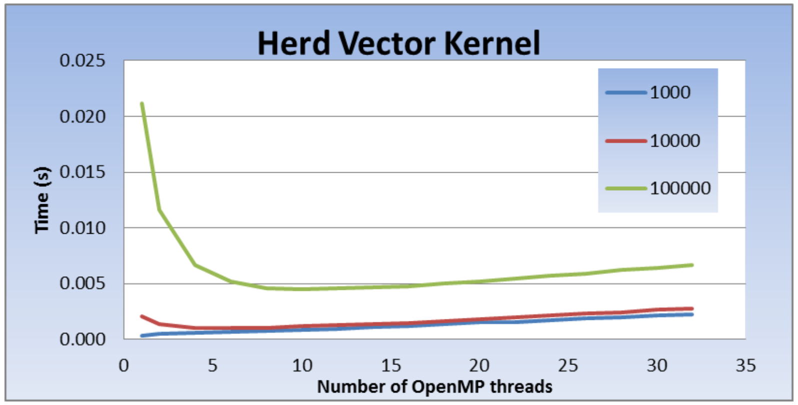
The SUNDIALS vector module is generic

- 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 operations provided for both serial and MPI parallel cases
- Can serve as templates for creating a user-supplied vector
- OpenMP and pThreads vector kernels coming soon. Preliminary performance tests indicate that 10K length required to see benefit





FASTMATH

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

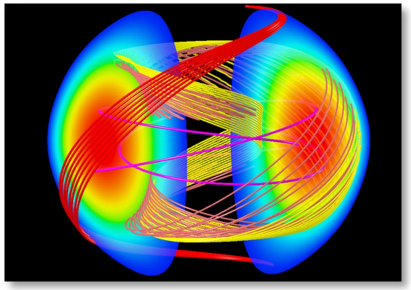
SUNDIALS code usage is similar across the suite

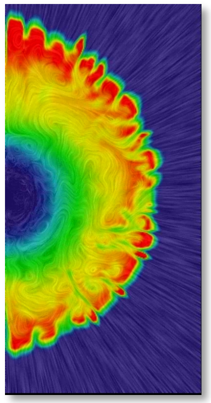
- Have a series of Set/Get routines to set options
- For CVODE with parallel vector implementation:

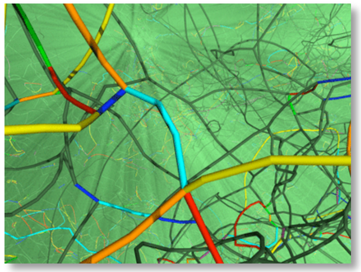
```
#include “cvode.h”
#include “cvode_spgmr.h”
#include “nvector_*.h”

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);
```

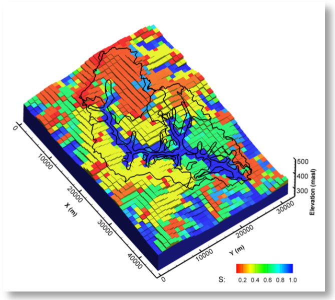
SUNDIALS has been used worldwide in applications from research and industry

- Power grid modeling (RTE France, ISU)
- Simulation of clutches and power train parts (LuK GmbH & Co.)
- Electrical and heat generation within battery cells (CD-adapco)
- 3D parallel fusion (SMU, U. York, LLNL)
- Implicit hydrodynamics in core collapse supernova (Stony Brook)
- Dislocation dynamics (LLNL)
- Sensitivity analysis of chemically reacting flows (Sandia)
- Large-scale subsurface flows (CO Mines, LLNL)
- Optimization in simulation of energy-producing algae (NREL)
- Micromagnetic simulations (U. Southampton)


Magnetic reconnection


Core collapse supernova


Dislocation dynamics



Subsurface flow

More than 3,000 downloads each year

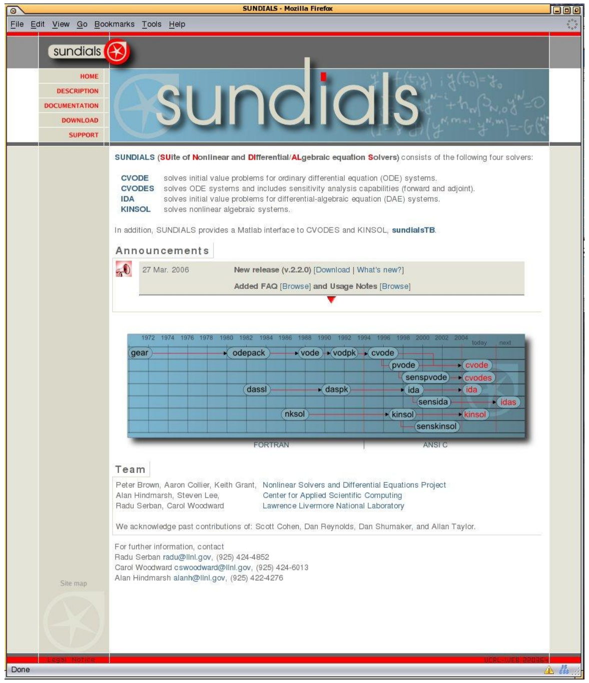
Availability

Open source BSD license

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

Publications

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



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SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers) consists of the following four solvers:

CVODE	solves initial value problems for ordinary differential equation (ODE) systems.
CVODES	solves ODE systems and includes sensitivity analysis capabilities (forward and adjoint).
IDA	solves initial value problems for differential-algebraic equation (DAE) systems.
KINSOL	solves nonlinear algebraic systems.

In addition, SUNDIALS provides a Matlab interface to CVODES and KINSOL, **sundialsTB**.

Announcements

27 Mar. 2006 — **New release (v.2.2.0)** [Download | What's new?]

Added FAQ [Browse] **and Usage Notes** [Browse]

Team

Peter Brown, Aaron Collier, Keith Grant, Alan Hindmarsh, Steven Lee, Radu Serban, Carol Woodward — Nonlinear Solvers and Differential Equations Project, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory

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Web site:

- Individual codes download
- SUNDIALS suite download
- User manuals
- User group email list

The SUNDIALS Team:

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