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, $\text{ATOL}^i$
- A relative tolerance is specified for all solution components, $\text{RTOL}$
- Norm calculations are weighted by:

$$e_{wt}^i = \frac{1}{\text{RTOL}|y^i| + \text{ATOL}^i}$$

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

- 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

\[ \dot{y} = f(y) \]

\[ M \approx I - \gamma \frac{\partial f}{\partial y} \quad \gamma = \beta_0 \Delta t_n \]

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

DAE

\[ \begin{align*}
F(\dot{y}, y) & = 0 \\
M & \approx \frac{\partial F}{\partial y} + \gamma \frac{\partial F}{\partial \dot{y}} \\
\gamma & = 1 / (\beta_0 \Delta t_n) \\
G(y_n) & \equiv F \left( t, (\beta_0 \Delta t_n)^{-1} \sum_{i=1}^{k} \alpha_{n,i} y_{n-i}, y_n \right) = 0
\end{align*} \]
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:

\[
Mz_i = My_{n-1} + h_n \sum_{j=0}^{i-1} A_{i,j}^{E} f_E(t_{n-1} + c_j h_n, z_j) + h_n \sum_{j=0}^{i} A_{i,j}^{I} f_I(t_{n-1} + c_j h_n, z_j),
\]

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

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

- 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

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

- If $\frac{\partial F}{\partial \dot{x}}$ 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 \( \delta \) 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 (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,

  \[
  \text{Initialize } h^0.
  
  \text{For } k = 0, 1, \ldots, \text{ until } \|F(h^k)\| < \epsilon
  
  \text{Set } h^{k+1} = G(h^k).
  \text{end}
  \]

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

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

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

- Fixed point iteration has a global but linear convergence theory

- Requires $G$ to be a contraction

  \[
  \|G(x) - G(y)\| \leq \gamma \|x - y\|, \quad \gamma < 1
  \]

KINSOL will have both Picard and fixed point iterations \textit{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 $I - \gamma \tilde{J}$, $\tilde{J} \approx J$
- 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 NVVECTOR 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 ↔ 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

For CVODE with parallel vector implementation and GMRES solver:

```c
#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

<table>
<thead>
<tr>
<th>Optional Input</th>
<th>Function Name</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>User data</td>
<td>CVodeSetUserData</td>
<td>NULL</td>
</tr>
<tr>
<td>Max. int. order</td>
<td>CvodeSetMaxOrd</td>
<td>5 (BDF)</td>
</tr>
<tr>
<td>Enable stability limit</td>
<td>CVodeSetStabLimDet</td>
<td>FALSE</td>
</tr>
<tr>
<td>detection</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Initial step size</td>
<td>CVodeSetInitStep</td>
<td>Est.</td>
</tr>
<tr>
<td>Min. step size</td>
<td>CVodeSetMinStep</td>
<td>0.0</td>
</tr>
<tr>
<td>Max. step size</td>
<td>CVodeSetMaxStep</td>
<td>infinity</td>
</tr>
<tr>
<td>Precond. Fcns</td>
<td>CVSpilsSetPreconditioner</td>
<td>NULL, NULL</td>
</tr>
<tr>
<td>Ratio between lin. &amp; nonlin. tols</td>
<td>CVSpilsSetEpsLin</td>
<td>0.05</td>
</tr>
<tr>
<td>Max. Krylov subspace size</td>
<td>CVSpilsSetMaxl</td>
<td>5</td>
</tr>
</tbody>
</table>

```c
flag = CVodeCreate(...);
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:

\[ c = (c^1, c^2, ..., c^{ns}) \]

and the PDE's are as follows for \( i = 1, \ldots, ns \):

\[ 0 = d(i) \times (c_{xx}^i + c_{yy}^i) + f_i(x, y, c) \]

where

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

The number of species is \( ns = 2 \times np \), 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 \( i \); \( a(i,j) = -GG \), \( i \leq np \), \( j > np \); \( a(i,j) = EE \), \( i > np \), \( j \leq np \)

\( b(i) = BB(1 + \alpha xy) \), \( i \leq np \); \( b(i) = -BB(1 + \alpha xy) \), \( i > np \)

\( d(i) = DPREY \), \( i \leq np \); \( d(i) = DPRED \), \( i > np \)

Solved on unit square with \( \nabla c \cdot n = 0 \) B.C. and constant initial iterate
Example food web problem for KINSOL

```c
#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 v, 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

```c
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 KINCreat/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);
/* 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)

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