Rsundials Version 1.6

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Contents

1. Summary

Rsundials implements the differential algebraic equation (DAE) and ordinary differential equation (ODE) solvers in the SUNDIALS suite (version 2.3.0 – http://www.llnl.gov/CASC/sundials/). The IDA module of SUNDIALS handles DAEs and the CVODES module solves ODE systems. Both modules utilize a dense linear solver and both require a user-defined (hard-coded) residual / right hand side function. Installation of the SUNDIALS libraries is not a prerequisite for this package.

2. IDA Example

The Problem

This example, due to Robertson[1], is a model of a three-species chemical kinetics system written in DAE form. Differential equations are given for species y_1 and y_2 while an algebraic equation determines y_3. The equations for the system concentrations $y_i(t)$ are:

$$\begin{aligned}\dot{y}_1 &= -0.4y_1 + 10^4 y_2 y_3\\ \dot{y}_2 &= 0.4y_1 - 10^4 y_2 y_3 - 30\cdot 10^7 y_2^2\\ 0 &= y_1 + y_2 + y_3 - 1\end{aligned}$$

The initial values are taken as $y_1 = 1$, $y_2 = 0$, and $y_3 = 0$. This example computes the three concentration components on the interval from t = 0 through t = $4*10^{10}$.

The Residual Function

The first step is to create a compilable file (preferably in c) that defines the residual (right hand side) function as called by the solver on each time step. A template for such a function can be described as:

```
#include "include/nvector_serial.h"
#include "include/sundials_dense.h"
```

```
int resrob(realtype tres, N_Vector yy, N_Vector yp, N_Vector rr,
           void *rdata)
{
  realtype *yval, *ypval, *rval;

  yval = NV_DATA_S(yy);
  ypval = NV_DATA_S(yp);
  rval = NV_DATA_S(rr);

  /* Set values of rval[0]...rval[n] here */

  return(0);
}
```

The function takes the arguments:

tres	the current value of the independent variable
yy	the current value of the dependent variable vector, y(t)
yp	the current value of y'(t)
rr	the output residual vector F(t, y, y')
rdata	a pointer to user data

The two includes are used to obtain the data types used by the SUNDIALS solver, namely N_Vector, a simple vector, and realtype, a primitive data type. By default, this is a double-precision floating-point numeric data type (double C-type). The header files are found in the *usrfcns* directory.

In order to write or read from the vectors, **`NV_DATA_S`** must be used on a realtype pointer. This sets the pointer to the first value of the vector. In general, nothing must be done with **`tres`** or **`rdata`**.

IDA works by attempting to minimize the residual of the equations presented. Thus, it is important to formulate the system properly by bringing everything over to one side. The output residual vector **`rr`** can be written to by writing to the elements of **`rval`**. For the above system, this can be done in the following way:

```
rval[0] = -0.04*yval[0] + 1.0e4*yval[1]*yval[2] - ypval[0];
rval[1] = 0.04*yval[0] - 1.0e4*yval[1]*yval[2]  -
          3.0e7*yval[1]*yval[1] - ypval[1]
rval[2] = yval[0] + yval[1] + yval[2] - 1;
```

If the complete function resrob is placed in the file idafcns.c, it can be compiled into a shared library useable by R by typing:

```
R CMD SHLIB ...path.../idafcns.c
```

in the command line as long as the header files nvector_serial.h and ida_dense.h are present in the same directory. This will compile the file and allow the functions within to be usable in R.

Solving the Problem in R

Once R is started, the defined functions must be loaded before running the IDA solver. To load dynamic libraries into R, use the command

```
dyn.load("...path.../idafcns.so") or
dyn.load("...path.../idafcns.dll")
```

depending on your system type. To execute the IDA solver in R, the following command might be used:

```
yvals <- ida(c(1,0,0), c(-0.04,0.04,0),
     gseq(.4,4e10,10), "idafcns", "resrob", jacfunc =
     "jacrob", rtol = 1E-4, atol = c(1E-8,1E-14,1E-6),
     verbose = TRUE)
```

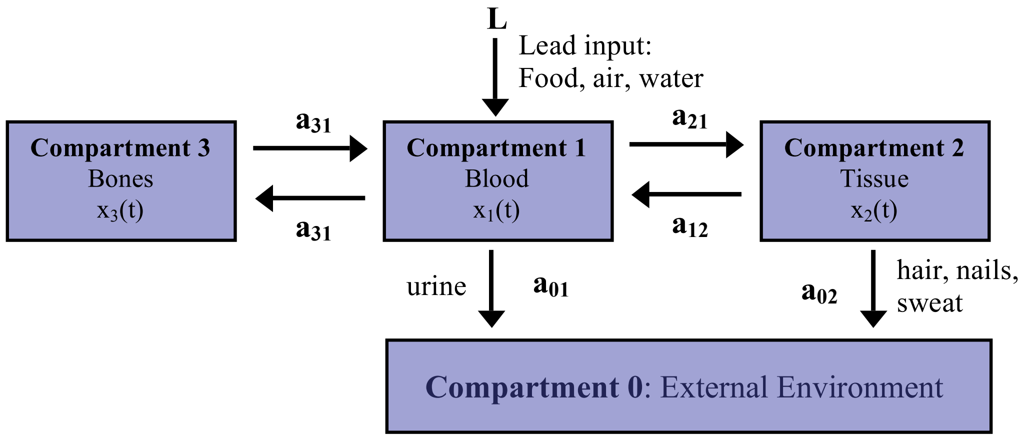
The following output should be obtained:

```
SUNDIALS IDADENSE Linear Solver
Number of Equations: 3
Integration Limits: 0.4 to 4e+10
Solver Memory Allocated
Max Number of Steps: 500
Max step size: 0
Relative Tolerance: 0.0001
Absolute Tolerances: 1e-08 1e-14 1e-06
Jacobian Function Initialized
IDADense Linear Solver Initialized
-----------------------------------------------------------------------
  t            y0           y1           y2      | nst  k      h
-----------------------------------------------------------------------
4.0000e+00   9.1172e-01   2.3133e-05   8.8253e-02  |  96  4   4.1520e-01
4.0000e+01   7.1686e-01   9.2258e-06   2.8313e-01  | 132  4   1.9421e+00
4.0000e+02   4.5066e-01   3.2247e-06   5.4933e-01  | 177  4   3.2576e+01
4.0000e+03   1.8321e-01   8.9427e-07   8.1679e-01  | 220  4   2.0527e+02
4.0000e+04   3.8985e-02   1.6218e-07   9.6102e-01  | 266  3   1.2965e+03
4.0000e+05   4.9391e-03   1.9853e-08   9.9506e-01  | 307  5   1.6802e+04
4.0000e+06   5.1672e-04   2.0679e-09   9.9948e-01  | 366  3   1.5150e+05
4.0000e+07   5.2026e-05   2.0811e-10   9.9995e-01  | 416  4   2.0066e+06
4.0000e+08   5.2132e-06   2.0853e-11   9.9999e-01  | 452  4   2.7282e+07
4.0000e+09   5.2178e-07   2.0871e-12   1.0000e+00  | 482  4   2.6574e+08
4.0000e+10   5.1049e-08   2.0420e-13   1.0000e+00  | 503  2   6.8880e+09

Final Run Statistics:

Number of steps                    = 503
Number of residual evaluations     = 703
Number of Jacobian evaluations     = 78
Number of nonlinear iterations     = 703
Number of error test failures      = 16
Number of nonlinear conv. failures = 0
Number of root fn. evaluations     = 0
       [,1]         [,2]         [,3]       [,4]
 [1,] 4e-01 1.000000e+00 0.000000e+00 0.00000000
 [2,] 4e+00 9.117237e-01 2.313333e-05 0.08825314
 [3,] 4e+01 7.168589e-01 9.225752e-06 0.28313186
 [4,] 4e+02 4.506627e-01 3.224737e-06 0.54933409
 [5,] 4e+03 1.832093e-01 8.942713e-07 0.81678983
 [6,] 4e+04 3.898477e-02 1.621830e-07 0.96101506
 [7,] 4e+05 4.939054e-03 1.985310e-08 0.99506093
 [8,] 4e+06 5.167204e-04 2.067937e-09 0.99948328
 [9,] 4e+07 5.202555e-05 2.081130e-10 0.99994797
[10,] 4e+08 5.213164e-06 2.085276e-11 0.99999479
[11,] 4e+09 5.217753e-07 2.087102e-12 0.99999948
[12,] 4e+10 5.104891e-08 2.041956e-13 0.99999995
```

3. CVODES Example

The Problem

This example from a presentation by Borrelli and Coleman[2] is a three-compartment model for lead in the human body. Lead is input to the system at a constant rate L. Three state variables, x_1, x_2, and x_3 describe the concentration of lead in the blood, tissue, and bones respectively. There exist transfer rates between the compartments as well as to the external environment via urine from the blood and via hair, nails, and sweat from the tissues.



For $\mathbf{i} = \mathbf{1}, \mathbf{2}, \mathbf{3}$, we let $\mathbf{x_i(t)}$ be the amount of lead in compartment $\mathbf{i}$ at time $\mathbf{t}$ and we assume that the rate of transfer from compartment $\mathbf{i}$ to $\mathbf{j}$ is proportional to $\mathbf{x_i(t)}$ with a proportionality constant of $\mathbf{a_{ji}}$. The units for amounts of lead are micrograms and the time $\mathbf{t}$ is measured in days.

The vector differential equation of this problem is in the form

$$\dot{\mathbf{x}} = \mathbf{Ax} + \mathbf{b}$$

where **A** is the matrix

$$\begin{bmatrix} -(a_{01}+a_{21}+a_{31}) & a_{12} & a_{13} \\ a_{21} & -(a_{02}+a_{12}) & 0 \\ a_{31} & 0 & -a_{13} \end{bmatrix}$$

and $\mathbf{b} = (\mathbf{L},\mathbf{0},\mathbf{0})^{\mathrm{T}}$.

In a paper published by Rabinowitz and colleagues[3], measurements of the concentration of lead in these compartments in a male subject living in Los Angeles allowed for the calculation of the rates of transfer. Relatively speaking, lead is somewhat slow to enter the bones and very slow to leave them.

Lead Transfer Coefficients (Rabinowitz, et al.)

Units: days^{-1}

$a_{21} = 0.011$	$a_{12} = 0.012$	**from blood to tissue and back**
$a_{31} = 0.0039$	$a_{13} = 0.000035$	**from blood to bone and back**
$a_{01} = 0.021$	$a_{02} = 0.016$	**excretion from blood and tissue**

The study also showed that the average rate of ingestion of lead (**L**) in Los Angeles over the period studied was **49.3** micrograms per day.

The Right Hand Side Function

The first step is to create a compilable file (preferably in c) that defines the right hand side function as called by the solver on each time step. A template for such a function can be described as:

```c
#include "include/nvector_serial.h"
#include "include/sundials_dense.h"

int rhs(realtype t, N_Vector y, N_Vector ydot, void *f_data)
{
  realtype y1, y2, y3;
  y1 = Ith(y,1); y2 = Ith(y,2); y3 = Ith(y,3);

  /* Change values of ydot here using Ith(ydot,i) */

  return(0);
}
```

The function takes the arguments:

`t`	the current value of the independent variable
`y`	the current value of the dependent variable vector, y(t)
`ydot`	the current value of y'(t)
`fdata`	a pointer to user data

The two includes are used to obtain the data types used by the SUNDIALS solver, namely N_Vector, a simple vector, and realtype, a primitive data type. By default, this is a double-precision floating-point numeric data type (double C-type). The header files are found in the *usrfcns* directory.

The realtypes y_1, y_2 and y_3 are first set to the corresponding value in the y vector using the macro `Ith` with indices from 1 to n (not from 0 to n-1). These can then be modified to reflect the proper value. For the above problem, the values of **`ydot`** can be updated using the following code:

```
double L = 49.3;
double a21 = 0.011; double a12 = 0.012;
double a31 = 0.0039; double a13 = 0.000035;
double a01 = 0.021; double a02 = 0.016;

Ith(ydot, 1) = -(a01 + a21 + a31)*y1 + a12*y2 + a13*y3 + L;
Ith(ydot, 2) = a21*y1 - (a02 + a12)*y2;
Ith(ydot, 3) = a31*y1 - a13*y3;
```

If the complete function *rhs* is placed in the file cvodesfcns.c, it can be compiled into a shared library useable by R by typing:

```
R CMD SHLIB ...path.../cvodesfcns.c
```

in the command line as long as the header files nvector_serial.h and cvodes_dense.h are present in the same directory. This will compile the file and allow the functions within to be usable in R.

The user may supply a method for computing the Jacobian; this can be placed in the same file as the RHS method.

Solving the Problem in R

Using the model defined above, let's take a look at an individual who moves to Los Angles with no lead in her body. We can use Rsundials to determine the levels in her system after a set number of days, say 400.

Once R is started, the defined functions must be loaded before running the CVODES solver. To load dynamic libraries into R, use the command

`dyn.load("...path.../cvodesfcns.so")` or
`dyn.load("...path.../cvodesfcns.dll")`

depending on your system type. To execute the CVODES solver in R, the following command might be used:

```
yvals <-
     cvodes(c(0.0,0.0,0.0),seq(0,400,20),"cvodesfcns",
          "rhs", rtol = 1E-4,atol = c(1E-8,1E-14,1E-
          6),verbose = TRUE)
```

The following output should be obtained:

```
SUNDIALS CVODES Linear Solver
Number of Equations: 3
Integration Limits: 0 to 400
Initial Values:  y0 = 0   y1 = 0   y2 = 0
Solver Memory Allocated
Relative Tolerance: 0.0001
Absolute Tolerances: 1e-08   1e-14   1e-06
CVDENSE Solver Initiated
Max number of steps: 500
Max step size: 0
Requesting data for all time points.

At t = 2.0000e+01        7.088272e+02    7.198569e+01    3.079803e+01
At t = 4.0000e+01        1.073435e+03    1.972720e+02    1.017541e+02
At t = 6.0000e+01        1.272270e+03    3.134134e+02    1.938759e+02
At t = 8.0000e+01        1.386870e+03    4.047548e+02    2.978071e+02
At t = 1.0000e+02        1.456042e+03    4.716999e+02    4.086610e+02
At t = 1.2000e+02        1.499400e+03    5.189813e+02    5.237255e+02
At t = 1.4000e+02        1.527143e+03    5.518129e+02    6.414478e+02
At t = 1.6000e+02        1.545141e+03    5.743737e+02    7.608681e+02
At t = 1.8000e+02        1.557178e+03    5.896541e+02    8.813493e+02
At t = 2.0000e+02        1.565419e+03    5.999263e+02    1.002498e+03
At t = 2.2000e+02        1.570973e+03    6.069031e+02    1.124084e+03
At t = 2.4000e+02        1.574665e+03    6.116752e+02    1.245947e+03
At t = 2.6000e+02        1.577182e+03    6.149088e+02    1.367965e+03
At t = 2.8000e+02        1.578955e+03    6.170854e+02    1.490058e+03
At t = 3.0000e+02        1.580190e+03    6.185755e+02    1.612180e+03
At t = 3.2000e+02        1.581042e+03    6.196108e+02    1.734300e+03
At t = 3.4000e+02        1.581648e+03    6.203337e+02    1.856392e+03
At t = 3.6000e+02        1.582106e+03    6.208375e+02    1.978440e+03
At t = 3.8000e+02        1.582467e+03    6.211930e+02    2.100434e+03
At t = 4.0000e+02        1.582768e+03    6.214457e+02    2.222365e+03

Final Run Statistics:

Number of steps                    = 73
Number of RHS evaluations          = 89
Number of linear solver setups     = 31
Number of nonlinear iterations     = 85
Number of error test failures      = 1
Number of nonlinear conv. failures = 0
Number of root fn. evaluations     = 0
      [,1]      [,2]      [,3]       [,4]
 [1,]    0    0.0000   0.00000    0.00000
 [2,]   20  708.8272  71.98569   30.79803
 [3,]   40 1073.4351 197.27204  101.75408
 [4,]   60 1272.2696 313.41340  193.87588
 [5,]   80 1386.8700 404.75483  297.80714
 [6,]  100 1456.0422 471.69985  408.66104
 [7,]  120 1499.4004 518.98131  523.72549
 [8,]  140 1527.1425 551.81292  641.44779
 [9,]  160 1545.1407 574.37374  760.86810
[10,]  180 1557.1780 589.65408  881.34927
[11,]  200 1565.4186 599.92632 1002.49768
[12,]  220 1570.9726 606.90308 1124.08405
```

```
[13,]  240 1574.6646 611.67520 1245.94737
[14,]  260 1577.1821 614.90883 1367.96547
[15,]  280 1578.9551 617.08536 1490.05834
[16,]  300 1580.1895 618.57552 1612.18045
[17,]  320 1581.0423 619.61078 1734.29997
[18,]  340 1581.6483 620.33370 1856.39243
[19,]  360 1582.1063 620.83745 1978.44042
[20,]  380 1582.4672 621.19300 2100.43377
[21,]  400 1582.7678 621.44568 2222.36541
```

[1] H. H. Robertson. The solution of a set of reaction rate equations. In J. Walsh, editor, Numerical analysis: an introduction, pages 178–182. Academ. Press, 1966.

[2] *Differential Equations: A Modeling Approach*, by R. Borrelli and C. Coleman, Prentice-Hall, 1987.

[3] Rabinowitz MB, Wetherill GW, Kopple JD. *Lead metabolism in the normal human: stable isotope studies*. Science. 1973 Nov 16;182(113):725–727.