Example Programs for kINSOL v5.2.0

Aaron M. Collier and Radu Serban
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory

March 31, 2020
DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

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

Approved for public release; further dissemination unlimited
Contents

1 Introduction 1

2 C example problems 3
   2.1 A serial dense example: kinFerTron_dns .......................... 3
   2.2 A serial Krylov example: kinFoodWeb_kry .......................... 6
   2.3 A parallel example: kinFoodWeb_kry_bbd_p ........................ 8

3 Fortran example problems 11
   3.1 A serial example: fkinDiagon_kry .................................. 11
   3.2 A parallel example: fkinDiagon_kry_p .............................. 13

References 14
1 Introduction

This report is intended to serve as a companion document to the User Documentation of KINSOL [1]. It provides details, with listings, on the example programs supplied with the KINSOL distribution package.

The KINSOL distribution contains examples of types: serial C examples, parallel C examples, serial and parallel FORTRAN examples, and an OpenMP example. With the exception of "demo"-type example files, the names of all the examples distributed with SUNDIALS are of the form [slv][PbName]_[strat]_[ls]_[prec]_[p], where

[slv] identifies the solver (for KINSOL examples this is kin, while for FKINSOL examples, this is fkin);

[PbName] identifies the problem;

[strat] identifies the strategy (absent if “none” or “linesearch”);

[ls] identifies the linear solver module used;

[prec] indicates the KINSOL preconditioner module used (only if applicable, for examples using a Krylov linear solver and the KBBDPRE module, this will be bbd);

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

The following lists summarize all examples distributed with KINSOL.

Supplied in the srcdir/examples/kinsol/serial directory are the following serial examples (using the NVVECTOR_SERIAL module):

- kinRoberts_fp solves the backward Euler time step for a three-species chemical kinetics system, using the fixed point strategy.

- kinFerTron_dns solves the Ferraris-Tronconi problem. This program solves the problem with the SUNLINSOL_DENSE linear solver and uses different combinations of globalization and Jacobian update strategies with different initial guesses.

- kinFerTron_klu solves the same problem as in kinFerTron_dns, but uses the sparse direct solver KLU via the SUNLINSOL_KLU module.

- kinRoboKin_dns solves a nonlinear system from robot kinematics. This program solves the problem with the SUNLINSOL_DENSE linear solver and a user-supplied Jacobian routine.

- kinRoboKin slu is the same as kinRoboKin_dns but uses the SuperLUMT sparse direct linear solver via the SUNLINSOL_SUPERLUMT module.

- kinLaplace_bnd solves a simple 2-D elliptic PDE on a unit square. This program solves the problem with the SUNLINSOL_BAND linear solver.

- kinLaplace_picard_bnd is the same as kinLaplace_bnd but uses the Picard strategy.
• **kinFoodWeb.kry** solves a food web model. This is a nonlinear system that arises from a system of partial differential equations describing a six-species food web population model, with predator-prey interaction and diffusion on the unit square in two dimensions. This program solves the problem with the SUNLINSOL_SPGMR linear solver module and a user-supplied preconditioner. The preconditioner is a block-diagonal matrix based on the partial derivatives of the interaction terms only.

• **kinKrylovDemo ls** solves the same problem as **kinFoodWeb.kry**, but with three Krylov linear solvers: SUNLINSOL_SPGMR, SUNLINSOL_SPCGS, and SUNLINSOL_SPTFQMR.

Supplied in the *srcdir/examples/kinsol/parallel* directory are the following parallel examples (using the NVECTO_PARALLEL module):

• **kinFoodWeb.kry.p** is a parallel implementation of **kinFoodWeb.kry**.

• **kinFoodWeb.kry_bbd.p** solves the same problem as **kinFoodWeb.kry.p**, with a block-diagonal matrix with banded blocks as a preconditioner, generated by difference quotients, using the KINBBDPRE module.

As part of the FKINSOL module, in the directories *srcdir/examples/kinsol/fcmix_serial* and *srcdir/examples/kinsol/fcmix_parallel*, respectively, are the following examples for the FORTRAN-C interface:

• **fkinDiagon.kry** is a serial example, which solves a nonlinear system of the form $u_i^2 = i^2$ using an approximate diagonal preconditioner.

• **fkinDiagon.kry.p** is a parallel implementation of **fkinDiagon.kry**.

Supplied in directory *srcdir/examples/kinsol/C_openmp* is an example using the OpenMP NVECTO module. **kin_FoodWeb_kry_omp** solves the same problem as **kin_FoodWeb_kry** but uses the OpenMP module.

In the following sections, we give detailed descriptions of some (but not all) of these examples. We also give our output files for each of these examples, 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 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 KINSOL User Document [1]. All citations to specific sections (e.g. §4.2) are references to parts of that User Document, unless explicitly stated otherwise.

**Note.** The examples in the KINSOL distribution are written in such a way as to compile and run for any combination of configuration options used during the installation of SUNDIALS (see Appendix A in the User Guide). As a consequence, they contain portions of code that will not be typically present in a user program. For example, all C 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.
2 C example problems

2.1 A serial dense example: kinFerTron_dns

As an initial illustration of the use of the KINSOL package for the solution of nonlinear systems, we give a sample program called kinFerTron_dns.c. It uses the KINSOL dense linear solver module SUNLINSOL_DENSE and the NVECTOR_SERIAL module (which provides a serial implementation of NVECTOR) for the solution of the Ferraris-Tronconi test problem [2].

This problem involves a blend of trigonometric and exponential terms:

\[
0 = 0.5 \sin(x_1 x_2) - 0.25 x_2 / \pi - 0.5 x_1 \\
0 = (1 - 0.25 / \pi)(e^{2x_1} - e) + e x_2 / \pi - 2 e x_1
\]

subject to
\[
\begin{align*}
x_{1 \text{min}} &= 0.25 \leq x_1 \leq 1 = x_{1 \text{max}} \\
x_{2 \text{min}} &= 1.5 \leq x_2 \leq 2 \pi = x_{2 \text{max}}.
\end{align*}
\]

The bounds constraints on \(x_1\) and \(x_2\) are treated by introducing four additional variables and using KINSOL’s optional constraints feature to enforce non-positivity and non-negativity:

\[
\begin{align*}
l_1 &= x_1 - x_{1 \text{min}} \geq 0 \\
L_1 &= x_1 - x_{1 \text{max}} \leq 0 \\
l_2 &= x_2 - x_{2 \text{min}} \geq 0 \\
L_2 &= x_2 - x_{2 \text{max}} \leq 0.
\end{align*}
\]

The Ferraris-Tronconi problem has two known solutions. We solve it with KINSOL using two sets of initial guesses for \(x_1\) and \(x_2\) (first their lower bounds and secondly the middle of their feasible regions), both with an exact and modified Newton method, with and without line search.

Following the initial comment block, this program has a number of \#include lines, which allow access to useful items in CVODE header files. The kinsol.h file provides prototypes for the KINSOL functions to be called (excluding the linear solver selection function), and also a number of constants that are to be used in setting input arguments and testing the return value of KINSol. The nvector_serial.h file is the header file for the serial implementation of the NVECTOR module and includes definitions of the N_Vector type, a macro to access vector components, and prototypes for the serial implementation specific machine environment memory allocation and freeing functions. The sunmatrix_dense.h file provides the prototype for the SUNDenseMatrix function. The sunlinsol_dense.h file provides the prototype for the SUNLinSol_Dense function. The sundials_types.h file provides the definition of the type realtype (see §4.2 for details). For now, it suffices to read realtype as double. Finally, sundials_math.h is included for the definition of the exponential function RExp.

Next, the program defines some problem-specific constants, which are isolated to this early location to make it easy to change them as needed. This program includes a user-defined accessor macro, Ith, that is useful in writing the problem functions in a form closely matching the mathematical description of the system, i.e. with components numbered from 1 instead of from 0. The Ith macro is used to access components of a vector of type N_Vector with a serial implementation. It is defined using the NVECTOR_SERIAL accessor macro NV_Ith_S which numbers components starting with 0. The program prologue ends with prototypes of the user-supplied system function func and several private helper functions.
The main program begins with some dimensions and type declarations, including use of the type \texttt{N\_Vector}, initializations, and allocation and definitions for the user data structure \texttt{data} which contains two arrays with lower and upper bounds for \(x_1\) and \(x_2\). Next, we create five serial vectors of type \texttt{N\_Vector} for the two different initial guesses, the solution vector \(u\), the scaling factors, and the constraint specifications.

The initial guess vectors \(u_1\) and \(u_2\) are set by the private functions \texttt{SetInitialGuess1} and \texttt{SetInitialGuess2} and the constraint vector \(c\) is initialized to \([0, 0, 1, -1, 1, -1]\) indicating that there are no additional constraints on the first two components of \(u\) (i.e. \(x_1\) and \(x_2\)) and that the 3rd and 5th components should be non-negative, while the 4th and 6th should be non-positive.

The calls to \texttt{N\_VNew\_Serial}, and also later calls to various \texttt{KIN***} functions, make use of a private function, \texttt{check\_flag}, which examines the return value and prints a message if there was a failure. The \texttt{check\_flag} function was written to be used for any serial SUNDIALS application.

The call to \texttt{KINCreate} creates the \texttt{knsol} solver memory block. Its return value is a pointer to that memory block for this problem. In the case of failure, the return value is \texttt{NULL}. This pointer must be passed in the remaining calls to \texttt{KINSOL} functions.

The next four calls to \texttt{KINSOL} optional input functions specify the pointer to the user data structure (to be passed to all subsequent calls to \texttt{func}), the vector of additional constraints, and the function and scaled step tolerances, \texttt{fnormtol} and \texttt{scsteptol}, respectively.

Solver memory is allocated through the call to \texttt{KINInit} which specifies the system function \texttt{func} and provides the vector \(u\) which will be used internally as a template for cloning additional necessary vectors of the same type as \(u\). The use of the dense linear solver is specified by calling \texttt{SUNDenseMatrix} to create the template Jacobian matrix (which also specifies the problem size \texttt{NEQ}), then calling \texttt{SUNLinSol\_Dense} to create the dense-direct linear solver, and finally calling \texttt{KINSetLinearSolver} to attach these to \texttt{KINSOL}.

The main program proceeds by solving the nonlinear system eight times, using each of the two initial guesses \(u_1\) and \(u_2\) (which are first copied into the vector \(u\) using \texttt{N\_VScale\_Serial} from the \texttt{NVECTOR\_SERIAL} module), with and without globalization through line search (specified by setting \texttt{glstr} to \texttt{KIN\_LINESEARCH} and \texttt{KIN\_NONE}, respectively), and applying either an exact or a modified Newton method. The switch from exact to modified Newton is done by changing the number of nonlinear iterations after which a Jacobian evaluation is enforced, a value \texttt{mset} = 1 thus resulting in re-evaluating the Jacobian at every single iteration of the nonlinear solver (exact Newton method). Note that passing \texttt{mset} = 0 indicates using the default \texttt{KINSOL} value of 10.

The actual problem solution is carried out in the private function \texttt{SolveIt} which calls the main solver function \texttt{KINSol} after first setting the optional input \texttt{mset}. After a successful return from \texttt{KINSol}, the solution \([x_1, x_2]\) and some solver statistics are printed.

The function \texttt{func} is a straightforward expression of the extended nonlinear system. It uses the macro \texttt{NV\_DATA\_S} (defined by the \texttt{NVECTOR\_SERIAL} module) to extract the pointers to the data arrays of the \texttt{N\_Vectors} \(u\) and \(f\) and sets the components of \texttt{fdata} using the current values for the components of \texttt{udata}. See §4.6.1 for a detailed specification of \(f\).

The output generated by \texttt{kinFerTron\_dns} is shown below.

---

Ferraris and Tronconi test problem
Tolerance parameters:
fnormtol = 1e-05
scsteptol = 1e-05

------------------------------------------
Initial guess on lower bounds
[x1, x2] = 0.25 1.5

Exact Newton
Solution:
[x1, x2] = 0.299449 2.83693
Final Statistics:
nni = 3  nfe = 4
nje = 3  nfeD = 18

Exact Newton with line search
Solution:
[x1, x2] = 0.299449 2.83693
Final Statistics:
nni = 3  nfe = 4
nje = 3  nfeD = 18

Modified Newton
Solution:
[x1, x2] = 0.299449 2.83693
Final Statistics:
nni = 11  nfe = 12
nje = 2  nfeD = 12

Modified Newton with line search
Solution:
[x1, x2] = 0.299449 2.83693
Final Statistics:
nni = 11  nfe = 12
nje = 2  nfeD = 12

------------------------------------------

Initial guess in middle of feasible region
[x1, x2] = 0.625 3.89159

Exact Newton
Solution:
[x1, x2] = 0.5 3.14159
Final Statistics:
nni = 5  nfe = 6
nje = 5  nfeD = 30

Exact Newton with line search
Solution:
[x1, x2] = 0.5 3.14159
Final Statistics:
nni = 5  nfe = 6
nje = 5  nfeD = 30

Modified Newton
Solution:
[x1, x2] = 0.500003 3.1416
Final Statistics:
Modified Newton with line search

Solution:

\[ [x_1, x_2] = 0.500003 \quad 3.1416 \]

Final Statistics:

\[ n_{ni} = 12 \quad n_{fe} = 13 \]
\[ n_{je} = 2 \quad n_{feD} = 12 \]

\section*{2.2 A serial Krylov example: kinFoodWeb\_kry}

We give here an example that illustrates the use of \textsc{kinsol} with the Krylov method \textsc{spgmr}, via the \textsc{sunlinsol\_spgmr} module, as the linear system solver.

This program solves a nonlinear system that arises from a discretized system of partial differential equations. The PDE system is a six-species food web population model, with predator-prey interaction and diffusion on the unit square in two dimensions. Given the dependent variable vector of species concentrations \( c = [c_1, c_2, ..., c_{n_s}]^T \), where \( n_s = 2n_p \) is the number of species and \( n_p \) is the number of predators and of prey, then the PDEs can be written as

\[
d_i \cdot \left( \frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} \right) + f_i(x, y, c) = 0 \quad (i = 1, ..., n_s),
\]

where the subscripts \( i \) are used to distinguish the species, and where

\[
f_i(x, y, c) = c_i \cdot \left( b_i + \sum_{j=1}^{n_s} a_{ij} \cdot c_j \right).
\]

The problem coefficients are given by

\[
a_{ij} = \begin{cases} 
-1 & i = j \\
-0.5 \cdot 10^{-6} & i \leq n_p, \; j > n_p \\
10^4 & i > n_p, \; j \leq n_p \\
0 & \text{all other} 
\end{cases}
\]

\[
b_i = b_i(x, y) = \begin{cases} 
1 + \alpha xy & i \leq n_p \\
-1 - \alpha xy & i > n_p,
\end{cases}
\]

and

\[
d_i = \begin{cases} 
1 & i \leq n_p \\
0.5 & i > n_p.
\end{cases}
\]

The spatial domain is the unit square \((x, y) \in [0, 1] \times [0, 1]\).

Homogeneous Neumann boundary conditions are imposed and the initial guess is constant in both \( x \) and \( y \). For this example, the equations (2) are discretized spatially with standard central finite differences on a \( 8 \times 8 \) mesh with \( n_s = 6 \), giving a system of size 384.

Among the initial \#include lines in this case are lines to include \textsc{sunlinsol\_spgmr.h} and \textsc{sundials\_math.h}. The first contains constants and function prototypes associated with the \textsc{spgmr} solver module. The inclusion of \textsc{sundials\_math.h} is done to access the \textsc{sunmax}...
and SUNRabs macros, and the SUNRsqrt function to compute the square root of a realtype number.

The main program calls KINCreate and then calls KINInit with the name of the user-supplied system function func and solution vector as arguments. The main program then calls a number of KINSet* routines to notify KINSOL of the user data pointer, the positivity constraints on the solution, and convergence tolerances on the system function and step size. It calls SUNLinSol_SPGMR (see §4.5.2) to create the spgmr linear solver module, supplying the maxl value of 15 as the maximum Krylov subspace dimension. It then calls KINSetLinearSolver to attach this solver module to KINSOL. Next, a maximum value of maxlrst = 2 restarts is imposed through a call to SUNLinSol_SPGMRSetMaxRestarts. Finally, the user-supplied preconditioner setup and solve functions, PrecSetupBD and PrecSolveBD, are specified through a call to KINSetPreconditioner (see §4.5.4). The data pointer passed to KINSetUserData is passed to PrecSetupBD and PrecSolveBD whenever these are called.

Next, KINSol is called, the return value is tested for error conditions, and the approximate solution vector is printed via a call to PrintOutput. After that, PrintFinalStats is called to get and print final statistics, and memory is freed by calls to N_VDestroy_Serial, FreeUserData and KINFree. The statistics printed are the total numbers of nonlinear iterations (nni), of func evaluations (excluding those for Jv product evaluations) (nfe), of func evaluations for Jv evaluations (nfeSG), of linear (Krylov) iterations (nli), of preconditioner evaluations (npe), and of preconditioner solves (nps). All of these optional outputs and others are described in §4.5.5.

Mathematically, the dependent variable has three dimensions: species number, x mesh point, and y mesh point. But in nvector_serial, a vector of type N_Vector works with a one-dimensional contiguous array of data components. The macro IJ_Vptr isolates the translation from three dimensions to one. Its use results in clearer code and makes it easy to change the underlying layout of the three-dimensional data. Here the problem size is 384, so we use the NV_DATA_S macro for efficient N_Vector access. The NV_DATA_S macro gives a pointer to the first component of a serial N_Vector which is then passed to the IJ_Vptr macro.

The preconditioner used here is the block-diagonal part of the true Newton matrix and is based only on the partial derivatives of the interaction terms \( f \) in (3) and hence its diagonal blocks are \( n_s \times n_s \) matrices (\( n_s = 6 \)). It is generated and factored in the PrecSetupBD routine and backsolved in the PrecSolveBD routine. See §4.6.7 for detailed descriptions of these preconditioner functions.

The program kinFoodWeb_kry.c uses the “small” dense functions for all operations on the 6\( \times \)6 preconditioner blocks. Thus it includes sundials_dense.h, and calls the small dense matrix functions newDenseMat, denseGETRF, and denseGETRS. The small dense functions are generally available for KINSOL user programs (for more information, see the comments in the header file sundials_dense.h).

In addition to the functions called by KINSOL, kinFoodWeb_kry.c includes definitions of several private functions. These are: AllocUserData to allocate space for the preconditioner and the pivot arrays; InitUserData to load problem constants in the data block; FreeUserData to free that block; SetInitialProfiles to load the initial values in cc; PrintHeader to print the heading for the output; PrintOutput to retrieve and print selected solution values; PrintFinalStats to print statistics; and check_flag to check return values for error conditions.

The output generated by kinFoodWeb_kry is shown below. Note that the solution involved 10 Newton iterations, with an average of about 38 Krylov iterations per Newton iteration.
2.3 A parallel example: kinFoodWeb_kry_bbd_p

In this example, kinFoodWeb_kry_bbd_p, we solve the same problem as with kinFoodWeb_kry above, but in parallel, and instead of supplying the preconditioner we use the KINBBDPRE module.

In this case, we think of the parallel MPI processes as being laid out in a rectangle, and each process being assigned a subgrid of size \( MX\times MY \) of the \( x-y \) grid. If there are \( NPEX \) processes in the \( x \) direction and \( NPEY \) processes in the \( y \) direction, then the overall grid size is \( MX\times MY \) with \( MX=NPEX\times MXSUB \) and \( MY=NPEY\times MYSUB \), and the size of the nonlinear system is \( \text{NUM\_SPECIES}\times MX\times MY \).

The evaluation of the nonlinear system function is performed in func. In this parallel setting, the processes first communicate the subgrid boundary data and then compute the local components of the nonlinear system function. The MPI communication is isolated in the private function ccomm (which in turn calls BRecvPost, BSend, and BRecvWait) and the subgrid boundary data received from neighboring processes is loaded into the work array cext. The computation of the nonlinear system function is done in func_local which starts by copying the local segment of the \( cc \) vector into cext, and then by imposing the boundary conditions by copying the first interior mesh line from \( cc \) into cext. After this, the nonlinear system function is evaluated by using central finite-difference approximations using the data in cext exclusively.

KINBBDPRE uses a band-block-diagonal preconditioner, generated by difference quotients.
The upper and lower half-bandwidths of the Jacobian block generated on each process are both equal to $2 \cdot n_s - 1$, and that is the value passed as \texttt{mudq} and \texttt{mldq} in the call to \texttt{KINBBDPrecInit}. These values are much less than the true half-bandwidths of the Jacobian blocks, which are $n_s \cdot \text{MXSUB}$. However, an even narrower band matrix is retained as the preconditioner, with half-bandwidths equal to $n_s$, and this is the value passed to \texttt{KINBBDPrecInit} for \texttt{mukeep} and \texttt{mlkeep}.

The function \texttt{func	extunderscore local} is also passed as the \texttt{gloc} argument to \texttt{KINBBDPrecInit}. Since all communication needed for the evaluation of the local approximation of $f$ used in building the band-block-diagonal preconditioner is already done for the evaluation of $f$ in \texttt{func}, a NULL pointer is passed as the \texttt{gcomm} argument to \texttt{KINBBDPrecInit}.

The \texttt{main} program resembles closely that of the \texttt{kinFoodWeb\_kry} example, with particularization arising from the use of the parallel MPI \texttt{nvector\_parallel} module. It begins by initializing MPI and obtaining the total number of processes and the rank of the local process. The local length of the solution vector is then computed as \texttt{NUM\_SPECIES\_MXSUB\_MYSUB}. Distributed vectors are created by calling the constructor defined in \texttt{nvector\_parallel} with the MPI communicator and the local and global problem sizes as arguments. All output is performed only from the process with id equal to 0. Finally, after \texttt{KINSol} is called and the results are printed, all memory is deallocated, and the MPI environment is terminated by calling \texttt{MPI\_Finalize}.

The output generated by \texttt{kinFoodWeb\_kry\_bbd\_p} is shown below. Note that 9 Newton iterations were required, with an average of about 51.6 Krylov iterations per Newton iteration.

---

**Predator-prey test problem -- KINSol (parallel-BBD version)**

- Mesh dimensions = 20 X 20
- Number of species = 6
- Total system size = 2400

- Subgrid dimensions = 10 X 10
- Processor array is 2 X 2

- Flag globalstrategy = 0 (0 = None, 1 = Linesearch)
- Linear solver is SPGMR with maxl = 20, maxlrst = 2
- Preconditioning uses band-block-diagonal matrix from \texttt{KINBBDPRE}
  - Difference quotient half-bandwidths: mudq = 11, mldq = 11
  - Retained band block half-bandwidths: mukeep = 6, mlkeep = 6
- Tolerance parameters: fnormtol = 1e-07 scsteptol = 1e-13

Initial profile of concentration
At all mesh points: 1 1 1 30000 30000 30000

Computed equilibrium species concentrations:
At bottom left:
1.165 1.165 1.165 34949 34949 34949

At top right:
1.25552 1.25552 1.25552 37663.2 37663.2 37663.2

Final Statistics..

nni = 9  nli = 464
<table>
<thead>
<tr>
<th>nfe</th>
<th>10</th>
<th>nfeSG</th>
<th>473</th>
</tr>
</thead>
<tbody>
<tr>
<td>nps</td>
<td>473</td>
<td>npe</td>
<td>1</td>
</tr>
<tr>
<td>ncfl</td>
<td>6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3 Fortran example problems

The FORTRAN example problem programs supplied with the KINSOL package are all written in standard F77 Fortran and use double precision arithmetic. Before running any of these examples, the user should make sure that the FORTRAN data types for real and integer variables appropriately match the C types. See §5.3 in the KINSOL User Document for details.

However, when the FORTRAN examples are built, the source code is automatically modified according to the configure options supplied by the user and the system type. Integer variables are declared as INTEGER*n, where n denotes the number of bytes in the corresponding C type (long int or int). Floating-point variable declarations remain unchanged if double precision is used, but are changed to REAL*n, where n denotes the number of bytes in the SUNDIALS type realtype, if using single precision. Also, if using single precision, declarations of floating-point constants are appropriately modified, e.g. 0.5D-4 is changed to 0.5E-4.

The two examples supplied with the fkinsol module are very simple tests of the FORTRAN-C interface module. They solve the nonlinear system

$$F(u) = 0, \quad \text{where } f_i(u) = u_i^2 - i^2, 1 \leq i \leq N.$$  

3.1 A serial example: fkinDiagon_kry

The fkinDiagon_kry program solves the above problem using the NVECTOR_SERIAL module.

The main program begins by calling fnvinits to initialize computations with the NVECTOR_SERIAL module. Next, the array uu is set to contain the initial guess $u_i = 2i$, the array scale is set with all components equal to 1.0 (meaning that no scaling is done), and the array constr is set with all components equal to 0.0 to indicate that no inequality constraints should be imposed on the solution vector.

The KINSOL solver is initialized and memory for it is allocated by calling fkinmalloc, which also specifies the iout and rout arrays which are used to store integer and real outputs, respectively (see Table 5.4). Also, various integer, real, and vector parameters are specified by calling the kinsetiin, kinsetrin, and kinsetvin subroutines, respectively. In particular, the maximum number of iterations between calls to the preconditioner setup routine (msbpre = 5), the tolerance for stopping based on the function norm (fnormtol = 10^{-5}), and the tolerance for stopping based on the step length (scsteptol = 10^{-4}) are specified.

Next, the SUNLINSOL_SPGMR linear solver module is attached to KINSOL by calling fsunspgmrinit, which also specifies the maximum Krylov subspace dimension (maxl = 10). This is then attached to KINSOL by calling fkinlsinit. The maximum number of restarts allowed for SPGMR is then updated to maxlrst = 2 by calling fsunspgmrsetmaxrs. The SUNLINSOL_SPGMR module is then directed to use the supplied preconditioner by calling the fkinlssetprec routine with a first argument equal to 1. The solution of the nonlinear system is obtained after a successful return from fkinsol, which is then printed to unit 6 (stdout). Finally, memory allocated for the KINSOL solver is released by calling fkinfree.

The user-supplied routine fkfun contains a straightforward transcription of the nonlinear system function $f$, while the routinefkpset sets the array pp (in the common block pcom) to contain an approximation to the reciprocals of the Jacobian diagonal elements. The components of pp are then used in fkpsol to solve the preconditioner linear system $Px = v$ through simple multiplications.

The following is sample output from fkinDiagon_kry, using $N = 128$. 

11
Example program fkinDiagon_kry:

This FKINSOL example solves a 128 eqn diagonal algebraic system. Its purpose is to demonstrate the use of the Fortran interface in a serial environment.

globalstrategy = KIN_NONE

FKINSOL return code is 0

The resultant values of uu are:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00000</td>
<td>2.00000</td>
<td>3.00000</td>
<td>4.00000</td>
</tr>
<tr>
<td>5</td>
<td>5.00000</td>
<td>6.00000</td>
<td>7.00000</td>
<td>8.00000</td>
</tr>
<tr>
<td>9</td>
<td>9.00000</td>
<td>10.00000</td>
<td>11.00000</td>
<td>12.00000</td>
</tr>
<tr>
<td>13</td>
<td>13.00000</td>
<td>14.00000</td>
<td>15.00000</td>
<td>16.00000</td>
</tr>
<tr>
<td>17</td>
<td>17.00000</td>
<td>18.00000</td>
<td>19.00000</td>
<td>20.00000</td>
</tr>
<tr>
<td>21</td>
<td>21.00000</td>
<td>22.00000</td>
<td>23.00000</td>
<td>24.00000</td>
</tr>
<tr>
<td>25</td>
<td>25.00000</td>
<td>26.00000</td>
<td>27.00000</td>
<td>28.00000</td>
</tr>
<tr>
<td>29</td>
<td>29.00000</td>
<td>30.00000</td>
<td>31.00000</td>
<td>32.00000</td>
</tr>
<tr>
<td>33</td>
<td>33.00000</td>
<td>34.00000</td>
<td>35.00000</td>
<td>36.00000</td>
</tr>
<tr>
<td>37</td>
<td>37.00000</td>
<td>38.00000</td>
<td>39.00000</td>
<td>40.00000</td>
</tr>
<tr>
<td>41</td>
<td>41.00000</td>
<td>42.00000</td>
<td>43.00000</td>
<td>44.00000</td>
</tr>
<tr>
<td>45</td>
<td>45.00000</td>
<td>46.00000</td>
<td>47.00000</td>
<td>48.00000</td>
</tr>
<tr>
<td>49</td>
<td>49.00000</td>
<td>50.00000</td>
<td>51.00000</td>
<td>52.00000</td>
</tr>
<tr>
<td>53</td>
<td>53.00000</td>
<td>54.00000</td>
<td>55.00000</td>
<td>56.00000</td>
</tr>
<tr>
<td>57</td>
<td>57.00000</td>
<td>58.00000</td>
<td>59.00000</td>
<td>60.00000</td>
</tr>
<tr>
<td>61</td>
<td>61.00000</td>
<td>62.00000</td>
<td>63.00000</td>
<td>64.00000</td>
</tr>
<tr>
<td>65</td>
<td>65.00000</td>
<td>66.00000</td>
<td>67.00000</td>
<td>68.00000</td>
</tr>
<tr>
<td>69</td>
<td>69.00000</td>
<td>70.00000</td>
<td>71.00000</td>
<td>72.00000</td>
</tr>
<tr>
<td>73</td>
<td>73.00000</td>
<td>74.00000</td>
<td>75.00000</td>
<td>76.00000</td>
</tr>
<tr>
<td>77</td>
<td>77.00000</td>
<td>78.00000</td>
<td>79.00000</td>
<td>80.00000</td>
</tr>
<tr>
<td>81</td>
<td>81.00000</td>
<td>82.00000</td>
<td>83.00000</td>
<td>84.00000</td>
</tr>
<tr>
<td>85</td>
<td>85.00000</td>
<td>86.00000</td>
<td>87.00000</td>
<td>88.00000</td>
</tr>
<tr>
<td>89</td>
<td>89.00000</td>
<td>90.00000</td>
<td>91.00000</td>
<td>92.00000</td>
</tr>
<tr>
<td>93</td>
<td>93.00000</td>
<td>94.00000</td>
<td>95.00000</td>
<td>96.00000</td>
</tr>
<tr>
<td>97</td>
<td>97.00000</td>
<td>98.00000</td>
<td>99.00000</td>
<td>100.00000</td>
</tr>
<tr>
<td>101</td>
<td>101.00000</td>
<td>102.00000</td>
<td>103.00000</td>
<td>104.00000</td>
</tr>
<tr>
<td>105</td>
<td>105.00000</td>
<td>106.00000</td>
<td>107.00000</td>
<td>108.00000</td>
</tr>
<tr>
<td>109</td>
<td>109.00000</td>
<td>110.00000</td>
<td>111.00000</td>
<td>112.00000</td>
</tr>
<tr>
<td>113</td>
<td>113.00000</td>
<td>114.00000</td>
<td>115.00000</td>
<td>116.00000</td>
</tr>
<tr>
<td>117</td>
<td>117.00000</td>
<td>118.00000</td>
<td>119.00000</td>
<td>120.00000</td>
</tr>
<tr>
<td>121</td>
<td>121.00000</td>
<td>122.00000</td>
<td>123.00000</td>
<td>124.00000</td>
</tr>
<tr>
<td>125</td>
<td>125.00000</td>
<td>126.00000</td>
<td>127.00000</td>
<td>128.00000</td>
</tr>
</tbody>
</table>

Final statistics:

nni = 7, nli = 21
nfe = 8, npe = 2
nps = 28, ncfl = 0
3.2 A parallel example: fkinDiagon_kry_p

The program fkinDiagon_kry_p is a straightforward modification of fkinDiagon_kry to use the MPI-enabled NVIRTUAL_PARALLEL module.

After initialization of MPI, the NVIRTUAL_PARALLEL module is initialized by calling fnvinitp with the default MPI communicator mpi_comm_world and the local and global vector sizes as its first three arguments. The rank of the local process, mype, is used in both the initial guess and the system function, inasmuch as the global and local indices to the vector u are related by the equation iglobal = ilocal + mype*nlocal. In other respects, the problem setup (KINSOL initialization, SUNLINSOL_SPGMR specification) and solution steps are the same as in fkinDiagon_kry. Upon successful return from fkinsol, the solution segment local to the process with id equal to 0 is printed to unit 6. Finally, the KINSOL memory is released and the MPI environment is terminated.

For this simple example, no inter-process communication is required to evaluate the non-linear system function f or the preconditioner. As a consequence, the user-supplied routines fkfun, fpset, and fkspsol are basically identical to those in fkinDiagon_kry.

Sample output from fkinDiagon_kry_p, for \( N = 128 \), follows.

--- fkinDiagon_kry_p sample output ---

Example program fkinDiagon_kry_p:

This FKINSOL example solves a 128 eqn diagonal algebraic system. Its purpose is to demonstrate the use of the Fortran interface in a parallel environment.

FKINSOL return code is 0

The resultant values of uu (process 0) are:


Final statistics:

nmi = 7, nli = 21
nfe = 8, npe = 2
nps = 28, ncf1 = 0

13
References
