

# Example Programs for IDAS

v3.0.0-dev

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May 7, 2018



LLNL-TR-437091

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Forward sensitivity analysis example problems</b>	<b>6</b>
2.1	A serial dense example: idasSlCrank_FSA_dns . . . . .	6
2.2	A parallel example using IDABBDPRE: idasBruss_FSA_kry_bbd_p . . . . .	9
<b>3</b>	<b>Adjoint sensitivity analysis example problems</b>	<b>12</b>
3.1	A serial dense example: idasAkzoNob_AS Ai_dns . . . . .	12
3.2	A parallel example using IDABBDPRE: idasBruss_AS Ap_kry_bbd_p . . . . .	13
	<b>References</b>	<b>15</b>



# 1 Introduction

This report is intended to serve as a companion document to the User Documentation of IDAS [4]. It provides details, with listings, on the example programs supplied with the IDAS distribution package.

The IDAS distribution contains examples of the following types: serial and parallel examples of Initial Value Problem (IVP) integration, serial and parallel examples of forward sensitivity analysis (FSA), and serial and parallel examples of adjoint sensitivity analysis (ASA). The names of all the examples are given in the following table.

	Serial examples	Parallel examples
IVP	idasRoberts_dns idasRoberts_klu idasRoberts_sps idasAkzoNob_dns idasSlCrank_dns idasHeat2D_bnd idasHeat2D_kry idasFoodWeb_bnd idasFoodWeb_bnd_omp idasFoodWeb_kry_omp idasKrylovDemo_ls	idasHeat2D_kry_p idasHeat2D_kry_bbd_p idasFoodWeb_kry_p idasFoodWeb_kry_bbd_p idasBruss_kry_bbd_p
FSA	idasRoberts_FSA_dns idasRoberts_FSA_klu idasRoberts_FSA_sps idasSlCrank_FSA_dns	idasBruss_FSA_kry_bbd_p idasHeat2D_FSA_kry_bbd_p
ASA	idasRoberts_AS Ai_dns idasRoberts_AS Ai_klu idasRoberts_AS Ai_sps idasAkzoNob_AS Ai_dns idasHessian_AS A_FSA	idasBruss_AS Ap_kry_bbd_p

With the exception of "demo"-type example files, the names of all the examples distributed with SUNDIALS are of the form [slv] [PbName]\_[SA]\_[ls]\_[prec]\_[p], where

[slv] identifies the solver (for IDAS examples this is `idas`);

[PbName] identifies the problem;

[SA] identifies sensitivity analysis examples. This field can be one of: `FSA` for forward sensitivity examples, `AS Ai` for adjoint sensitivity examples using an integral-form model output, or `AS Ap` for adjoint sensitivity examples using an pointwise model output;

[ls] identifies the linear solver module used;

[prec] indicates the IDAS preconditioner module used (if applicable — for examples using a Krylov linear solver and the IDABBDPRE module, this will be `bbd`);

[p] indicates an example using the parallel vector module `NVECTOR_PARALLEL`.

The examples are briefly described next. Note that the IDAS distribution includes all of the IDA C examples (denoted here as examples for IVP integration). More details on these can be found in the IDA Example Program document [2].

Supplied in the `srcdir/examples/idas/serial` directory are the following serial examples (using the `NVECTOR_SERIAL` module):

- `idasRoberts_dns` solves the Robertson chemical kinetics problem [3], which consists of two differential equations and one algebraic constraint. It also uses the rootfinding feature of IDAS.

The problem is solved with the IDADENSE linear solver using a user-supplied Jacobian.

- `idasRoberts_klu` is the same as `idasRoberts_dns` but uses the KLU sparse direct linear solver.
- `idasRoberts_sps` is the same as `idasRoberts_dns` but uses the SuperLUMT sparse direct linear solver (with one thread).
- `idasAkzoNob_dns` solves the Akzo-Nobel chemical kinetics problem, which consists of six nonlinear DAEs of index 1. The problem originates from Akzo Nobel Central research in Arnheren, The Netherlands, and describes a chemical process in which two species are mixed, while carbon dioxide is continuously added.

The problem is solved with the IDADENSE linear solver using the default difference quotient dense Jacobian approximation.

- `idasHeat2D_bnd` solves a 2-D heat equation, semidiscretized to a DAE on the unit square.

This program solves the problem with the IDABAND linear solver and the default difference-quotient Jacobian approximation. For purposes of illustration, `IDACalcIC` is called to compute correct values at the boundary, given incorrect values as input initial guesses. The constraint  $u > 0.0$  is imposed for all components.

- `idasHeat2D_kry` solves the same 2-D heat equation problem as `idasHeat2D_bnd`, with the Krylov linear solver IDASPGMR. The preconditioner uses only the diagonal elements of the Jacobian.
- `idasFoodWeb_bnd` solves a system of PDEs modeling a food web problem, with predator-prey interaction and diffusion, on the unit square in 2-D.

The PDEs are discretized in space to a system of DAEs which are solved using the IDABAND linear solver with the default difference-quotient Jacobian approximation.

- `idasSlCrank_dns` solves a system of index-2 DAEs, modeling a planar slider-crank mechanism.

The problem is obtained through a stabilized index reduction (Gear-Gupta-Leimkuhler) starting from the index-3 DAE equations of motion derived using three generalized coordinates and two algebraic position constraints. The program also computes the time-averaged kinetic energy as a quadrature.

- `idasKrylovDemo_ls` solves the same problem as `idasHeat2D_kry`, with three Krylov linear solvers IDASPGMR, IDASPCG, and IDASPTFQMR. The preconditioner uses only the diagonal elements of the Jacobian.

- `idasRoberts_FSA_dns` solves the same kinetics problem as in `idasRoberts_dns`. IDAS also computes both its solution and solution sensitivities with respect to the three reaction rate constants appearing in the model. This program solves the problem with the IDADENSE linear solver, and a user-supplied Jacobian routine.

- `idasRoberts_FSA_klu` solves the same problem as in `idasRoberts_FSA_dns` but uses the sparse direct solver KLU.
- `idasRoberts_FSA_sps` solves the same problem as in `idasRoberts_FSA_dns` but uses the sparse solver SuperLUMT.
- `idasSlCrank_FSA_dns` solves a system of index-2 DAEs, modeling a planar slider-crank mechanism.

This example computes both its solution and solution sensitivities with respect to the problem parameters  $k$  (spring constant) and  $c$  (damper constant), and then uses them to evaluate the gradient of the cumulative kinetic energy of the system.

- `idasRoberts_ASai_dns` solves the same kinetics problem as in `idasRoberts_dns`. Here the adjoint capability of IDAS is used to compute gradients of a functional of the solution with respect to the three reaction rate constants appearing in the model. This program solves both the forward and backward problems with the IDADENSE linear solver, and user-supplied Jacobian routines.
- `idasRoberts_ASai_klu` solves the same problem as in `idasRoberts_ASai_dns`, but uses the sparse direct solver KLU.
- `idasRoberts_ASai_sps` solves the same problem as in `idasRoberts_ASai_dns`, but uses the sparse solver SuperLUMT.
- `idasAkzoNob_ASai_dns` solves the Akzo-Nobel chemical kinetics problem. The adjoint capability of IDAS is used to compute gradients with respect to the initial conditions of the integral over time of the concentration of the first species.
- `idasHessian_ASA_FSA` is an example of using the *forward-over-adjoint* method for computing 2nd-order derivative information, in the form of Hessian-times-vector products.

Supplied in the `srcdir/examples/idas/parallel` directory are the following parallel examples (using the `NVECTOR_PARALLEL` module):

- `idasHeat2D_kry_p` solves the same 2-D heat equation problem as `idasHeat2D_kry`, with IDASPGMR in parallel, and with a user-supplied diagonal preconditioner,
- `idasHeat2D_kry_bbd_p` solves the same problem as `idasHeat2D_kry_p`.  
This program uses the IDASPGMR linear solver in parallel, and the band-block-diagonal preconditioner IDABBDPRE with half-bandwidths equal to 1.
- `idasFoodWeb_kry_p` solves the same food web problem as `idasFoodWeb_bnd`, but with IDASPGMR and a user-supplied preconditioner.  
The preconditioner supplied to IDASPGMR is the block-diagonal part of the Jacobian with  $n_s \times n_s$  blocks arising from the reaction terms only ( $n_s$  = number of species).
- `idasFoodWeb_kry_bbd_p` solves the same food web problem as `idasFoodWeb_kry_p`.  
This program solves the problem using IDASPGMR in parallel and the IDABBDPRE preconditioner.

- `idasBruss_kry_bbd_p` solves the two-species time-dependent PDE known as the Brusselator problem, using the IDASPGMR linear solver and the IDABBDPRE preconditioner. The PDEs are discretized by central differencing on a 2D spatial mesh. The system is actually implemented on submeshes, processor by processor.
- `idasBruss_FSA_kry_bbd_p` solves the Brusselator problem with the forward sensitivity capability in IDAS used to compute solution sensitivities with respect to two of the problem parameters, and then the gradient of a model output functional, written as the final time value of the spatial integral of the first PDE component.
- `idasHeat2D_FSA_kry_bbd_p` solves the same problem as `idaHeat2D_kry_p`, but using the IDABBDPRE preconditioner, and with forward sensitivity enabled to compute the solution sensitivity with respect to two coefficients of the original PDE.
- `idasBruss_ASAP_kry_bbd_p` solves the same problem as `idasBruss_FSA_kry_bbd_p` but using an adjoint sensitivity approach for computing the gradient of the model output functional.

Supplied in the `srcdir/examples/idas/C_openmp` directory are the following examples, using the OpenMP NVECTOR module:

- `idasFoodWeb_bnd_omp` solves the same problem as in `idasFoodWeb_bnd` but uses the OpenMP module.
- `idasFoodWeb_kry_omp` solves the same problem as in `idasFoodWeb_kry` but uses the OpenMP module.

In the following sections, we give detailed descriptions of some (but not all) of the sensitivity analysis examples. We do not discuss the examples for IVP integration; for those, the interested reader should consult the IDA Examples document [2]. Any IDA problem will work with IDAS with only two modifications: (1) the main program should include the header file `idas.h` instead of `ida.h`, and (2) the loader command must reference `build-dir/lib/libsundials_idas.lib` instead of `builddir/lib/libsundials_ida.lib`.

We also give our output files for each of these examples described below, but users should be cautioned that their results may differ slightly from these. Differences in solution values may differ within the tolerances, and differences in cumulative counters, such as numbers of steps or Newton iterations, may differ from one machine environment to another by as much as 10% to 20%.

In the descriptions below, we make frequent references to the IDAS User Guide [4]. All citations to specific sections (e.g. §4.2) are references to parts of that user guide, unless explicitly stated otherwise.

**Note** The examples in the IDAS distribution were written in such a way as to compile and run for any combination of configuration options during the installation of SUNDIALS (see Appendix A in the User Guide). As a consequence, they contain portions of code that will not typically be present in a user program. For example, all example programs make use of the variables `SUNDIALS_EXTENDED_PRECISION` and `SUNDIALS_DOUBLE_PRECISION` to test if the



solver libraries were built in extended or double precision, and use the appropriate conversion specifiers in `printf` functions. Similarly, all forward sensitivity examples can be run with or without sensitivity computations enabled and, in the former case, with various combinations of methods and error control strategies. This is achieved in these example through the program arguments.

## 2 Forward sensitivity analysis example problems

For all the IDAS examples, either of the two sensitivity method options, `IDA_SIMULTANEOUS` or `IDA_STAGGERED`, can be used, and sensitivities may be included in the error test or not (`errconS` set to `SUNTRUE` or `SUNFALSE`, respectively, in the call to `IDASetSensErrCon`).

Descriptions of one serial example (`idasSlCrank_FSA_dns`) and one parallel example (`idasBruss_FSA_kry_bbd_p`) are provided in the following two subsections. For details on the other examples, the reader is directed to the comments in their source files.

### 2.1 A serial dense example: `idasSlCrank_FSA_dns`

To illustrate the use of IDAS in a forward sensitivity analysis (FSA) problem, using the serial vector representation, we present in this section a problem from multibody system dynamics. Besides introducing the FSA capabilities of IDAS, this example also illustrates the proper treatment of such problems within IDA and IDAS (a stabilized index reduction is required).

The multibody system considered here consists of two bodies (crank and connecting rod) with a translational-spring-damper (TSD) and a constant force acting on the connecting rod. The system has a single degree of freedom. It is modeled with the three generalized coordinates indicated in Fig. 1 (crank angle, horizontal position of the translational joint, and angle of the connecting rod) and therefore has two constraints. The local reference frame on the crank is positioned at the revolute joint on the ground. The crank has length  $a$ , mass  $m_1$ , and moment of inertia  $J_1$  (with respect to the local frame). The local reference frame on the connecting rod is positioned at the translational joint. The connecting rod has length 2, mass  $m_2$ , and moment of inertia  $J_2$ . The TSD has spring constant  $k$ , damping constant  $c$ , and free length  $l_0$ . A constant horizontal force  $F$  acts on the connecting rod.

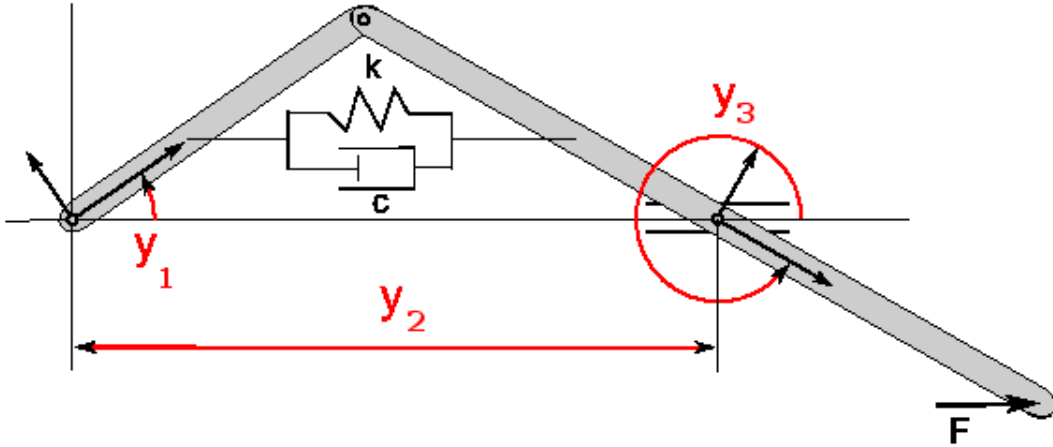


Figure 1: Slider-crank mechanism modeled with three generalized coordinates.

The equations of motion can be written as

$$\begin{aligned} M(y)\ddot{y} &= Q(y, \dot{y}) - \Phi_y^T(y)\lambda \\ \Phi(y) &= 0, \end{aligned}$$

where  $y \in R^3$  is the vector of generalized coordinates,  $M(y)$  is the generalized mass matrix, and  $Q$  is a vector of generalized applied forces.  $\Phi(y) \in R^2$  represents the (algebraic) position-level constraints and  $\Phi_y$  is its Jacobian with respect to  $y$ .  $\lambda \in R^2$  are Lagrange multipliers corresponding to the constraint forces. For its solution with IDAS, the above index-3 DAE is reformulated as a stabilized index-2 DAE (Gear-Gupta-Leimkuhler formulation, [1]) by introducing two additional Lagrange multipliers  $\mu$  and appending the velocity constraints. Converting to first order differential equations, we obtain:

$$\begin{aligned} \dot{y} &= v - \Phi_y^T(y)\mu \\ M(y)\dot{v} &= Q(y, v) - \Phi_y^T(y)\lambda \\ \Phi(y) &= 0 \\ \Phi_y(y)v &= 0 \end{aligned} \tag{1}$$

where  $v = \dot{y}$  are the generalized velocities.

For the mechanical system under consideration, the position constraints can be written as

$$\Phi(y) = \begin{bmatrix} y_2 - a \cos(y_1) - a \cos(y_3) \\ a \sin(y_1) + \sin(y_3) \end{bmatrix}$$

while the generalized force takes the form

$$Q(y, v) = \begin{bmatrix} -(f/\ell)a[\sin(y_3 - y_1)/2 + y_2 \sin(y_1)]/2 \\ (f/\ell)[\cos(y_3)/2 - y_2 + a \cos(y_1)/2] + F \\ -(f/\ell)[y_2 \sin(y_3) - a \sin(y_3 - y_1)/2]/2 - F \sin(y_3) \end{bmatrix},$$

where

$$\begin{aligned} f &= k(\ell - \ell_0) + c\ell' \\ \ell^2 &= y_2^2 - y_2[\cos(y_3) + a \cos(y_1)] + (1 + a^2)/4 + a \cos(y_3 - y_1)/2 \\ 2\ell\ell' &= 2y_2v_2 - v_2[\cos(y_3) + a \cos(y_1)] + y_2[\sin(y_3)v_3 + a \sin(y_1)v_1] \\ &\quad - a \sin(y_3 - y_1)(v_3 - v_1)/2. \end{aligned}$$

The generalized mass matrix is diagonal:  $M = \text{diag}\{J_1, m_2, J_2\}$ .

In the case treated here,  $a = .5$ ,  $J_1 = 1$ ,  $J_2 = 2$ ,  $m_1 = m_2 = 1$ ,  $F = 1$ ,  $k = 1$ ,  $c = 1$ , and  $\ell_0 = 1$ . The final time is  $t_f = 10$ .

The system (1) is solved with IDAS using a state vector  $Y = [y, v, \lambda, \mu] \in R^{10}$ . The initial conditions (at  $t = 0$ ) are set to consistent values, given as follows:

$$\begin{aligned} y_1 &= \pi/2 \\ y_3 &= \arcsin(-a) \\ y_2 &= \cos(y_3) \\ v_1 &= v_2 = v_3 = 0 \\ \lambda_1 &= \lambda_2 = \mu_1 = \mu_2 = 0 \\ dy_1/dt &= dy_2/dt = dy_3/dt = 0 \\ dv_1/dt &= [Q_1]_{t=0}/J_1 \\ dv_2/dt &= [Q_2]_{t=0}/m_2 \\ dv_3/dt &= [Q_3]_{t=0}/J_2 \\ d\lambda_1/dt &= d\lambda_2/dt = d\mu_1/dt = d\mu_2/dt = 0. \end{aligned}$$

The problem is solved with a relative tolerance of  $10^{-6}$  and a (scalar) absolute tolerance of  $10^{-7}$ . Note that the algebraic variables  $\lambda$  and  $\mu$  are excluded from the error test (by specifying them through `IDASetId` and invoking `IDASetSuppressAlg`).

The two parameters of the TSD,  $k$  and  $c$ , are considered in a forward sensitivity analysis of this model. Solution sensitivities with respect to those parameters are computed and then used to estimate the gradient of the integrated kinetic energy of the system,

$$G = \int_{t_0}^{t_f} \left( \frac{1}{2} J_1 \dot{y}_1^2 + \frac{1}{2} m_2 \dot{y}_2^2 + \frac{1}{2} J_2 \dot{y}_3^2 \right) dt. \quad (2)$$

This is then compared against gradient approximations based on (backward, forward, and central) finite differences. The sensitivity residuals are evaluated using the IDAS internal finite-difference approximation. Computation of the gradient of the integral in  $G$  takes advantage of the IDAS feature for computing sensitivities of pure quadrature equations.

Figure 2 shows the sensitivities of the horizontal position of the translational joint ( $x = y_2$ ) with respect to the TSD parameters  $k$  and  $c$ , superimposed over the solution itself.

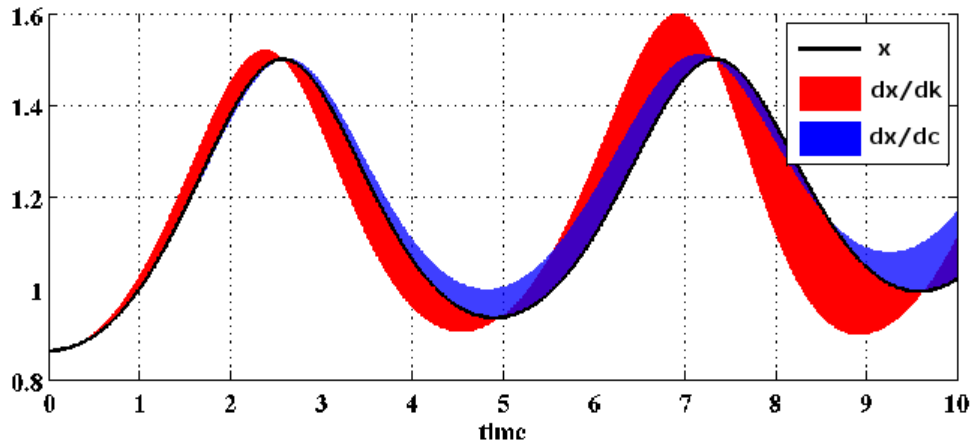


Figure 2: Sensitivities of the solution component  $y_2$  with respect to the TSD parameters.

The following output is generated by `idasSlCrank_FSA_dns` when computing sensitivities with the `IDA_SIMULTANEOUS` method and full error control:

```

idasSlCrank_FSA_dns sample output

Slider-Crank example for IDAS:

Forward integration ... done!

Final Run Statistics:

Number of steps                = 233
Number of residual evaluations  = 1194
Number of Jacobian evaluations = 47
Number of nonlinear iterations  = 724
Number of error test failures   = 0
Number of nonlinear conv. failures = 1
-----
G = 3.3366156425216897

```

```

-----
-----F O R W A R D-----
dG/dp:      3.3346e-01   -3.6375e-01
-----

      Checking using Finite Differences

-----BACKWARD-----
dG/dp:      3.3345e-01   -3.6375e-01
-----

-----FORWARD-----
dG/dp:      3.3345e-01   -3.6374e-01
-----

-----CENTERED-----
dG/dp:      3.3345e-01   -3.6375e-01
-----

```

## 2.2 A parallel example using IDABBDPRE: idasBruss\_FSA\_kry\_bbd\_p

The `idasBruss_FSA_kry_bbd_p` program solves the two-species time-dependent PDE known as the Brusselator problem, using the IDASPGMR linear solver and the IDABBDPRE preconditioner.

With subscripts on  $u$  and  $v$  denoting partial derivatives, the PDEs are as follows:

$$\begin{aligned}\partial u / \partial t &= \epsilon_1(u_{xx} + u_{yy}) + u^2 v - (B + 1)u + A \\ \partial v / \partial t &= \epsilon_2(v_{xx} + v_{yy}) - u^2 v + Bu\end{aligned}$$

on the unit square in  $(x, y)$ , and for  $0 \leq t \leq t_f = 1$ . The constants involved are  $\epsilon_1 = \epsilon_2 = 0.002$ ,  $A = 1$ , and  $B = 3.4$ . The boundary conditions are Neumann (zero derivatives). The initial conditions are given by:

$$\begin{aligned}u &= 1 - 0.5 \cos(\pi y) \\ v &= 3.5 - 2.5 \cos(\pi x)\end{aligned}$$

The PDEs are discretized by central differencing on a uniform 2D spatial mesh. The boundary conditions are handled by copying values from the first interior mesh line to a line of ghost values on each side of the square. The system is actually implemented on submeshes, processor by processor.

Here the forward sensitivity capability in IDAS is used to compute solution sensitivities with respect to the two parameters  $\epsilon_i$ . From those, we compute the corresponding sensitivities of the final spatial average of  $u$ ,

$$g = \int \int u(x, y, t_f) \, dx \, dy$$

by means of a spatial integration of the sensitivities:

$$dg/d\epsilon_i = \int \int \partial u(x, y, t_f) / \partial \epsilon_i \, dx \, dy .$$

The following output is generated by `idasBruss_FSA_kry_bbd_p` when computing sensitivities with the `IDA_SIMULTANEOUS` method and full error control:

```
mpirun -np 4 idasBruss_FSA_kry_bbd_p -sensi sim t
```

idasBruss_FSA_kry_bbd_p sample output					
Brusselator PDE - DAE parallel example problem for IDA					
Number of species ns: 2      Mesh dimensions: 82 x 82					
Total system size: 13448					
Subgrid dimensions: 41 x 41      Processor array: 2 x 2					
Tolerance parameters: rtol = 1e-05      atol = 1e-05					
Linear solver: SUNSPGMR      Max. Krylov dimension maxl: 16					
Preconditioner: band-block-diagonal (IDABBDPRE), with parameters					
mudq = 82, mldq = 82, mukeep = 2, mlkeep = 2					
CalcIC called to correct initial concentrations					
-----					
t	bottom-left	top-right	nst	k	h
-----					
0.00e+00	5.0038e-01	1.4996e+00	0	0	1.0000e-07
	1.0019e+00	5.9981e+00			
1.00e-03	4.9944e-01	1.5076e+00	11	1	5.1200e-04
	1.0034e+00	5.9896e+00			
1.00e-02	4.9119e-01	1.5832e+00	17	2	2.0480e-03
	1.0170e+00	5.9082e+00			
1.00e-01	4.2223e-01	3.0684e+00	31	4	7.4353e-03
	1.1419e+00	4.3097e+00			
4.00e-01	3.0652e-01	5.4104e+00	72	5	7.4353e-03
	1.4714e+00	6.1133e-01			
7.00e-01	2.7048e-01	4.1053e+00	112	5	7.4353e-03
	1.7403e+00	7.8907e-01			
1.00e+00	2.6100e-01	3.1024e+00	152	5	7.4353e-03
	1.9881e+00	1.0113e+00			
-----					
Final statistics:					
Number of steps = 152					
Number of residual evaluations = 1243					
Number of nonlinear iterations = 165					
Number of error test failures = 1					
Number of nonlinear conv. failures = 1					
Number of linear iterations = 1047					
Number of linear conv. failures = 0					
Number of preconditioner setups = 16					
Number of preconditioner solves = 1635					
Number of local residual evals. = 2656					

```
The average of u on the domain:  
g = 1.62453
```

```
Sensitivities of g:  
w.r.t. eps0 = 16.1571399862  
w.r.t. eps1 = -3.7188305042
```

### 3 Adjoint sensitivity analysis example problems

The next two subsections describe a serial example (`idasAkzoNob_ASAi_dns`) and a parallel one (`idasBruss_ASAP_kry_bbd_p`). For details on the other examples, the reader is directed to the comments in their source files.

#### 3.1 A serial dense example: `idasAkzoNob_ASAi_dns`

The `idasAkzoNob_ASAi_dns` program solves the Akzo-Nobel chemical kinetics problem, which consists of six nonlinear DAEs. The system has index 1. The problem originates from Akzo Nobel Central research in Arnhem, The Netherlands, and describes a chemical process in which two species are mixed, while carbon dioxide is continuously added.

The problem is of the form

$$\begin{aligned} y' &= f(y, z) \\ 0 &= g(y, z) \end{aligned} \tag{3}$$

with  $y \in R^5$  and  $z \in R$ . The function  $f$  is defined by

$$f(y, z) = \begin{bmatrix} -2r_1 & +r_2 & -r_3 & -r_4 & & \\ -\frac{1}{2}r_1 & & & -r_4 & -\frac{1}{2}r_5 & +F_{in} \\ r_1 & -r_2 & +r_3 & & & \\ & -r_2 & +r_3 & -2r_4 & & \\ & r_2 & -r_3 & & +r_5 & \end{bmatrix}$$

where the  $r_i$  and  $F_{in}$  are auxiliary variables, given by

$$\begin{aligned} r_1 &= k_1 y_1^4 y_2^{1/2} \\ r_2 &= k_2 y_3 y_4 \\ r_3 &= \frac{k_2}{K} y_1 y_5 \\ r_4 &= k_3 y_1 y_4^{1/2} \\ r_5 &= k_4 z^2 y_2^{1/2} \\ F_{in} &= klA \left( \frac{p(CO_2)}{H} - y_2 \right) . \end{aligned}$$

The function  $g$  in the algebraic equation is defined by

$$g(y, z) = K_s y_1 y_4 - z .$$

It is clear from the fact that the Jacobian  $\partial g / \partial z$  is non-singular that the DAE (3) has (differentiation) index 1. See <http://pitagora.dm.uniba.it/~testset/report/chemakzo.pdf> for details.

The problem is solved with the IDADENSE linear solver using the default difference quotient dense Jacobian approximation. The adjoint capability of IDAS is used to compute gradients with respect to the initial conditions of the integral

$$G = \int_0^{t_f} y_1 dt ,$$



where  $y_1$  is the concentration of the first species. The sensitivity of  $G$  is the solution of the adjoint system, evaluated at  $t = 0$ .

The output generated by `idasAkzoNob_ASAi_dns` is shown below.

```

----- idasAkzoNob_ASAi_dns sample output -----

Adjoint Sensitivity Example for Akzo-Nobel Chemical Kinetics
-----
Sensitivity of G = int_t0^tf (y1) dt with respect to IC.
-----

Forward integration ... done ( nst = 457 )
G:                31.2642162580311549
-----

Backward integration ... done ( nst = 274 )
dG/dy0:           2.2207e+01
                  -6.2695e+01
                  -2.5115e+00
                  9.1837e+01
                  3.5176e+00
                  3.6976e-01
-----

```

### 3.2 A parallel example using IDABBDPRE: `idasBruss_ASAP_kry_bbd_p`

The `idasBruss_ASAP_kry_bbd_p` program solves the same problem as `idasBruss_kry_bbd_p` and `idasBruss_FSA_kry_bbd_p`, namely the Brusselator PDE system. (See §2.2 above.) In addition, it uses an adjoint sensitivity approach to compute the gradients of the model output functional

$$g(t) = \int \int u(t, x, y) \, dx \, dy .$$

For perturbations  $\delta u_0$  and  $\delta v_0$  in the initial profiles  $u$  and  $v$ , the perturbation of  $g$  at the final time is

$$\delta g(t_f) = \int \int [\lambda(0, x, y) \delta u_0 + \mu(0, x, y) \delta v_0] \, dx \, dy ,$$

where  $\lambda(t, x, y)$  and  $\mu(t, x, y)$  are the solutions of the adjoint PDEs,

$$\begin{aligned} \partial \lambda / \partial t &= -\epsilon_1 (\lambda_{xx} + \lambda_{yy}) - (2uv - B - 1)\lambda + (2uv - B)\mu \\ \partial \mu / \partial t &= -\epsilon_2 (\mu_{xx} + \mu_{yy}) - u^2 \lambda + u^2 \mu , \end{aligned}$$

with Neumann boundary conditions, and initial (final time) conditions

$$\lambda(t_f, x, y) = 1 , \quad \mu(t_f, x, y) = 0 .$$

The adjoint PDEs are discretized and solved in the same way as the Brusselator PDEs.

A sample output generated by `idasBruss_ASAP_kry_bbd_p` is shown below.

```

----- idasBruss_ASAP_kry_bbd_p sample output -----

Starting integration of the FORWARD problem

```

BRUSSELATOR: chemically reacting system

Number of species ns: 2      Mesh dimensions: 42 x 42  
Total system size: 3528  
Subgrid dimensions: 21 x 21      Processor array: 2 x 2  
Tolerance parameters: rtol = 1e-05    atol = 1e-05  
Linear solver: SUNSPGMR      Max. Krylov dimension maxl: 16  
Preconditioner: band-block-diagonal (IDABBDPRE), with parameters  
                 mudq = 42, mldq = 42, mukeep = 2, mlkeep = 2

t	bottom-left	top-right	nst	k	h
1.00e+00	2.6132e-01	3.0982e+00	154	5	1.1112e-02
	1.9993e+00	1.0125e+00			

Final statistics:

Number of steps                                = 154  
Number of residual evaluations               = 392  
Number of nonlinear iterations               = 174  
Number of error test failures                = 2  
Number of nonlinear conv. failures = 0  
  
Number of linear iterations                   = 216  
Number of linear conv. failures              = 0  
  
Number of preconditioner setups              = 17  
Number of preconditioner solves              = 392  
Number of local residual evals.              = 1462

BACKWARD problem

Final statistics:

Number of steps                                = 99  
Number of residual evaluations               = 268  
Number of nonlinear iterations               = 118  
Number of error test failures                = 0  
Number of nonlinear conv. failures = 0  
  
Number of linear iterations                   = 150  
Number of linear conv. failures              = 0  
  
Number of preconditioner setups              = 16  
Number of preconditioner solves              = 268  
Number of local residual evals.              = 1376

## References

- [1] C.W. Gear, B. Leimkuhler, and G.K. Gupta. Automatic Integration of Euler-Lagrange Equations with Constraints. *J. Comput. Appl. Math.*, 12/13:77–90, 1985.
- [2] A. C. Hindmarsh, R. Serban, and A. Collier. Example Programs for IDA v4.0.0-dev. Technical Report UCRL-SM-208113, LLNL, 2017.
- [3] 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.
- [4] R. Serban, C. Petra, and A. C. Hindmarsh. User Documentation for IDAS v3.0.0-dev. Technical Report UCRL-SM-234051, LLNL, 2017.

