SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers

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Outline

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

SUite of Nonlinear and DIfferential-ALgebraic Solvers

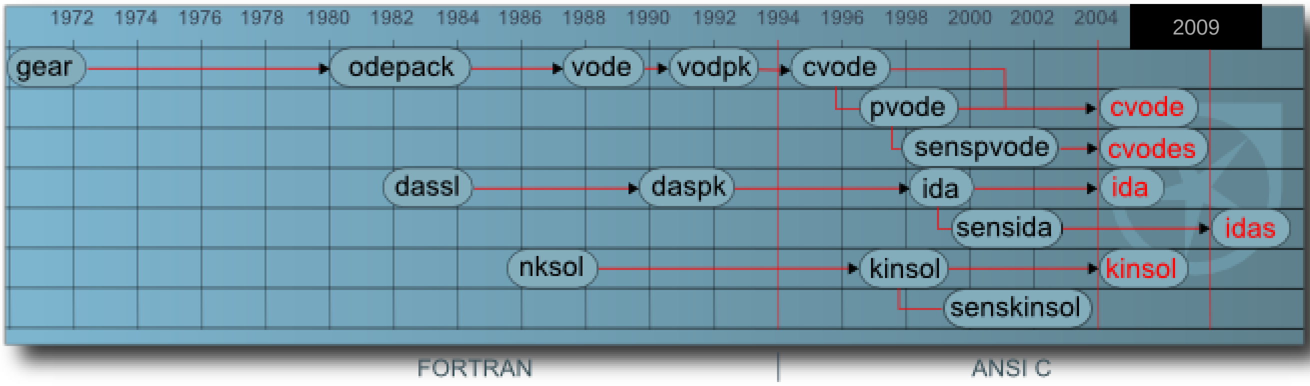
- Suite of time integrators and nonlinear solvers
  - ODE and DAE time integrators with forward and adjoint sensitivity capabilities, Newton-Krylov nonlinear solver
  - Written in C with interfaces to Fortran and Matlab
  - Designed to be incorporated into existing codes
  - Modular implementation: users 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

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



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); $K_1 = 1$, $K_2 = k$, $k = 1,\ldots,12$
- Backward Differentiation Formulas [BDF] (stiff); $K_1 = k$, $K_2 = 0$, $k = 1,\ldots,5$
- Optional stability limit detection based on linear analysis only
- 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:

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

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, $\Delta t'$, 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

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

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

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

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)
- 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.
- Implicit RK methods require multiple nonlinear solves per time step
- 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:

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

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

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

- 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 (no Adams)
- 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 (no functional iteration)

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

CVODE and IDA are equipped with a rootfinding capability

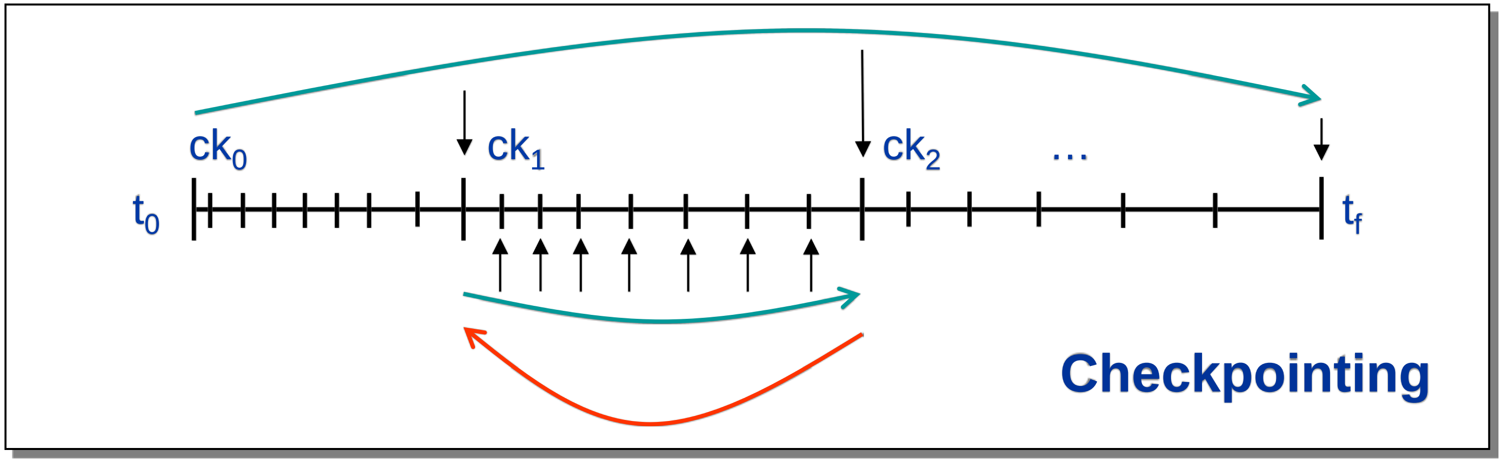
- Finds roots of user-defined functions, $g_i(t,y)$ or $g_i(t,y, y')$
- Important in applications where problem definition may change based on a function of the solution
- Roots are found by looking at sign changes, so only roots of odd multiplicity are found
- Checks each time interval for sign change
- When sign changes are found, apply a modified secant method with a tight tolerance to identify root
- If $g_i(t^*,y) = 0$ for some t^*
  - $g_i(t^*+\delta,y)$ is computed for some small δ in direction of integration
  - Integration stops if any $g_i(t+\delta,y) = 0$
  - Ensures values of g_i are nonzero at some past value of t, beyond which a search for roots is done

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 – augment state system with sensitivity equations
  - Adjoint sensitivity analysis – solve a backward in time adjoint problem (user supplies the adjoint problem)

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
- 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 for use with iterative linear solvers

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

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,..., until $\|F(h^k)\| <$
    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

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

  - 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

Our next release of SUNDIALS will include interfaces 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 release of this capability will support
  - SuperLU_MT (multi-threaded version of SuperLU)
  - KLU (serial)
- Also considering PARDISO (threaded) for future releases

Preconditioning is essential for large problems as Krylov methods can stagnate

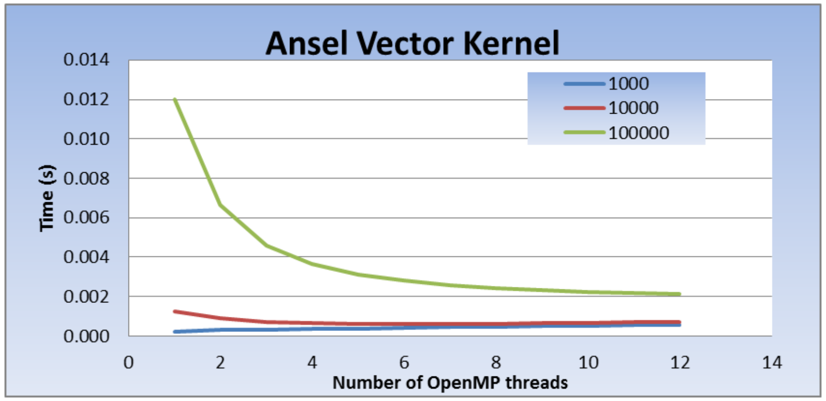
- Preconditioner P must approximate Newton matrix, yet be reasonably efficient to evaluate and solve.
- Typical P (for time-dep. ODE problem) is $I - \gamma \tilde{J}, \quad \tilde{J} \approx J$
- The user must supply two routines for treatment of P:
  - Setup: evaluate and preprocess P (infrequently)
  - 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 …

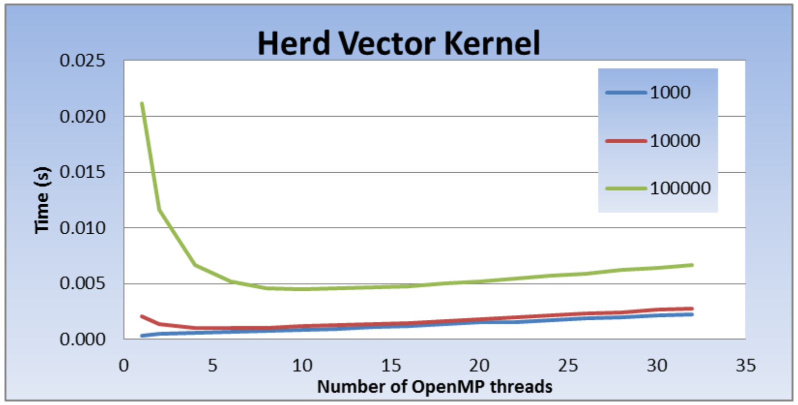
The SUNDIALS vector module is generic

- 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 in next release. Preliminary performance tests indicate that 10K length required to see benefit





SUNDIALS provides Fortran interfaces

- CVODE, IDA, and KINSOL
- Cross-language calls go in both directions:
- Fortran user code $\leftarrow\rightarrow$ interfaces $\leftarrow\rightarrow$ CVODE/KINSOL/IDA

- Fortran main $\rightarrow$ interfaces to solver routines
- Solver routines $\rightarrow$ 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

For CVODE with parallel vector implementation and GMRES solver:

```
#include “cvode.h”
#include “cvode_spgmr.h”
#include “nvector_parallel.h”

y = N_VNew_Parallel(comm, local_n, NEQ);
cvmem = CVodeCreate(CV_BDF,CV_NEWTON);
flag = CVodeSet*(…);
flag = CVodeInit(cvmem,rhs,t0,y,…);
flag = CVSpgmr(cvmem,…);
flag = CVSpilsSet*(cvmem, …);
for(tout = …) {
   flag = CVode(cvmem, …,y,…);  }

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

Set/Get routines also customization of solver parameters and output information

Some CVODE optional inputs

Optional Input	Function Name	Default
User data	CVodeSetUserData	NULL
Max. int. order	CvodeSetMaxOrd	5 (BDF)
Enable stability limit detection	CVodeSetStabLimDet	FALSE
Initial step size	CVodeSetInitStep	Est.
Min. step size	CVodeSetMinStep	0.0
Max. step size	CVodeSetMaxStep	infinity
Precond. Fcns	CVSpilsSet Preconditioner	NULL, NULL
Ratio between lin. & nonlin. tols	CVSpilsSetEpsLin	0.05
Max. Krylov subspace size	CVSpilsSetMaxl	5

```
cvmem = CVodeCreate(…);
flag = CVodeSet*(cvmem,…);
flag = CVodeInit(cvmem,…);
```

```
flag = CVSpgmr(cvmem,…);
flag =
   CVSpilsSet*(cvmem, …);
flag =
   CVSpilsSetPreconditioner(
   cvmem,PrecondSet,PSolve);
```

Example food web problem for KINSOL

A food web population model, with predator-prey interaction and diffusion on the unit square in 2D. The dependent variable vector is the following:

$$c = (c^1, c^2, \ldots, c^{ns})$$

and the PDE's are as follows for i = 1, …, ns:

$$0 = d(i) * (c^i_{xx} + c^i_{yy}) + f_i(x, y, c)$$

where

$$f_i(x, y, c) = c^i * (b(i) + \sum_{j=1}^{ns} (a(i,j) * c^j))$$

Solved on unit square with $\nabla c \bullet n = 0$ B.C. and constant initial iterate

The number of species is ns = 2 * np, with the first np being prey and the last np being predators. The coefficients a(i,j), b(i), d(i) are:

a(i,i) = -AA, all i; a(i,j) = -GG, i <= np , j > np; a(i,j) = EE, i > np, j <= np
b(i) = BB(1 + αxy), i <= np; b(i) = - BB(1 + αxy), i > np
d(i) = DPREY, i <= np; d(i) = DPRED, i > np

Example food web problem for KINSOL

```
#include <kinsol/kinsol.h>
#include <kinsol/kinsol_spgmr.h>
#include <nvector/nvector_parallel.h>
#include <sundials/sundials_dense.h>
#include <sundials/sundials_types.h>
#include <sundials/sundials_math.h>
#include <mpi.h>

#define NPEX       2
#define NPEY       2
#define MXSUB      10
#define MYSUB      10

#define MX         (NPEX*MXSUB)
#define MY         (NPEY*MYSUB)

#define NEQ    (NUM_SPECIES*MX*MY)
```

```
/* Type : UserData contains preconditioner
blocks, pivot arrays, and problem param */

typedef struct {
  realtype **P[MXSUB][MYSUB];
  long int *pivot[MXSUB][MYSUB];
  realtype **acoef, *bcoef;
  N_Vector rates;
  realtype *cox, *coy;
  realtype ax, ay, dx, dy;
  realtype uround, sqruround;
  int mx, my, ns, np;
  realtype cext[NUM_SPECIES *
        (MXSUB+2)*(MYSUB+2)];
  int my_pe, isubx, isuby, nsmxsub,
        nsmxsub2;
  MPI_Comm comm;
} *UserData;
```

Example food web problem for KINSOL

/* Functions Called by the KINSol Solver */

static int funcprpr(N_Vector cc, N_Vector fval, void *user_data);

static int Precondbd(N_Vector cc, N_Vector cscale, N_Vector fval, N_Vector fscale, void *user_data, N_Vector vtemp1, N_Vector vtemp2);

static int PSolvebd(N_Vector cc, N_Vector cscale, N_Vector fval, N_Vector fscale, N_Vector vv, void *user_data, N_Vector vtemp);

/* Private Helper Functions */

AllocUserData
InitUserData
FreeUserData
SetInitialProfiles
PrintHeader
PrintOutput
PrintFinalStats
WebRate
DotProd
Bsend
BRecvPost
BRecvWait
ccomm
fcalcprpr
check_flag

Example food web problem for KINSOL

```
int main(int argc, char *argv[])
{
/* Get processor number and total
number of pe's */
MPI_Init(&argc, &argv);
comm = MPI_COMM_WORLD;
MPI_Comm_size(comm, &npes);
MPI_Comm_rank(comm, &my_pe);

/* Set local vector length */
local_N =
NUM_SPECIES*MXSUB*MYSUB;

/* Allocate and init. user data*/
data = AllocUserData();
InitUserData(my_pe, comm, data);
/* Set global strategy flag */
globalstrategy = KIN_NONE;
```

```
/* Allocate and initialize vectors */
cc = N_VNew_Parallel(comm, local_N, NEQ);
sc = N_VNew_Parallel(comm, local_N, NEQ);
data->rates = N_VNew_Parallel(comm,
local_N, NEQ);
constraints = N_VNew_Parallel(comm,
local_N, NEQ);
N_VConst(ZERO, constraints);

SetInitialProfiles(cc, sc);
fnormtol=FTOL; scsteptol=STOL;

/* Call KINCreate/KINInit to initialize KINSOL:
A pointer to KINSOL problem memory is
returned and stored in kmem. */
kmem = KINCreate();
```

Example food web problem for KINSOL

```
/* Vector cc passed as template vector.
*/
flag = KINInit(kmem, funcprpr, cc);

flag = KINSetNumMaxIters(kmem, 250);
flag = KINSetUserData(kmem, data);
flag = KINSetConstraints(kmem,
constraints);
flag = KINSetFuncNormTol(kmem,
fnormtol);
flag = KINSetScaledStepTol(kmem,
scsteptol);

 /* We no longer need the constraints
vector since KINSetConstraints creates a
private copy for KINSOL to use. */
N_VDestroy_Parallel(constraints);
```

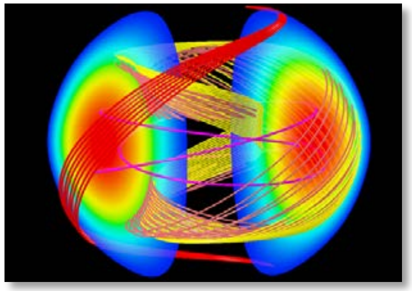
```
/* Call KINSpgmr to specify the linear
solver KINSPGMR with preconditioner
routines Precondbd and PSolvebd, and
the pointer to the user data block. */

maxl = 20; maxlrst = 2;

flag = KINSpgmr(kmem, maxl);
flag = KINSpilsSetMaxRestarts(kmem,
maxlrst);
flag =
KINSpilsSetPreconditioner(kmem,
Precondbd, PSolvebd);
```

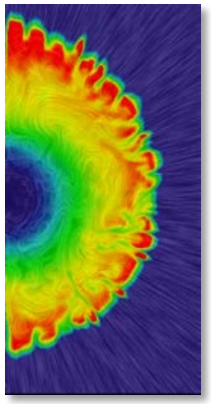
Example food web problem for KINSOL

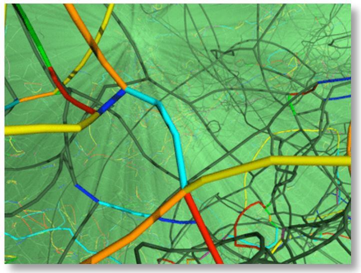
```
/* Call KINSol and print output profile */
flag = KINSol(kmem,   /* KINSol memory*/
       cc,  /* initial guess input; sol'n output*/
       globalstrategy, /* nonlinear strategy*/
       sc, /* scaling vector for variable cc */
       sc); /* scaling vector for function vals*/

/* Print final statistics and free memory */
if (my_pe == 0) PrintFinalStats(kmem);

N_VDestroy_Parallel(cc);
N_VDestroy_Parallel(sc);
KINFree(&kmem);
FreeUserData(data);

MPI_Finalize();
return(0);
}
```

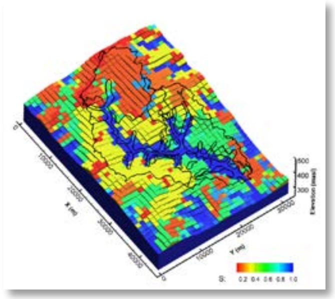
SUNDIALS has been used worldwide in applications from research and industry

- 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 3,500 downloads each year

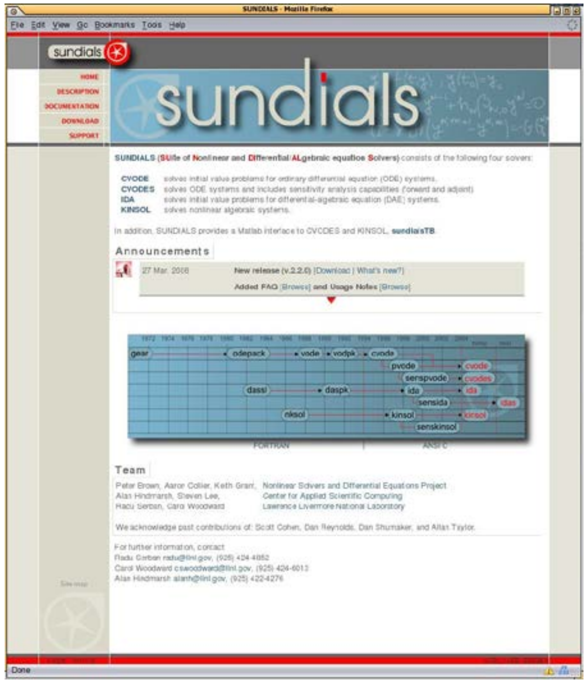
Availability

Open source BSD license

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

Publications

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



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

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