Example Programs for CVODE v2.4.0

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Contents

1 Introduction

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

The CVODE distribution contains examples of four types: serial C examples, parallel C examples, and serial and parallel FORTRAN examples. The following lists summarize all of these examples.

Supplied in the `sundials/examples/cvode/serial` directory are the following six serial examples (using the NVECTOR_SERIAL module):

- `cvdenx` solves a chemical kinetics problem consisting of three rate equations.
  This program solves the problem with the BDF method and Newton iteration, with the CVDENSE linear solver and a user-supplied Jacobian routine. It also uses the rootfinding feature of CVODE.

- `cvdenx_uw` is the same as `cvdenx` but demonstrates the user-supplied error weight function feature of CVODE.

- `cvbanx` solves the semi-discrete form of an advection-diffusion equation in 2-D.
  This program solves the problem with the BDF method and Newton iteration, with the CVBAND linear solver and a user-supplied Jacobian routine.

- `cvkryx` solves the semi-discrete form of a two-species diurnal kinetics advection-diffusion PDE system in 2-D.
  The problem is solved with the BDF/GMRES method (i.e. using the CVSPGMR linear solver) and the block-diagonal part of the Newton matrix as a left preconditioner. A copy of the block-diagonal part of the Jacobian is saved and conditionally reused within the preconditioner setup routine.

- `cvkryx_bp` solves the same problem as `cvkryx`, with the BDF/GMRES method and a banded preconditioner, generated by difference quotients, using the module CVBANDPRE.
  The problem is solved twice: with preconditioning on the left, then on the right.

- `cvkrydem_lin` solves the same problem as `cvkryx`, with the BDF method, but with three Krylov linear solvers: CVSPGMR, CVSPBCG, and CVSPTFQMR.

- `cvdirectdem` is a demonstration program for CVODE with direct linear solvers.
  Two separate problems are solved using both the Adams and BDF linear multistep methods in combination with functional and Newton iterations.
  The first problem is the Van der Pol oscillator for which the Newton iteration cases use the following types of Jacobian approximations: (1) dense, user-supplied, (2) dense, difference-quotient approximation, (3) diagonal approximation. The second problem is a linear ODE with a banded lower triangular matrix derived from a 2-D advection PDE. In this case, the Newton iteration cases use the following types of Jacobian approximation: (1) banded, user-supplied, (2) banded, difference-quotient approximation, (3) diagonal approximation.

- `cvkrydem_pre` is a demonstration program for CVODE with the Krylov linear solver.
  This program solves a stiff ODE system that arises from a 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.
The ODE system is solved using Newton iteration and the CVSPGMR linear solver (scaled preconditioned GMRES).
The preconditioner matrix used is the product of two matrices: (1) a matrix, only defined implicitly, based on a fixed number of Gauss-Seidel iterations using the diffusion terms only; and (2) a block-diagonal matrix based on the partial derivatives of the interaction terms only, using block-grouping.
Four different runs are made for this problem. The product preconditoner is applied on the left and on the right. In each case, both the modified and classical Gram-Schmidt options are tested.

Supplied in the `sundials/examples/cvode/parallel` directory are the following three parallel examples (using the NVECTOR_PARALLEL module):

- `cvnonx_p` solves the semi-discrete form of an advection-diffusion equation in 1-D.
  This program solves the problem with the option for nonstiff systems, i.e. Adams method and functional iteration.

- `cvkryx_p` is the parallel implementation of `cvkryx`.

- `cvkryx_bbd_p` solves the same problem as `cvkryx_p`, with the BDF/GMRES method and a block-diagonal matrix with banded blocks as a preconditioner, generated by difference quotients, using the module CVBBDPRE.

With the FCVODE module, in the directories `sundials/examples/cvode/fcmix_serial` and `sundials/examples/cvode/fcmix_parallel`, are the following examples for the FORTRAN-C interface:

- `fcvdenx` is a serial chemical kinetics example (`BDF`/DENSE) with rootfinding.

- `fcvbanx` is a serial advection-diffusion example (`BDF`/BAND).

- `fcvkryx` is a serial kinetics-transport example (`BDF`/SPGMR).

- `fcvkryx_bp` is the `fcvkryx` example with FCVBP.

- `fcvnonx_p` is a parallel diagonal ODE example (`ADAMS`/`FUNCTIONAL`).

- `fcvkryx_p` is a parallel diagonal ODE example (`BDF`/SPGMR).

- `fcvkryx_bbd_p` is a parallel diagonal ODE example (`BDF`/SPGMR with FCVBBD).

In the following sections, we give detailed descriptions of some (but not all) of these examples. The Appendices contain complete listings of those examples described below. 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 steps or Newton iterations, may differ from one machine environment to another by as much as 10% to 20%.

The final section of this report describes a set of tests done with the parallel version of CVODE, using a problem based on the `cvkryx`/`cvkryx_p` example.

In the descriptions below, we make frequent references to the CVODE User Document [1]. All citations to specific sections (e.g. §5.2) are references to parts of that User Document, unless explicitly stated otherwise.

Note. The examples in the CVODE distribution are written in such a way as to compile and run for any combination of configuration options during the installation of SUNDIALS (see §2). 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 variable `SUNDIALS_EXTENDED_PRECISION` to test if the solver libraries were built in extended precision and use the appropriate conversion specifiers in `printf` functions. Similarly, the FORTRAN examples in FCVODE are automatically pre-processed to generate source code that corresponds to the manner in which the CVODE libraries were built (see §4 in this document for more details).

2 Serial example problems

2.1 A dense example: cvdenx

As an initial illustration of the use of the CVODE package for the integration of IVP ODEs, we give a sample program called `cvdenx.c`. It uses the CVODE dense linear solver module CVDENSE and the NVECTOR_SERIAL module (which provides a serial implementation of NVECTOR) in the solution of a 3-species chemical kinetics problem.

The problem consists of the following three rate equations:

$$\begin{aligned} \dot{y}_1 &= -0.04 \cdot y_1 + 10^4 \cdot y_2 \cdot y_3 \\ \dot{y}_2 &= 0.04 \cdot y_1 - 10^4 \cdot y_2 \cdot y_3 - 3 \cdot 10^7 \cdot y_2^2 \\ \dot{y}_3 &= 3 \cdot 10^7 \cdot y_2^2 \end{aligned} \tag{1}$$

on the interval $t \in [0,\ 4 \cdot 10^{10}]$, with initial conditions $y_1(0) = 1.0$, $y_2(0) = y_3(0) = 0.0$. While integrating the system, we also use the rootfinding feature to find the points at which $y_1 = 10^{-4}$ or at which $y_3 = 0.01$.

For the source, listed in Appendix A, we give a rather detailed explanation of the parts of the program and their interaction with CVODE.

Following the initial comment block, this program has a number of `#include` lines, which allow access to useful items in CVODE header files. The `sundials_types.h` file provides the definition of the type `realtype` (see §5.2 for details). For now, it suffices to read `realtype` as `double`. The `cvode.h` file provides prototypes for the CVODE 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 `CVode`. The `cvode_dense.h` file provides the prototype for the `CVDense` function. 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 `sundials_dense.h` file provides the definition of the dense matrix type `DenseMat` and a macro for accessing matrix elements. We have explicitly included `sundials_dense.h`, but this is not necessary because it is included by `cvode_dense.h`.

This program includes two user-defined accessor macros, `Ith` and `IJth` that are useful in writing the problem functions in a form closely matching the mathematical description of the ODE 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 `IJth` macro is used to access elements of a dense matrix of type `DenseMat`. It is defined using the DENSE accessor macro `DENSE_ELEM` which numbers matrix rows and columns starting with 0. The macro `NV_Ith_S` is fully described in §7.1. The macro `DENSE_ELEM` is fully described in §5.6.4.

Next, the program includes some problem-specific constants, which are isolated to this early location to make it easy to change them as needed. The program prologue ends with prototypes of four private helper functions and the three user-supplied functions that are called by CVODE.

The `main` program begins with some dimensions and type declarations, including use of the type `N_Vector`. The next several lines allocate memory for the `y` and `abstol` vectors using `N_VNew_Serial` with a length argument of `NEQ` (= 3). The lines following that load

the initial values of the dependendent variable vector into `y` and the absolute tolerances into `abstol` using the `Ith` macro.

The calls to `N_VNew_Serial`, and also later calls to `CVode***` functions, make use of a private function, `check_flag`, which examines the return value and prints a message if there was a failure. The `check_flag` function was written to be used for any serial SUNDIALS application.

The call to `CVodeCreate` creates the CVODE solver memory block, specifying the `CV_BDF` integration method with `CV_NEWTON` iteration. Its return value is a pointer to that memory block for this problem. In the case of failure, the return value is `NULL`. This pointer must be passed in the remaining calls to CVODE functions.

The call to `CVodeMalloc` allocates the solver memory block. Its arguments include the name of the C function `f` defining the right-hand side function $f(t, y)$, and the initial values of t and y. The argument `CV_ SV` specifies a vector of absolute tolerances, and this is followed by the value of the relative tolerance `reltol` and the absolute tolerance vector `abstol`. See §5.5.1 for full details of this call.

The call to `CVodeRootInit` specifies that a rootfinding problem is to be solved along with the integration of the ODE system, that the root functions are specified in the function `g`, and that there are two such functions. Specifically, they are set to $y_1 - 0.0001$ and $y_3 - 0.01$, respectively. See §5.7.1 for a detailed description of this call.

The calls to `CVDense` (see §5.5.3) and `CVDenseSetJacFn` (see §5.5.5) specify the CVDENSE linear solver with an analytic Jacobian supplied by the user-supplied function `Jac`.

The actual solution of the ODE initial value problem is accomplished in the loop over values of the output time `tout`. In each pass of the loop, the program calls `CVode` in the `CV_NORMAL` mode, meaning that the integrator is to take steps until it overshoots `tout` and then interpolate to $t =$`tout`, putting the computed value of y(`tout`) into `y`, with `t` = `tout`. The return value in this case is `CV_SUCCESS`. However, if `CVode` finds a root before reaching the next value of `tout`, it returns `CV_ROOT_RETURN` and stores the root location in `t` and the solution there in `y`. In either case, the program prints `t` and `y`. In the case of a root, it calls `CVodeGetRootInfo` to get a length-2 array `rootsfound` of bits showing which root function was found to have a root. If `CVode` returned any negative value (indicating a failure), the program breaks out of the loop. In the case of a `CV_SUCCESS` return, the value of `tout` is advanced (multiplied by 10) and a counter (`iout`) is advanced, so that the loop can be ended when that counter reaches the preset number of output times, `NOUT` = 12. See §5.5.4 for full details of the call to `CVode`.

Finally, the main program calls `PrintFinalStats` to get and print all of the relevant statistical quantities. It then calls `NV_Destroy` to free the vectors `y` and `abstol`, and `CVodeFree` to free the CVODE memory block.

The function `PrintFinalStats` used here is actually suitable for general use in applications of CVODE to any problem with a dense Jacobian. It calls various `CVodeGet***` and `CVDenseGet***` functions to obtain the relevant counters, and then prints them. Specifically, these are: the cumulative number of steps (`nst`), the number of `f` evaluations (`nfe`) (excluding those for difference-quotient Jacobian evaluations), the number of matrix factorizations (`nsetups`), the number of `f` evaluations for Jacobian evaluations (`nfeD` = 0 here), the number of Jacobian evaluations (`njeD`), the number of nonlinear (Newton) iterations (`nni`), the number of nonlinear convergence failures (`ncfn`), the number of local error test failures (`netf`), and the number of `g` (root function) evaluations (`nge`). These optional outputs are described in §5.5.7.

The function `f` is a straightforward expression of the ODEs. It uses the user-defined

macro `Ith` to extract the components of `y` and to load the components of `ydot`. See §5.6.1 for a detailed specification of `f`.

Similarly, the function `g` defines the two functions, g_0 and g_1, whose roots are to be found. See §5.7.2 for a detailed description of the `g` function.

The function `Jac` sets the nonzero elements of the Jacobian as a dense matrix. (Zero elements need not be set because `J` is preset to zero.) It uses the user-defined macro `IJth` to reference the elements of a dense matrix of type `DenseMat`. Here the problem size is small, so we need not worry about the inefficiency of using `NV_Ith_S` and `DENSE_ELEM` to access `N_Vector` and `DenseMat` elements. Note that in this example, `Jac` only accesses the `y` and `J` arguments. See §5.6.4 for a detailed description of the dense `Jac` function.

The output generated by `cvdenx` is shown below. It shows the output values at the 12 preset values of `tout`. It also shows the two root locations found, first at a root of g_1, and then at a root of g_0.

cvdenx sample output

```
3-species kinetics problem

At t = 2.6391e-01      y =  9.899653e-01    3.470564e-05    1.000000e-02
    rootsfound[] =   0   1
At t = 4.0000e-01      y =  9.851641e-01    3.386242e-05    1.480205e-02
At t = 4.0000e+00      y =  9.055097e-01    2.240338e-05    9.446793e-02
At t = 4.0000e+01      y =  7.157952e-01    9.183486e-06    2.841956e-01
At t = 4.0000e+02      y =  4.505420e-01    3.222963e-06    5.494548e-01
At t = 4.0000e+03      y =  1.831878e-01    8.941319e-07    8.168113e-01
At t = 4.0000e+04      y =  3.897868e-02    1.621567e-07    9.610212e-01
At t = 4.0000e+05      y =  4.940023e-03    1.985716e-08    9.950600e-01
At t = 4.0000e+06      y =  5.165107e-04    2.067097e-09    9.994835e-01
At t = 2.0807e+07      y =  1.000000e-04    4.000395e-10    9.999000e-01
    rootsfound[] =   1   0
At t = 4.0000e+07      y =  5.201457e-05    2.080690e-10    9.999480e-01
At t = 4.0000e+08      y =  5.207182e-06    2.082883e-11    9.999948e-01
At t = 4.0000e+09      y =  5.105811e-07    2.042325e-12    9.999995e-01
At t = 4.0000e+10      y =  4.511312e-08    1.804525e-13    1.000000e-00

Final Statistics:
nst = 515     nfe  = 755     nsetups = 110     nfeLS = 0      nje = 12
nni = 751     ncfn = 0       netf = 26      nge = 543
```

2.2 A banded example: cvbanx

The example program `cvbanx.c` solves the semi-discretized form of the 2-D advection-diffusion equation

$$\partial v/\partial t = \partial^2 v/\partial x^2 + .5\partial v/\partial x + \partial^2 v/\partial y^2 \tag{2}$$

on a rectangle, with zero Dirichlet boundary conditions. The PDE is discretized with standard central finite differences on a (`MX`+2) × (`MY`+2) mesh, giving an ODE system of size `MX*MY`. The discrete value v_{ij} approximates v at $x = i\Delta x$, $y = j\Delta y$. The ODEs are

$$\frac{dv_{ij}}{dt} = f_{ij} = \frac{v_{i-1,j} - 2v_{ij} + v_{i+1,j}}{(\Delta x)^2} + .5\frac{v_{i+1,j} - v_{i-1,j}}{2\Delta x} + \frac{v_{i,j-1} - 2v_{ij} + v_{i,j+1}}{(\Delta y)^2}, \tag{3}$$

where $1 \le i \le$MX and $1 \le j \le$MY. The boundary conditions are imposed by taking $v_{ij} = 0$ above if $i = 0$ or MX+1, or if $j = 0$ or MY+1. If we set $u_{(j-1)+(i-1)*\texttt{MY}} = v_{ij}$, so that the ODE system is $\dot{u} = f(u)$, then the system Jacobian $J = \partial f/\partial u$ is a band matrix with upper and lower half-bandwidths both equal to MY. In the example, we take MX = 10 and MY = 5. The source is listed in Appendix B.

The cvbanx.c program includes files cvode_band.h and sundials_band.h in order to use the CVBAND linear solver. The cvode_band.h file contains the prototype for the CVBand routine. The sundials_band.h file contains the definition for band matrix type BandMat and the BAND_COL and BAND_COL_ELEM macros for accessing matrix elements (see §9.2). We have explicitly included sundials_band.h, but this is not necessary because it is included by cvode_band.h. The file nvector_serial.h is included for the definition of the serial N_Vector type.

The include lines at the top of the file are followed by definitions of problem constants which include the x and y mesh dimensions, MX and MY, the number of equations NEQ, the scalar absolute tolerance ATOL, the initial time T0, and the initial output time T1.

Spatial discretization of the PDE naturally produces an ODE system in which equations are numbered by mesh coordinates (i, j). The user-defined macro IJth isolates the translation for the mathematical two-dimensional index to the one-dimensional N_Vector index and allows the user to write clean, readable code to access components of the dependent variable. The NV_DATA_S macro returns the component array for a given N_Vector, and this array is passed to IJth in order to do the actual N_Vector access.

The type UserData is a pointer to a structure containing problem data used in the f and Jac functions. This structure is allocated and initialized at the beginning of main. The pointer to it, called data, is passed to both CVodeSetFData and CVBandSetJacFn, and as a result it will be passed back to the f and Jac functions each time they are called. (If appropriate, two different data structures could be defined and passed to f and Jac.) The use of the data pointer eliminates the need for global program data.

The main program is straightforward. The CVodeCreate call specifies the CV_BDF method with a CV_NEWTON iteration. In the CVodeMalloc call, the parameter SS indicates scalar relative and absolute tolerances, and pointers &reltol and &abstol to these values are passed. The call to CVBand (see §5.5.3) specifies the CVBAND linear solver, and specifies that both half-bandwidths of the Jacobian are equal to MY. The call to CVBandSetJacFn (see §5.5.5) specifies that a user-supplied Jacobian function Jac is to be used and that a pointer to data shold be passed to Jac every time it is called. The actual solution of the problem is performed by the call to CVode within the loop over the output times tout. The max-norm of the solution vector (from a call to N_VMaxNorm) and the cumulative number of time steps (from a call to CVodeGetNumSteps) are printed at each output time. Finally, the calls to PrintFinalStats, N_VDestroy, and CVodeFree print statistics and free problem memory.

Following the main program in the cvbanx.c file are definitions of five functions: f, Jac, SetIC, PrintFinalStats, and check_flag. The last three functions are called only from within the cvbanx.c file. The SetIC function sets the initial dependent variable vector; PrintFinalStats gets and prints statistics at the end of the run; and check_flag aids in checking return values. The statistics printed include counters such as the total number of steps (nst), f evaluations (excluding those for Jaobian evaluations) (nfe), LU decompositions (nsetups), f evaluations for difference-quotient Jacobians (nfeB = 0 here), Jacobian evaluations (njeB), and nonlinear iterations (nni). These optional outputs are described in §5.5.7. Note that PrintFinalStats is suitable for general use in applications of CVODE to any problem with a banded Jacobian.

The `f` function implements the central difference approximation (3) with u identically zero on the boundary. The constant coefficients $(\Delta x)^{-2}$, $.5(2\Delta x)^{-1}$, and $(\Delta y)^{-2}$ are computed only once at the beginning of `main`, and stored in the locations `data->hdcoef`, `data->hacoef`, and `data->vdcoef`, respectively. When `f` receives the `data` pointer (renamed `f_data` here), it pulls out these values from storage in the local variables `hordc`, `horac`, and `verdc`. It then uses these to construct the diffusion and advection terms, which are combined to form `udot`. Note the extra lines setting out-of-bounds values of u to zero.

The `Jac` function is an expression of the derivatives

$$\begin{aligned} \partial f_{ij}/\partial v_{ij} &= -2[(\Delta x)^{-2} + (\Delta y)^{-2}] \\ \partial f_{ij}/\partial v_{i\pm1,j} &= (\Delta x)^{-2} \pm .5(2\Delta x)^{-1}, \quad \partial f_{ij}/\partial v_{i,j\pm1} = (\Delta y)^{-2} \ . \end{aligned}$$

This function loads the Jacobian by columns, and like `f` it makes use of the preset coefficients in `data`. It loops over the mesh points (`i`,`j`). For each such mesh point, the one-dimensional index `k = j-1 + (i-1)*MY` is computed and the `k`th column of the Jacobian matrix J is set. The row index k' of each component $f_{i',j'}$ that depends on $v_{i,j}$ must be identified in order to load the corresponding element. The elements are loaded with the `BAND_COL_ELEM` macro. Note that the formula for the global index k implies that decreasing (increasing) `i` by 1 corresponds to decreasing (increasing) `k` by `MY`, while decreasing (increasing) `j` by 1 corresponds of decreasing (increasing) `k` by 1. These statements are reflected in the arguments to `BAND_COL_ELEM`. The first argument passed to the `BAND_COL_ELEM` macro is a pointer to the diagonal element in the column to be accessed. This pointer is obtained via a call to the `BAND_COL` macro and is stored in `kthCol` in the `Jac` function. When setting the components of J we must be careful not to index out of bounds. The guards `(i != 1)` etc. in front of the calls to `BAND_COL_ELEM` prevent illegal indexing. See §5.6.5 for a detailed description of the banded `Jac` function.

The output generated by `cvbanx` is shown below.

cvbanx sample output

```
2-D Advection-Diffusion Equation
Mesh dimensions = 10 X 5
Total system size = 50
Tolerance parameters: reltol = 0   abstol = 1e-05

At t = 0      max.norm(u) =  8.954716e+01
At t = 0.10   max.norm(u) =  4.132889e+00   nst =   85
At t = 0.20   max.norm(u) =  1.039294e+00   nst =  103
At t = 0.30   max.norm(u) =  2.979829e-01   nst =  113
At t = 0.40   max.norm(u) =  8.765774e-02   nst =  120
At t = 0.50   max.norm(u) =  2.625637e-02   nst =  126
At t = 0.60   max.norm(u) =  7.830425e-03   nst =  130
At t = 0.70   max.norm(u) =  2.329387e-03   nst =  134
At t = 0.80   max.norm(u) =  6.953434e-04   nst =  137
At t = 0.90   max.norm(u) =  2.115983e-04   nst =  140
At t = 1.00   max.norm(u) =  6.556853e-05   nst =  142

Final Statistics:
nst = 142    nfe  = 174    nsetups = 23    nfeLS = 0    nje = 3
nni = 170    ncfn = 0      netf = 3
```

2.3 A Krylov example: cvkryx

We give here an example that illustrates the use of CVODE with the Krylov method SPGMR, in the CVSPGMR module, as the linear system solver. The source file, `cvkryx.c`, is listed in Appendix C.

This program solves the semi-discretized form of a pair of kinetics-advection-diffusion partial differential equations, which represent a simplified model for the transport, production, and loss of ozone and the oxygen singlet in the upper atmosphere. The problem includes nonlinear diurnal kinetics, horizontal advection and diffusion, and nonuniform vertical diffusion. The PDEs can be written as

$$\frac{\partial c^i}{\partial t} = K_h \frac{\partial^2 c^i}{\partial x^2} + V\frac{\partial c^i}{\partial x} + \frac{\partial}{\partial y}K_v(y)\frac{\partial c^i}{\partial y} + R^i(c^1, c^2, t) \quad (i = 1, 2) \ , \tag{4}$$

where the superscripts i are used to distinguish the two chemical species, and where the reaction terms are given by

$$\begin{aligned} R^1(c^1, c^2, t) &= -q_1 c^1 c^3 - q_2 c^1 c^2 + 2q_3(t)c^3 + q_4(t)c^2 \ , \\ R^2(c^1, c^2, t) &= q_1 c^1 c^3 - q_2 c^1 c^2 - q_4(t)c^2 \ . \end{aligned} \tag{5}$$

The spatial domain is $0 \le x \le 20$, $30 \le y \le 50$ (in km). The various constants and parameters are: $K_h = 4.0 \cdot 10^{-6}$, $V = 10^{-3}$, $K_v = 10^{-8}\exp(y/5)$, $q_1 = 1.63 \cdot 10^{-16}$, $q_2 = 4.66 \cdot 10^{-16}$, $c^3 = 3.7 \cdot 10^{16}$, and the diurnal rate constants are defined as:

$$q_i(t) = \left\{ \begin{array}{ll} \exp[-a_i/\sin\omega t], & \text{for } \sin\omega t > 0 \\ 0, & \text{for } \sin\omega t \le 0 \end{array} \right\} \quad (i = 3, 4) \ ,$$

where $\omega = \pi/43200$, $a_3 = 22.62$, $a_4 = 7.601$. The time interval of integration is $[0, 86400]$, representing 24 hours measured in seconds.

Homogeneous Neumann boundary conditions are imposed on each boundary, and the initial conditions are

$$\begin{aligned} c^1(x, y, 0) = 10^6\alpha(x)\beta(y) \ , \quad c^2(x, y, 0) = 10^{12}\alpha(x)\beta(y) \ , \\ \alpha(x) = 1 - (0.1x - 1)^2 + (0.1x - 1)^4/2 \ , \\ \beta(y) = 1 - (0.1y - 4)^2 + (0.1y - 4)^4/2 \ . \end{aligned} \tag{6}$$

For this example, the equations (4) are discretized spatially with standard central finite differences on a 10×10 mesh, giving an ODE system of size 200.

Among the initial `#include` lines in this case are lines to include `cvode_spgmr.h` and `sundials_math.h`. The first contains constants and function prototypes associated with the SPGMR method, including the values of the `pretype` argument to `CVSpgmr`. The inclusion of `sundials_math.h` is done to access the `SQR` macro for the square of a `realtype` number.

The `main` program calls `CVodeCreate` specifying the `CV_BDF` method and `CV_NEWTON` iteration, and then calls `CVodeMalloc` with scalar tolerances. It calls `CVSpgmr` (see §5.5.3) to specify the CVSPGMR linear solver with left preconditioning, and the default value (indicated by a zero argument) for `maxl`. The Gram-Schmidt orthogonalization is set to `MODIFIED_GS` through the function `CVSpilsSetGSType`. Next, user-supplied preconditioner setup and solve functions, `Precond` and `PSolve`, as well as the `data` pointer passed to `Precond` and `PSolve` whenever these are called, See §5.5.5 for details on the `CVSpilsSetPreconditioner` function.

Then for a sequence of `tout` values, `CVode` is called in the `CV_NORMAL` mode, sampled output is printed, and the return value is tested for error conditions. After that, `PrintFinalStats`

is called to get and print final statistics, and memory is freed by calls to N_VDestroy, FreeUserData, and CVodeFree. The printed statistics include various counters, such as the total numbers of steps (nst), of f evaluations (excluding those for Jv product evaluations) (nfe), of f evaluations for Jv evaluations (nfel), of nonlinear iterations (nni), of linear (Krylov) iterations (nli), of preconditioner setups (nsetups), of preconditioner evaluations (npe), and of preconditioner solves (nps), among others. Also printed are the lengths of the problem-dependent real and integer workspaces used by the main integrator CVode, denoted lenrw and leniw, and those used by CVSPGMR, denoted llrw and lliw. All of these optional outputs are described in §5.5.7. The PrintFinalStats function is suitable for general use in applications of CVODE to any problem with the SPGMR linear solver.

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 IJKth 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 200, 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 an N_Vector which we pass to the IJKth macro to do an N_Vector access.

The preconditioner used here is the block-diagonal part of the true Newton matrix. It is generated and factored in the Precond routine (see §5.6.8) and backsolved in the PSolve routine (see §5.6.7). Its diagonal blocks are 2×2 matrices that include the interaction Jacobian elements and the diagonal contribution of the diffusion Jacobian elements. The block-diagonal part of the Jacobian itself, J_{bd}, is saved in separate storage each time it is generated, on calls to Precond with jok == FALSE. On calls with jok == TRUE, signifying that saved Jacobian data can be reused, the preconditioner $P = I - \gamma J_{bd}$ is formed from the saved matrix J_{bd} and factored. (A call to Precond with jok == TRUE can only occur after a prior call with jok == FALSE.) The Precond routine must also set the value of jcur, i.e. *jcurPtr, to TRUE when J_{bd} is re-evaluated, and FALSE otherwise, to inform CVSPGMR of the status of Jacobian data.

We need to take a brief detour to explain one last important aspect of the cvkryx.c program. The generic DENSE solver contains two sets of functions: one for "large" matrices and one for "small" matrices. The large dense functions work with the type DenseMat, while the small dense functions work with realtype ** as the underlying dense matrix types. The CVDENSE linear solver uses the type DenseMat for the $N \times N$ dense Jacobian and Newton matrices, and calls the large matrix functions. But to avoid the extra layer of function calls, cvkryx.c uses the small dense functions for all operations on the 2×2 preconditioner blocks. Thus it includes sundials_smalldense.h, and calls the small dense matrix functions denalloc, dencopy, denscale, denaddI, denfree, denfreepiv, denGETRF, and denGETRS. The macro IJth defined near the top of the file is used to access individual elements in each preconditioner block, numbered from 1. The small dense functions are available for CVODE user programs generally, and are documented in §9.1.

In addition to the functions called by CVODE, cvkryx.c includes definitions of several private functions. These are: AllocUserData to allocate space for J_{bd}, P, 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 y; PrintOutput to retreive and print selected solution values and statistics; PrintFinalStats to print statistics; and check_flag to check return values for error conditions.

The output generated by cvkryx.c is shown below. Note that the number of precondi-

tioner evaluations, `npe`, is much smaller than the number of preconditioner setups, `nsetups`, as a result of the Jacobian re-use scheme.

cvkryx sample output

```
2-species diurnal advection-diffusion problem

t = 7.20e+03   no. steps = 219   order = 5   stepsize = 1.59e+02
c1 (bot.left/middle/top rt.) =    1.047e+04     2.964e+04     1.119e+04
c2 (bot.left/middle/top rt.) =    2.527e+11     7.154e+11     2.700e+11

t = 1.44e+04   no. steps = 251   order = 5   stepsize = 3.77e+02
c1 (bot.left/middle/top rt.) =    6.659e+06     5.316e+06     7.301e+06
c2 (bot.left/middle/top rt.) =    2.582e+11     2.057e+11     2.833e+11

t = 2.16e+04   no. steps = 277   order = 5   stepsize = 2.75e+02
c1 (bot.left/middle/top rt.) =    2.665e+07     1.036e+07     2.931e+07
c2 (bot.left/middle/top rt.) =    2.993e+11     1.028e+11     3.313e+11

t = 2.88e+04   no. steps = 301   order = 5   stepsize = 3.87e+02
c1 (bot.left/middle/top rt.) =    8.702e+06     1.292e+07     9.650e+06
c2 (bot.left/middle/top rt.) =    3.380e+11     5.029e+11     3.751e+11

t = 3.60e+04   no. steps = 343   order = 3   stepsize = 2.34e+01
c1 (bot.left/middle/top rt.) =    1.404e+04     2.029e+04     1.561e+04
c2 (bot.left/middle/top rt.) =    3.387e+11     4.894e+11     3.765e+11

t = 4.32e+04   no. steps = 421   order = 4   stepsize = 5.26e+02
c1 (bot.left/middle/top rt.) =   -4.385e-06    -1.528e-06    -4.905e-06
c2 (bot.left/middle/top rt.) =    3.382e+11     1.355e+11     3.804e+11

t = 5.04e+04   no. steps = 445   order = 3   stepsize = 1.98e+02
c1 (bot.left/middle/top rt.) =    4.461e-07     1.869e-07     4.842e-07
c2 (bot.left/middle/top rt.) =    3.358e+11     4.930e+11     3.864e+11

t = 5.76e+04   no. steps = 462   order = 5   stepsize = 2.35e+02
c1 (bot.left/middle/top rt.) =    3.204e-09     1.203e-09     3.555e-09
c2 (bot.left/middle/top rt.) =    3.320e+11     9.650e+11     3.909e+11

t = 6.48e+04   no. steps = 474   order = 5   stepsize = 6.02e+02
c1 (bot.left/middle/top rt.) =   -1.066e-09    -3.409e-10    -1.206e-09
c2 (bot.left/middle/top rt.) =    3.313e+11     8.922e+11     3.963e+11

t = 7.20e+04   no. steps = 486   order = 5   stepsize = 6.02e+02
c1 (bot.left/middle/top rt.) =    2.614e-09     9.722e-10     2.904e-09
c2 (bot.left/middle/top rt.) =    3.330e+11     6.186e+11     4.039e+11

t = 7.92e+04   no. steps = 498   order = 5   stepsize = 6.02e+02
c1 (bot.left/middle/top rt.) =    4.649e-11     1.729e-11     5.161e-11
c2 (bot.left/middle/top rt.) =    3.334e+11     6.669e+11     4.120e+11

t = 8.64e+04   no. steps = 510   order = 5   stepsize = 6.02e+02
c1 (bot.left/middle/top rt.) =   -8.856e-14    -3.348e-14    -9.785e-14
c2 (bot.left/middle/top rt.) =    3.352e+11     9.107e+11     4.163e+11


Final Statistics..
```

```
lenrw   =  2089     leniw   =    50
lenrwLS =  2046     leniwLS =    10
nst     =   510
nfe     =   675     nfeLS   =   641
nni     =   671     nli     =   641
nsetups =    94     netf    =    36
npe     =     9     nps     =  1243
ncfn    =     0     ncfl    =     0
```

3 Parallel example problems

3.1 A nonstiff example: cvnonx_p

This problem begins with a simple diffusion-advection equation for $u = u(t, x)$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 0.5\frac{\partial u}{\partial x} \tag{7}$$

for $0 \le t \le 5$, $0 \le x \le 2$, and subject to homogeneous Dirichlet boundary conditions and initial values given by

$$\begin{aligned} u(t,0) &= 0\ , \quad u(t,2) = 0\ , \\ u(0,x) &= x(2-x)e^{2x}\ . \end{aligned} \tag{8}$$

A system of `MX` ODEs is obtained by discretizing the x-axis with `MX`+2 grid points and replacing the first and second order spatial derivatives with their central difference approximations. Since the value of u is constant at the two endpoints, the semi-discrete equations for those points can be eliminated. With u_i as the approximation to $u(t, x_i)$, $x_i = i(\Delta x)$, and $\Delta x = 2/(\texttt{MX}+1)$, the resulting system of ODEs, $\dot{u} = f(t, u)$, can now be written:

$$\dot{u}_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + 0.5\frac{u_{i+1} - u_{i-1}}{2(\Delta x)}\ . \tag{9}$$

This equation holds for $i = 1, 2, \ldots,$ `MX`, with the understanding that $u_0 = u_{\texttt{MX}+1} = 0$.

In the parallel processing environment, we may think of the several processors as being laid out on a straight line with each processor to compute its contiguous subset of the solution vector. Consequently the computation of the right hand side of Eq. (9) requires that each interior processor must pass the first component of its block of the solution vector to its left-hand neighbor, acquire the last component of that neighbor's block, pass the last component of its block of the solution vector to its right-hand neighbor, and acquire the first component of that neighbor's block. If the processor is the first (0th) or last processor, then communication to the left or right (respectively) is not required.

The source file for this problem, `cvnonx_p.c`, is listed in Appendix D. It uses the Adams (non-stiff) integration formula and functional iteration. This problem is unrealistically simple, but serves to illustrate use of the parallel version of CVODE.

The `cvnonx_p.c` file begins with `#include` lines, including lines for `nvector_parallel` to access the parallel `N_Vector` type and related macros, and for `mpi.h` to access MPI types and constants. Following that are definitions of problem constants and a data block for communication with the `f` routine. That block includes the number of PEs, the index of the local PE, and the MPI communicator.

The `main` program begins with MPI calls to initialize MPI and to set multi-processor environment parameters `npes` (number of PEs) and `my_pe` (local PE index). The local vector length is set according to `npes` and the problem size `NEQ` (which may or may not be multiple of `npes`). The value `my_base` is the base value for computing global indices (from 1 to `NEQ`) for the local vectors. The solution vector `u` is created with a call to `N_VNew_Parallel` and loaded with a call to `SetIC`. The calls to `CVodeCreate` and `CVodeMalloc` specify a CVODE solution with the nonstiff method and scalar tolerances. The call to `CVodeSetFdata` insures that the pointer `data` is passed to the `f` routine whenever it is called. A heading is printed (if on processor 0). In a loop over `tout` values, `CVode` is called, and the return value checked for

errors. The max-norm of the solution and the total number of time steps so far are printed at each output point. Finally, some statistical counters are printed, memory is freed, and MPI is finalized.

The `SetIC` routine uses the last two arguments passed to it to compute the set of global indices (`my_base`+1 to `my_base+my_length`) corresponding to the local part of the solution vector `u`, and then to load the corresponding initial values. The `PrintFinalStats` routine uses `CVodeGet***` calls to get various counters, and then prints these. The counters are: `nst` (number of steps), `nfe` (number of `f` evaluations), `nni` (number of nonlinear iterations), `netf` (number of error test failures), and `ncfn` (number of nonlinear convergence failures). This routine is suitable for general use with CVODE applications to nonstiff problems.

The `f` function is an implementation of Eq. (9), but preceded by communication operations appropriate for the parallel setting. It copies the local vector `u` into a larger array `z`, shifted by 1 to allow for the storage of immediate neighbor components. The first and last components of `u` are sent to neighboring processors with `MPI_Send` calls, and the immediate neighbor solution values are received from the neighbor processors with `MPI_Recv` calls, except that zero is loaded into `z[0]` or `z[my_length+1]` instead if at the actual boundary. Then the central difference expressions are easily formed from the `z` array, and loaded into the data array of the `udot` vector.

The `cvnonx_p.c` file includes a routine `check_flag` that checks the return values from calls in `main`. This routine was written to be used by any parallel SUNDIALS application.

The output below is for `cvnonx_p` with `MX` = 10 and four processors. Varying the number of processors will alter the output, only because of roundoff-level differences in various vector operations. The fairly high value of `ncfn` indicates that this problem is on the borderline of being stiff.

cvnonx_p sample output

```
 1-D advection-diffusion equation, mesh size = 10

 Number of PEs =   4

At t = 0.00   max.norm(u) =  1.569909e+01  nst =   0
At t = 0.50   max.norm(u) =  3.052881e+00  nst = 113
At t = 1.00   max.norm(u) =  8.753188e-01  nst = 191
At t = 1.50   max.norm(u) =  2.494926e-01  nst = 265
At t = 2.00   max.norm(u) =  7.109707e-02  nst = 339
At t = 2.50   max.norm(u) =  2.026223e-02  nst = 418
At t = 3.00   max.norm(u) =  5.777332e-03  nst = 486
At t = 3.50   max.norm(u) =  1.650483e-03  nst = 563
At t = 4.00   max.norm(u) =  4.754357e-04  nst = 646
At t = 4.50   max.norm(u) =  1.374222e-04  nst = 715
At t = 5.00   max.norm(u) =  3.937469e-05  nst = 795

Final Statistics:

nst = 795     nfe  = 1465    nni = 1461    ncfn = 146     netf = 5
```

3.2 A user preconditioner example: cvkryx_p

As an example of using CVODE with the Krylov linear solver CVSPGMR and the parallel MPI NVECTOR_PARALLEL module, we describe a test problem based on the system PDEs given above for the `cvkryx` example. As before, we discretize the PDE system with central differencing, to obtain an ODE system $\dot{u} = f(t, u)$ representing (4). But in this case, the discrete solution vector is distributed over many processors. Specifically, we may think of the processors as being laid out in a rectangle, and each processor being assigned a subgrid of size `MXSUB`×`MYSUB` of the $x - y$ grid. If there are `NPEX` processors in the x direction and `NPEY` processors in the y direction, then the overall grid size is `MX`×`MY` with `MX`=`NPEX`×`MXSUB` and `MY`=`NPEY`×`MYSUB`, and the size of the ODE system is 2·`MX`·`MY`.

To compute f in this setting, the processors pass and receive information as follows. The solution components for the bottom row of grid points in the current processor are passed to the processor below it and the solution for the top row of grid points is received from the processor below the current processor. The solution for the top row of grid points for the current processor is sent to the processor above the current processor, while the solution for the bottom row of grid points is received from that processor by the current processor. Similarly the solution for the first column of grid points is sent from the current processor to the processor to its left and the last column of grid points is received from that processor by the current processor. The communication for the solution at the right edge of the processor is similar. If this is the last processor in a particular direction, then message passing and receiving are bypassed for that direction.

The code listing for this example is given in Appendix E. The purpose of this code is to provide a more realistic example than that in `cvnonx_p`, and to provide a template for a stiff ODE system arising from a PDE system. The solution method is BDF with Newton iteration and SPGMR. The left preconditioner is the block-diagonal part of the Newton matrix, with 2×2 blocks, and the corresponding diagonal blocks of the Jacobian are saved each time the preconditioner is generated, for re-use later under certain conditions.

The organization of the `cvkryx_p` program deserves some comments. The right-hand side routine `f` calls two other routines: `ucomm`, which carries out inter-processor communication; and `fcalc`, which operates on local data only and contains the actual calculation of $f(t, u)$. The `ucomm` function in turn calls three routines which do, respectively, non-blocking receive operations, blocking send operations, and receive-waiting. All three use MPI, and transmit data from the local `u` vector into a local working array `uext`, an extended copy of `u`. The `fcalc` function copies `u` into `uext`, so that the calculation of $f(t, u)$ can be done conveniently by operations on `uext` only. Most other features of `cvkryx_p.c` are the same as in `cvkryx.c`.

The following is a sample output from `cvkryx_p`, for four processors (in a 2×2 array) with a 5×5 subgrid on each. The output will vary slightly if the number of processors is changed.

cvkryx_p sample output

```
2-species diurnal advection-diffusion problem

t = 7.20e+03   no. steps = 219   order = 5   stepsize = 1.59e+02
At bottom left:  c1, c2 =    1.047e+04    2.527e+11
At top right:    c1, c2 =    1.119e+04    2.700e+11

t = 1.44e+04   no. steps = 251   order = 5   stepsize = 3.77e+02
At bottom left:  c1, c2 =    6.659e+06    2.582e+11
```

```
At top right:    c1, c2 =    7.301e+06    2.833e+11

t = 2.16e+04   no. steps = 277   order = 5   stepsize = 2.75e+02
At bottom left:  c1, c2 =    2.665e+07    2.993e+11
At top right:    c1, c2 =    2.931e+07    3.313e+11

t = 2.88e+04   no. steps = 307   order = 4   stepsize = 1.98e+02
At bottom left:  c1, c2 =    8.702e+06    3.380e+11
At top right:    c1, c2 =    9.650e+06    3.751e+11

t = 3.60e+04   no. steps = 335   order = 5   stepsize = 1.17e+02
At bottom left:  c1, c2 =    1.404e+04    3.387e+11
At top right:    c1, c2 =    1.561e+04    3.765e+11

t = 4.32e+04   no. steps = 388   order = 4   stepsize = 4.48e+02
At bottom left:  c1, c2 =   -5.732e-07    3.382e+11
At top right:    c1, c2 =   -6.367e-07    3.804e+11

t = 5.04e+04   no. steps = 406   order = 5   stepsize = 3.97e+02
At bottom left:  c1, c2 =   -4.317e-09    3.358e+11
At top right:    c1, c2 =   -8.233e-09    3.864e+11

t = 5.76e+04   no. steps = 418   order = 5   stepsize = 4.74e+02
At bottom left:  c1, c2 =   -2.576e-09    3.320e+11
At top right:    c1, c2 =   -1.259e-09    3.909e+11

t = 6.48e+04   no. steps = 428   order = 5   stepsize = 7.70e+02
At bottom left:  c1, c2 =    3.451e-09    3.313e+11
At top right:    c1, c2 =    2.081e-09    3.963e+11

t = 7.20e+04   no. steps = 437   order = 5   stepsize = 7.70e+02
At bottom left:  c1, c2 =    1.630e-11    3.330e+11
At top right:    c1, c2 =    1.843e-11    4.039e+11

t = 7.92e+04   no. steps = 447   order = 5   stepsize = 7.70e+02
At bottom left:  c1, c2 =   -1.704e-11    3.334e+11
At top right:    c1, c2 =   -1.131e-11    4.120e+11

t = 8.64e+04   no. steps = 456   order = 5   stepsize = 7.70e+02
At bottom left:  c1, c2 =    1.496e-12    3.352e+11
At top right:    c1, c2 =    8.085e-13    4.163e+11


Final Statistics:

lenrw   =  2089     leniw   =   120
lenrwls =  2046     leniwls =    80
nst     =   456
nfe     =   586     nfels   =   619
nni     =   582     nli     =   619
nsetups =    73     netf    =    25
npe     =     8     nps     =  1149
ncfn    =     0     ncfl    =     0
```

3.3 A CVBBDPRE preconditioner example: cvkryx_bbd_p

In this example, `cvkryx_bbd_p`, we solve the same problem in `cvkryx_p` above, but instead of supplying the preconditioner, we use the CVBBDPRE module, which generates and uses a band-block-diagonal preconditioner. The half-bandwidths of the Jacobian block on each processor are both equal to 2·`MXSUB`, and that is the value supplied as `mudq` and `mldq` in the call to `CVBBDPrecAlloc`. But in order to reduce storage and computation costs for preconditioning, we supply the values `mukeep` = `mlkeep` = 2 (= `NVARS`) as the half-bandwidths of the retained band matrix blocks. This means that the Jacobian elements are computed with a difference quotient scheme using the true bandwidth of the block, but only a narrow band matrix (bandwidth 5) is kept as the preconditioner. The source is listed in Appendix F.

As in `cvkryx_p.c`, the `f` routine in `cvkryx_bbd_p.c` simply calls a

communication routine, `fucomm`, and then a strictly computational routine, `flocal`. However, the call to `CVBBDPrecAlloc` specifies the pair of routines to be called as `ucomm` and `flocal`, where `ucomm` is an *empty* routine. This is because each call by the solver to `ucomm` is preceded by a call to `f` with the same `(t,u)` arguments, and therefore the communication needed for `flocal` in the solver's calls to it have already been done.

In `cvkryx_bbd_p.c`, the problem is solved twice — first with preconditioning on the left, and then on the right. Thus prior to the second solution, calls are made to reset the initial values (`SetInitialProfiles`), the main solver memory (`CVodeReInit`), the CVBBDPRE memory (`CVBBDPrecReInit`), as well as the preconditioner type (`CVSpilsSetPrecType`).

Sample output from `cvkryx_bbd_p` follows, again using 5×5 subgrids on a 2×2 processor grid. The performance of the preconditioner, as measured by the number of Krylov iterations per Newton iteration, `nli/nni`, is very close to that of `cvkryx_p` when preconditioning is on the left, but slightly poorer when it is on the right.

cvkryx_bbd_p sample output

```
2-species diurnal advection-diffusion problem
  10 by 10 mesh on 4 processors
  Using CVBBDPRE preconditioner module
    Difference-quotient half-bandwidths are mudq = 10,  mldq = 10
    Retained band block half-bandwidths are mukeep = 2,  mlkeep = 2

Preconditioner type is:  jpre = PREC_LEFT

t = 7.20e+03   no. steps = 190   order = 5   stepsize = 1.61e+02
At bottom left:  c1, c2 =    1.047e+04    2.527e+11
At top right:    c1, c2 =    1.119e+04    2.700e+11

t = 1.44e+04   no. steps = 221   order = 5   stepsize = 3.85e+02
At bottom left:  c1, c2 =    6.659e+06    2.582e+11
At top right:    c1, c2 =    7.301e+06    2.833e+11

t = 2.16e+04   no. steps = 247   order = 5   stepsize = 3.00e+02
At bottom left:  c1, c2 =    2.665e+07    2.993e+11
At top right:    c1, c2 =    2.931e+07    3.313e+11

t = 2.88e+04   no. steps = 272   order = 4   stepsize = 4.05e+02
At bottom left:  c1, c2 =    8.702e+06    3.380e+11
At top right:    c1, c2 =    9.650e+06    3.751e+11

t = 3.60e+04   no. steps = 309   order = 4   stepsize = 7.53e+01
```

```
At bottom left:  c1, c2 =    1.404e+04    3.387e+11
At top right:    c1, c2 =    1.561e+04    3.765e+11

t = 4.32e+04   no. steps = 377   order = 4   stepsize = 4.02e+02
At bottom left:  c1, c2 =    1.908e-07    3.382e+11
At top right:    c1, c2 =    2.345e-07    3.804e+11

t = 5.04e+04   no. steps = 392   order = 5   stepsize = 3.67e+02
At bottom left:  c1, c2 =   -6.408e-10    3.358e+11
At top right:    c1, c2 =   -6.654e-10    3.864e+11

t = 5.76e+04   no. steps = 403   order = 5   stepsize = 4.72e+02
At bottom left:  c1, c2 =    2.017e-08    3.320e+11
At top right:    c1, c2 =    3.353e-08    3.909e+11

t = 6.48e+04   no. steps = 415   order = 5   stepsize = 7.47e+02
At bottom left:  c1, c2 =   -2.502e-10    3.313e+11
At top right:    c1, c2 =    2.005e-10    3.963e+11

t = 7.20e+04   no. steps = 424   order = 5   stepsize = 7.47e+02
At bottom left:  c1, c2 =    4.217e-12    3.330e+11
At top right:    c1, c2 =   -2.693e-12    4.039e+11

t = 7.92e+04   no. steps = 434   order = 5   stepsize = 7.47e+02
At bottom left:  c1, c2 =    2.779e-12    3.334e+11
At top right:    c1, c2 =   -1.865e-12    4.120e+11

t = 8.64e+04   no. steps = 444   order = 5   stepsize = 7.47e+02
At bottom left:  c1, c2 =    2.331e-13    3.352e+11
At top right:    c1, c2 =   -1.599e-13    4.163e+11


Final Statistics:

lenrw   =  2089     leniw   =   120
lenrwls =  2046     leniwls =    80
nst     =   444
nfe     =   581     nfels   =   526
nni     =   577     nli     =   526
nsetups =    75     netf    =    28
npe     =     8     nps     =  1057
ncfn    =     0     ncfl    =     0

In CVBBDPRE: real/integer local work space sizes = 600, 50
             no. flocal evals. = 176


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


Preconditioner type is:  jpre = PREC_RIGHT

t = 7.20e+03   no. steps = 191   order = 5   stepsize = 1.22e+02
At bottom left:  c1, c2 =    1.047e+04    2.527e+11
At top right:    c1, c2 =    1.119e+04    2.700e+11

t = 1.44e+04   no. steps = 223   order = 5   stepsize = 2.79e+02
At bottom left:  c1, c2 =    6.659e+06    2.582e+11
At top right:    c1, c2 =    7.301e+06    2.833e+11
```

```
t = 2.16e+04   no. steps = 249   order = 5   stepsize = 4.31e+02
At bottom left:  c1, c2 =    2.665e+07    2.993e+11
At top right:    c1, c2 =    2.931e+07    3.313e+11

t = 2.88e+04   no. steps = 314   order = 3   stepsize = 9.38e+01
At bottom left:  c1, c2 =    8.702e+06    3.380e+11
At top right:    c1, c2 =    9.650e+06    3.751e+11

t = 3.60e+04   no. steps = 350   order = 5   stepsize = 9.78e+01
At bottom left:  c1, c2 =    1.404e+04    3.387e+11
At top right:    c1, c2 =    1.561e+04    3.765e+11

t = 4.32e+04   no. steps = 403   order = 4   stepsize = 3.87e+02
At bottom left:  c1, c2 =    1.504e-09    3.382e+11
At top right:    c1, c2 =    1.683e-09    3.804e+11

t = 5.04e+04   no. steps = 416   order = 5   stepsize = 5.91e+02
At bottom left:  c1, c2 =   -1.137e-11    3.358e+11
At top right:    c1, c2 =   -1.439e-11    3.864e+11

t = 5.76e+04   no. steps = 432   order = 5   stepsize = 1.73e+02
At bottom left:  c1, c2 =    1.293e-09    3.320e+11
At top right:    c1, c2 =    2.448e-10    3.909e+11

t = 6.48e+04   no. steps = 447   order = 5   stepsize = 6.38e+02
At bottom left:  c1, c2 =    7.963e-13    3.313e+11
At top right:    c1, c2 =   -2.943e-13    3.963e+11

t = 7.20e+04   no. steps = 459   order = 5   stepsize = 6.38e+02
At bottom left:  c1, c2 =   -2.414e-12    3.330e+11
At top right:    c1, c2 =    2.797e-13    4.039e+11

t = 7.92e+04   no. steps = 470   order = 5   stepsize = 6.38e+02
At bottom left:  c1, c2 =   -1.059e-13    3.334e+11
At top right:    c1, c2 =    3.557e-14    4.120e+11

t = 8.64e+04   no. steps = 481   order = 5   stepsize = 6.38e+02
At bottom left:  c1, c2 =    6.045e-15    3.352e+11
At top right:    c1, c2 =   -2.016e-15    4.163e+11


Final Statistics:

lenrw   =  2089     leniw   =   120
lenrwls =  2046     leniwls =    80
nst     =   481
nfe     =   622     nfels   =   769
nni     =   618     nli     =   769
nsetups =   104     netf    =    33
npe     =     9     nps     =  1281
ncfn    =     0     ncfl    =     0

In CVBBDPRE: real/integer local work space sizes = 600, 50
             no. flocal evals. = 198
```

4 Fortran example problems

The FORTRAN example problem programs supplied with the CVODE package are all written in standard FORTRAN77 and use double-precision arithmetic. 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, then declarations of floating-point constants are appropriately modified; e.g. `0.5D-4` is changed to `0.5E-4`.

4.1 A serial example: fcvkryx

The `fcvkryx` example is a FORTRAN equivalent of the `cvkryx` problem. (In fact, it was derived from an earlier FORTRAN example program for VODPK.) The source program `fcvkryx.f` is listed in Appendix G.

The main program begins with a call to `INITKX`, which sets problem parameters, loads these into arrays `IPAR` and `RPAR` for use by other routines, and loads `Y` with its initial values. It calls `FNVINITS`, `FCVMALLOC`, `FCVSPGMR`, `FCVSPGMRSETPSET`, and `FCVSPGMRSETPSOL` to initialize the NVECTOR_SERIAL module, the main solver memory, and the CVSPGMR module, and to specify user-supplied preconditioner setup and solve routines. It calls `FCVODE` in a loop over `TOUT` values, with printing of selected solution values and performance data (from the `IOUT` and `ROUT` arrays). At the end, it prints a number of performance counters, and frees memory with calls to `FCVFREE`.

In `fcvkryx.f`, the `FCVFUN` routine is a straightforward implementation of the discretized form of Eqns. (4). In `FCVPSET`, the block-diagonal part of the Jacobian, J_{bd}, is computed (and copied to `P`) if `JOK` $= 0$, but is simply copied from `BD` to `P` if `JOK` $= 1$. In both cases, the preconditioner matrix P is formed from J_{bd} and its 2×2 blocks are LU-factored. In `FCVPSOL`, the solution of a linear system $Px = z$ is solved by doing backsolve operations on the blocks. The remainder of `fcvkryx.f` consists of routines from LINPACK and the BLAS needed for matrix and vector operations.

The following is sample output from `fcvkryx`, using a 10×10 mesh. The performance of FCVODE here is quite similar to that of CVODE on the `cvkryx` problem, as expected.

fcvkryx sample output

```
Krylov example problem:

 Kinetics-transport, NEQ =  200


 t =   0.720E+04   nst =   219  q =  5  h =   0.158696E+03
  c1 (bot.left/middle/top rt.) =   0.104683E+05  0.296373E+05  0.111853E+05
  c2 (bot.left/middle/top rt.) =   0.252672E+12  0.715376E+12  0.269977E+12

 t =   0.144E+05   nst =   251  q =  5  h =   0.377205E+03
  c1 (bot.left/middle/top rt.) =   0.665902E+07  0.531602E+07  0.730081E+07
  c2 (bot.left/middle/top rt.) =   0.258192E+12  0.205680E+12  0.283286E+12

 t =   0.216E+05   nst =   277  q =  5  h =   0.274587E+03
  c1 (bot.left/middle/top rt.) =   0.266498E+08  0.103636E+08  0.293077E+08
```

```
  c2 (bot.left/middle/top rt.) =   0.299279E+12  0.102810E+12  0.331344E+12

 t =   0.288E+05   nst =   312  q =  4  h =   0.367517E+03
  c1 (bot.left/middle/top rt.) =   0.870209E+07  0.129197E+08  0.965002E+07
  c2 (bot.left/middle/top rt.) =   0.338035E+12  0.502929E+12  0.375096E+12

 t =   0.360E+05   nst =   350  q =  4  h =   0.683836E+02
  c1 (bot.left/middle/top rt.) =   0.140404E+05  0.202903E+05  0.156090E+05
  c2 (bot.left/middle/top rt.) =   0.338677E+12  0.489443E+12  0.376517E+12

 t =   0.432E+05   nst =   407  q =  4  h =   0.383863E+03
  c1 (bot.left/middle/top rt.) =   0.803367E-06  0.363858E-06  0.889797E-06
  c2 (bot.left/middle/top rt.) =   0.338233E+12  0.135487E+12  0.380352E+12

 t =   0.504E+05   nst =   436  q =  3  h =   0.215343E+03
  c1 (bot.left/middle/top rt.) =   0.375001E-05  0.665499E-06  0.454113E-05
  c2 (bot.left/middle/top rt.) =   0.335816E+12  0.493028E+12  0.386445E+12

 t =   0.576E+05   nst =   454  q =  5  h =   0.428080E+03
  c1 (bot.left/middle/top rt.) =   0.112301E-08  0.194567E-09  0.136087E-08
  c2 (bot.left/middle/top rt.) =   0.332031E+12  0.964985E+12  0.390900E+12

 t =   0.648E+05   nst =   466  q =  5  h =   0.690422E+03
  c1 (bot.left/middle/top rt.) =   0.353041E-08  0.590752E-09  0.428410E-08
  c2 (bot.left/middle/top rt.) =   0.331303E+12  0.892184E+12  0.396342E+12

 t =   0.720E+05   nst =   476  q =  5  h =   0.690422E+03
  c1 (bot.left/middle/top rt.) =  -0.121418E-09 -0.206756E-10 -0.147240E-09
  c2 (bot.left/middle/top rt.) =   0.332972E+12  0.618620E+12  0.403885E+12

 t =   0.792E+05   nst =   487  q =  5  h =   0.690422E+03
  c1 (bot.left/middle/top rt.) =  -0.341376E-11 -0.568210E-12 -0.414339E-11
  c2 (bot.left/middle/top rt.) =   0.333441E+12  0.666893E+12  0.412026E+12

 t =   0.864E+05   nst =   497  q =  5  h =   0.690422E+03
  c1 (bot.left/middle/top rt.) =   0.309841E-12  0.526192E-13  0.375773E-12
  c2 (bot.left/middle/top rt.) =   0.335178E+12  0.910652E+12  0.416251E+12


Final statistics:

 number of steps        =   497      number of f evals.     =  651
 number of prec. setups =    91
 number of prec. evals. =     9      number of prec. solves =  1233
 number of nonl. iters. =   647      number of lin. iters.  =   652
 average Krylov subspace dimension (NLI/NNI)  =   0.100773E+01
 number of conv. failures.. nonlinear =   0 linear =   0
 number of error test failures =  34
```

4.2 A parallel example: fcvkryx_bbd_p

This example, `fcvkryx_bbd_p`, uses a simple diagonal ODE system to illustrate the use of FCVODE in a parallel setting. The system is

$$\dot{y}_i = -\alpha\ i\ y_i \quad (i = 1, \ldots, N) \tag{10}$$

on the time interval $0 \leq t \leq 1$. In this case, we use $\alpha = 10$ and $N = 10*$NPES, where NPES is the number of processors and is specified at run time. The linear solver to be used is SPGMR with the CVBBDPRE (band-block-diagonal) preconditioner. Since the system Jacobian is diagonal, the half-bandwidths specified are all zero. The problem is solved twice — with preconditioning on the left, then on the right.

The source file, fcvkryx_bbd_p.f, is listed in Appendix H. It begins with MPI calls to initialize MPI and to get the number of processors and local processor index. The linear solver specification is done with calls to FCVBBDINIT and FCVBBDSPGMR. In a loop over TOUT values, it calls FCVODE and prints the step and f evaluation counters. After that, it computes and prints the maximum global error, and all the relevant performance counters. Those specific to CVBBDPRE are obtained by a call to FCVBBDOPT. To prepare for the second run, the program calls FCVREINIT, FCVBBDREINIT, and FCVSPGMRREINIT, in addition to resetting the initial conditions. Finally, it frees memory and terminates MPI. Notice that in the FCVFUN routine, the local processor index MYPE and the local vector size NLOCAL are used to form the global index values needed to evaluate the right-hand side of Eq. (10).

The following is a sample output from fcvkryx_bbd_p, with NPES = 4. As expected, the performance is identical for left vs right preconditioning.

fcvkryx_bbd_p sample output

```
Diagonal test problem:

 NEQ =  40
 parameter alpha =   10.000
 ydot_i = -alpha*i * y_i (i = 1,...,NEQ)
 RTOL, ATOL =    0.1E-04   0.1E-09
 Method is BDF/NEWTON/SPGMR
 Preconditioner is band-block-diagonal, using CVBBDPRE
 Number of processors =   4


Preconditioning on left

 t =   0.10E+00     no. steps =   221   no. f-s =   262
 t =   0.20E+00     no. steps =   265   no. f-s =   308
 t =   0.30E+00     no. steps =   290   no. f-s =   334
 t =   0.40E+00     no. steps =   306   no. f-s =   351
 t =   0.50E+00     no. steps =   319   no. f-s =   365
 t =   0.60E+00     no. steps =   329   no. f-s =   375
 t =   0.70E+00     no. steps =   339   no. f-s =   386
 t =   0.80E+00     no. steps =   345   no. f-s =   392
 t =   0.90E+00     no. steps =   352   no. f-s =   399
 t =   0.10E+01     no. steps =   359   no. f-s =   406

Max. absolute error is  0.28E-08


Final statistics:

 number of steps        =   359     number of f evals.     =   406
 number of prec. setups =    38
 number of prec. evals. =     7     number of prec. solves =   728
 number of nonl. iters. =   402     number of lin. iters.  =   364
 average Krylov subspace dimension (NLI/NNI) =   0.9055
 number of conv. failures.. nonlinear =   0  linear =   0
 number of error test failures =   5
```

```
 main solver real/int workspace sizes   =   489  120
 linear solver real/int workspace sizes =   446   80
In CVBBDPRE:
 real/int local workspace =    20   10
 number of g evals. =    14


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


Preconditioning on right

 t =   0.10E+00     no. steps =   221   no. f-s =   262
 t =   0.20E+00     no. steps =   265   no. f-s =   308
 t =   0.30E+00     no. steps =   290   no. f-s =   334
 t =   0.40E+00     no. steps =   306   no. f-s =   351
 t =   0.50E+00     no. steps =   319   no. f-s =   365
 t =   0.60E+00     no. steps =   329   no. f-s =   375
 t =   0.70E+00     no. steps =   339   no. f-s =   386
 t =   0.80E+00     no. steps =   345   no. f-s =   392
 t =   0.90E+00     no. steps =   352   no. f-s =   399
 t =   0.10E+01     no. steps =   359   no. f-s =   406

Max. absolute error is  0.28E-08


Final statistics:

 number of steps        =   359     number of f evals.     =   406
 number of prec. setups =    38
 number of prec. evals. =     7     number of prec. solves =   728
 number of nonl. iters. =   402     number of lin. iters.  =   364
 average Krylov subspace dimension (NLI/NNI) =   0.9055
 number of conv. failures.. nonlinear =   0  linear =   0
 number of error test failures =   5
 main solver real/int workspace sizes   =   489  120
 linear solver real/int workspace sizes =   446   80
In CVBBDPRE:
 real/int local workspace =    20   10
 number of g evals. =    14
```

5 Parallel tests

The stiff example problem `cvkryx` described above, or rather its parallel version `cvkry_p`, has been modified and expanded to form a test problem for the parallel version of CVODE. This work was largely carried out by M. Wittman and reported in [2].

To start with, in order to add realistic complexity to the solution, the initial profile for this problem was altered to include a rather steep front in the vertical direction. Specifically, the function $\beta(y)$ in Eq. (6) has been replaced by:

$$\beta(y) = .75 + .25 \tanh(10y - 400) \ . \tag{11}$$

This function rises from about .5 to about 1.0 over a y interval of about .2 (i.e. 1/100 of the total span in y). This vertical variation, together with the horizonatal advection and diffusion in the problem, demands a fairly fine spatial mesh to achieve acceptable resolution.

In addition, an alternate choice of differencing is used in order to control spurious oscillations resulting from the horizontal advection. In place of central differencing for that term, a biased upwind approximation is applied to each of the terms $\partial c^i/\partial x$, namely:

$$\partial c/\partial x|_{x_j} \approx \left[\frac{3}{2}c_{j+1} - c_j - \frac{1}{2}c_{j-1}\right] /(2\Delta x) \ . \tag{12}$$

With this modified form of the problem, we performed tests similar to those described above for the example. Here we fix the subgrid dimensions at `MXSUB = MYSUB =` 50, so that the local (per-processor) problem size is 5000, while the processor array dimensions, `NPEX` and `NPEY`, are varied. In one (typical) sequence of tests, we fix `NPEY` = 8 (for a vertical mesh size of `MY` = 400), and set `NPEX` = 8 (`MX` = 400), `NPEX` = 16 (`MX` = 800), and `NPEX` = 32 (`MX` = 1600). Thus the largest problem size N is $2 \cdot 400 \cdot 1600 = 1,280,000$. For these tests, we also raise the maximum Krylov dimension, `maxl`, to 10 (from its default value of 5).

For each of the three test cases, the test program was run on a Cray-T3D (256 processors) with each of three different message-passing libraries:

- MPICH: an implementation of MPI on top of the Chameleon library
- EPCC: an implementation of MPI by the Edinburgh Parallel Computer Centre
- SHMEM: Cray's Shared Memory Library

The following table gives the run time and selected performance counters for these 9 runs. In all cases, the solutions agreed well with each other, showing expected small variations with grid size. In the table, M-P denotes the message-passing library, RT is the reported run time in CPU seconds, `nst` is the number of time steps, `nfe` is the number of f evaluations, `nni` is the number of nonlinear (Newton) iterations, `nli` is the number of linear (Krylov) iterations, and `npe` is the number of evaluations of the preconditioner.

Some of the results were as expected, and some were surprising. For a given mesh size, variations in performance counts were small or absent, except for moderate (but still acceptable) variations for SHMEM in the smallest case. The increase in costs with mesh size can be attributed to a decline in the quality of the preconditioner, which neglects most of the spatial coupling. The preconditioner quality can be inferred from the ratio `nli/nni`, which is the average number of Krylov iterations per Newton iteration. The most interesting (and unexpected) result is the variation of run time with library: SHMEM is the most efficient,

NPEX	M-P	RT	nst	nfe	nni	nli	npe
8	MPICH	436.	1391	9907	1512	8392	24
8	EPCC	355.	1391	9907	1512	8392	24
8	SHMEM	349.	1999	10,326	2096	8227	34
16	MPICH	676.	2513	14,159	2583	11,573	42
16	EPCC	494.	2513	14,159	2583	11,573	42
16	SHMEM	471.	2513	14,160	2581	11,576	42
32	MPICH	1367.	2536	20,153	2696	17,454	43
32	EPCC	737.	2536	20,153	2696	17,454	43
32	SHMEM	695.	2536	20,121	2694	17,424	43

Table 1: Parallel CVODE test results vs problem size and message-passing library

but EPCC is a very close second, and MPICH loses considerable efficiency by comparison, as the problem size grows. This means that the highly portable MPI version of CVODE, with an appropriate choice of MPI implementation, is fully competitive with the Cray-specific version using the SHMEM library. While the overall costs do not prepresent a well-scaled parallel algorithm (because of the preconditioner choice), the cost per function evaluation is quite flat for EPCC and SHMEM, at .033 to .037 (for MPICH it ranges from .044 to .068).

For tests that demonstrate speedup from parallelism, we consider runs with fixed problem size: `MX` = 800, `MY` = 400. Here we also fix the vertical subgrid dimension at `MYSUB` = 50 and the vertical processor array dimension at `NPEY` = 8, but vary the corresponding horizontal sizes. We take `NPEX` = 8, 16, and 32, with `MXSUB` = 100, 50, and 25, respectively. The runs for the three cases and three message-passing libraries all show very good agreement in solution values and performance counts. The run times for EPCC are 947, 494, and 278, showing speedups of 1.92 and 1.78 as the number of processors is doubled (twice). For the SHMEM runs, the times were slightly lower and the ratios were 1.98 and 1.91. For MPICH, consistent with the earlier runs, the run times were considerably higher, and in fact show speedup ratios of only 1.54 and 1.03.

References

[1] A. C. Hindmarsh and R. Serban. User Documentation for CVODE v2.4.0. Technical Report UCRL-SM-208108, LLNL, 2005.

[2] M. R. Wittman. Testing of PVODE, a Parallel ODE Solver. Technical Report UCRL-ID-125562, LLNL, August 1996.

A Listing of cvdenx.c

```
/*
 * -----------------------------------------------------------------
 * $Revision: 1.1 $
 * $Date: 2006/07/05 15:50:05 $
 * -----------------------------------------------------------------
 * Programmer(s): Scott D. Cohen, Alan C. Hindmarsh and
 *                Radu Serban @ LLNL
 * -----------------------------------------------------------------
 * Example problem:
 *
 * The following is a simple example problem, with the coding
 * needed for its solution by CVODE. The problem is from
 * chemical kinetics, and consists of the following three rate
 * equations:
 *    dy1/dt = -.04*y1 + 1.e4*y2*y3
 *    dy2/dt = .04*y1 - 1.e4*y2*y3 - 3.e7*(y2)^2
 *    dy3/dt = 3.e7*(y2)^2
 * on the interval from t = 0.0 to t = 4.e10, with initial
 * conditions: y1 = 1.0, y2 = y3 = 0. The problem is stiff.
 * While integrating the system, we also use the rootfinding
 * feature to find the points at which y1 = 1e-4 or at which
 * y3 = 0.01. This program solves the problem with the BDF method,
 * Newton iteration with the CVDENSE dense linear solver, and a
 * user-supplied Jacobian routine.
 * It uses a scalar relative tolerance and a vector absolute
 * tolerance. Output is printed in decades from t = .4 to t = 4.e10.
 * Run statistics (optional outputs) are printed at the end.
 * -----------------------------------------------------------------
 */

#include <stdio.h>

/* Header files with a description of contents used in cvdenx.c */

#include <cvode/cvode.h>             /* prototypes for CVODE fcts. and consts. */
#include <nvector/nvector_serial.h>  /* serial N_Vector types, fcts., and macros */
#include <cvode/cvode_dense.h>       /* prototype for CVDense */
#include <sundials/sundials_dense.h> /* definitions DenseMat DENSE_ELEM */
#include <sundials/sundials_types.h> /* definition of type realtype */

/* User-defined vector and matrix accessor macros: Ith, IJth */

/* These macros are defined in order to write code which exactly matches
   the mathematical problem description given above.

   Ith(v,i) references the ith component of the vector v, where i is in
   the range [1..NEQ] and NEQ is defined below. The Ith macro is defined
   using the N_VIth macro in nvector.h. N_VIth numbers the components of
   a vector starting from 0.

   IJth(A,i,j) references the (i,j)th element of the dense matrix A, where
   i and j are in the range [1..NEQ]. The IJth macro is defined using the
   DENSE_ELEM macro in dense.h. DENSE_ELEM numbers rows and columns of a
   dense matrix starting from 0. */

#define Ith(v,i)    NV_Ith_S(v,i-1)       /* Ith numbers components 1..NEQ */
#define IJth(A,i,j) DENSE_ELEM(A,i-1,j-1) /* IJth numbers rows,cols 1..NEQ */
```

```
58
59
60  /* Problem Constants */
61
62  #define NEQ   3                /* number of equations  */
63  #define Y1    RCONST(1.0)      /* initial y components */
64  #define Y2    RCONST(0.0)
65  #define Y3    RCONST(0.0)
66  #define RTOL  RCONST(1.0e-4)   /* scalar relative tolerance            */
67  #define ATOL1 RCONST(1.0e-8)   /* vector absolute tolerance components */
68  #define ATOL2 RCONST(1.0e-14)
69  #define ATOL3 RCONST(1.0e-6)
70  #define T0    RCONST(0.0)      /* initial time           */
71  #define T1    RCONST(0.4)      /* first output time      */
72  #define TMULT RCONST(10.0)     /* output time factor     */
73  #define NOUT  12               /* number of output times */
74
75
76  /* Functions Called by the Solver */
77
78  static int f(realtype t, N_Vector y, N_Vector ydot, void *f_data);
79
80  static int g(realtype t, N_Vector y, realtype *gout, void *g_data);
81
82  static int Jac(long int N, DenseMat J, realtype t,
83                 N_Vector y, N_Vector fy, void *jac_data,
84                 N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
85
86  /* Private functions to output results */
87
88  static void PrintOutput(realtype t, realtype y1, realtype y2, realtype y3);
89  static void PrintRootInfo(int root_f1, int root_f2);
90
91  /* Private function to print final statistics */
92
93  static void PrintFinalStats(void *cvode_mem);
94
95  /* Private function to check function return values */
96
97  static int check_flag(void *flagvalue, char *funcname, int opt);
98
99
100 /*
101  *-------------------------------
102  * Main Program
103  *-------------------------------
104  */
105
106 int main()
107 {
108   realtype reltol, t, tout;
109   N_Vector y, abstol;
110   void *cvode_mem;
111   int flag, flagr, iout;
112   int rootsfound[2];
113
114   y = abstol = NULL;
115   cvode_mem = NULL;
116
```

```
117     /* Create serial vector of length NEQ for I.C. and abstol */
118     y = N_VNew_Serial(NEQ);
119     if (check_flag((void *)y, "N_VNew_Serial", 0)) return(1);
120     abstol = N_VNew_Serial(NEQ);
121     if (check_flag((void *)abstol, "N_VNew_Serial", 0)) return(1);
122
123     /* Initialize y */
124     Ith(y,1) = Y1;
125     Ith(y,2) = Y2;
126     Ith(y,3) = Y3;
127
128     /* Set the scalar relative tolerance */
129     reltol = RTOL;
130     /* Set the vector absolute tolerance */
131     Ith(abstol,1) = ATOL1;
132     Ith(abstol,2) = ATOL2;
133     Ith(abstol,3) = ATOL3;
134
135     /*
136        Call CVodeCreate to create the solver memory:
137
138        CV_BDF     specifies the Backward Differentiation Formula
139        CV_NEWTON  specifies a Newton iteration
140
141        A pointer to the integrator problem memory is returned and stored in cvode_mem.
142     */
143
144     cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
145     if (check_flag((void *)cvode_mem, "CVodeCreate", 0)) return(1);
146
147     /*
148        Call CVodeMalloc to initialize the integrator memory:
149
150        cvode_mem is the pointer to the integrator memory returned by CVodeCreate
151        f         is the user's right hand side function in y'=f(t,y)
152        T0        is the initial time
153        y         is the initial dependent variable vector
154        CV_SV     specifies scalar relative and vector absolute tolerances
155        &reltol   is a pointer to the scalar relative tolerance
156        abstol    is the absolute tolerance vector
157     */
158
159     flag = CVodeMalloc(cvode_mem, f, T0, y, CV_SV, reltol, abstol);
160     if (check_flag(&flag, "CVodeMalloc", 1)) return(1);
161
162     /* Call CVodeRootInit to specify the root function g with 2 components */
163     flag = CVodeRootInit(cvode_mem, 2, g, NULL);
164     if (check_flag(&flag, "CVodeRootInit", 1)) return(1);
165
166     /* Call CVDense to specify the CVDENSE dense linear solver */
167     flag = CVDense(cvode_mem, NEQ);
168     if (check_flag(&flag, "CVDense", 1)) return(1);
169
170     /* Set the Jacobian routine to Jac (user-supplied) */
171     flag = CVDenseSetJacFn(cvode_mem, Jac, NULL);
172     if (check_flag(&flag, "CVDenseSetJacFn", 1)) return(1);
173
174     /* In loop, call CVode, print results, and test for error.
175        Break out of loop when NOUT preset output times have been reached.  */
```

```
176   printf("␣\n3-species␣kinetics␣problem\n\n");
177
178   iout = 0;  tout = T1;
179   while(1) {
180     flag = CVode(cvode_mem, tout, y, &t, CV_NORMAL);
181     PrintOutput(t, Ith(y,1), Ith(y,2), Ith(y,3));
182
183     if (flag == CV_ROOT_RETURN) {
184       flagr = CVodeGetRootInfo(cvode_mem, rootsfound);
185       if (check_flag(&flagr, "CVodeGetRootInfo", 1)) return(1);
186       PrintRootInfo(rootsfound[0],rootsfound[1]);
187     }
188
189     if (check_flag(&flag, "CVode", 1)) break;
190     if (flag == CV_SUCCESS) {
191       iout++;
192       tout *= TMULT;
193     }
194
195     if (iout == NOUT) break;
196   }
197
198   /* Print some final statistics */
199   PrintFinalStats(cvode_mem);
200
201   /* Free y vector */
202   N_VDestroy_Serial(y);
203
204   /* Free integrator memory */
205   CVodeFree(&cvode_mem);
206
207   return(0);
208 }
209
210
211 /*
212  *-------------------------------
213  * Functions called by the solver
214  *-------------------------------
215  */
216
217 /*
218  * f routine. Compute function f(t,y).
219  */
220
221 static int f(realtype t, N_Vector y, N_Vector ydot, void *f_data)
222 {
223   realtype y1, y2, y3, yd1, yd3;
224
225   y1 = Ith(y,1); y2 = Ith(y,2); y3 = Ith(y,3);
226
227   yd1 = Ith(ydot,1) = RCONST(-0.04)*y1 + RCONST(1.0e4)*y2*y3;
228   yd3 = Ith(ydot,3) = RCONST(3.0e7)*y2*y2;
229         Ith(ydot,2) = -yd1 - yd3;
230
231   return(0);
232 }
233
234 /*
```

```
235   * g routine. Compute functions g_i(t,y) for i = 0,1.
236   */
237
238  static int g(realtype t, N_Vector y, realtype *gout, void *g_data)
239  {
240    realtype y1, y3;
241
242    y1 = Ith(y,1); y3 = Ith(y,3);
243    gout[0] = y1 - RCONST(0.0001);
244    gout[1] = y3 - RCONST(0.01);
245
246    return(0);
247  }
248
249  /*
250   * Jacobian routine. Compute J(t,y) = df/dy. *
251   */
252
253  static int Jac(long int N, DenseMat J, realtype t,
254                 N_Vector y, N_Vector fy, void *jac_data,
255                 N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
256  {
257    realtype y1, y2, y3;
258
259    y1 = Ith(y,1); y2 = Ith(y,2); y3 = Ith(y,3);
260
261    IJth(J,1,1) = RCONST(-0.04);
262    IJth(J,1,2) = RCONST(1.0e4)*y3;
263    IJth(J,1,3) = RCONST(1.0e4)*y2;
264    IJth(J,2,1) = RCONST(0.04);
265    IJth(J,2,2) = RCONST(-1.0e4)*y3-RCONST(6.0e7)*y2;
266    IJth(J,2,3) = RCONST(-1.0e4)*y2;
267    IJth(J,3,2) = RCONST(6.0e7)*y2;
268
269    return(0);
270  }
271
272  /*
273   *-------------------------------
274   * Private helper functions
275   *-------------------------------
276   */
277
278  static void PrintOutput(realtype t, realtype y1, realtype y2, realtype y3)
279  {
280  #if defined(SUNDIALS_EXTENDED_PRECISION)
281    printf("At␣t␣=␣%0.4Le␣␣␣␣␣␣␣y␣=%14.6Le␣␣%14.6Le␣␣%14.6Le\n", t, y1, y2, y3);
282  #elif defined(SUNDIALS_DOUBLE_PRECISION)
283    printf("At␣t␣=␣%0.4le␣␣␣␣␣␣␣y␣=%14.6le␣␣%14.6le␣␣%14.6le\n", t, y1, y2, y3);
284  #else
285    printf("At␣t␣=␣%0.4e␣␣␣␣␣␣␣y␣=%14.6e␣␣%14.6e␣␣%14.6e\n", t, y1, y2, y3);
286  #endif
287
288    return;
289  }
290
291  static void PrintRootInfo(int root_f1, int root_f2)
292  {
293    printf("␣␣␣␣rootsfound[]␣=␣%3d␣%3d\n", root_f1, root_f2);
```

```
294
295     return;
296   }
297
298   /*
299    * Get and print some final statistics
300    */
301
302   static void PrintFinalStats(void *cvode_mem)
303   {
304     long int nst, nfe, nsetups, nje, nfeLS, nni, ncfn, netf, nge;
305     int flag;
306
307     flag = CVodeGetNumSteps(cvode_mem, &nst);
308     check_flag(&flag, "CVodeGetNumSteps", 1);
309     flag = CVodeGetNumRhsEvals(cvode_mem, &nfe);
310     check_flag(&flag, "CVodeGetNumRhsEvals", 1);
311     flag = CVodeGetNumLinSolvSetups(cvode_mem, &nsetups);
312     check_flag(&flag, "CVodeGetNumLinSolvSetups", 1);
313     flag = CVodeGetNumErrTestFails(cvode_mem, &netf);
314     check_flag(&flag, "CVodeGetNumErrTestFails", 1);
315     flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
316     check_flag(&flag, "CVodeGetNumNonlinSolvIters", 1);
317     flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);
318     check_flag(&flag, "CVodeGetNumNonlinSolvConvFails", 1);
319
320     flag = CVDenseGetNumJacEvals(cvode_mem, &nje);
321     check_flag(&flag, "CVDenseGetNumJacEvals", 1);
322     flag = CVDenseGetNumRhsEvals(cvode_mem, &nfeLS);
323     check_flag(&flag, "CVDenseGetNumRhsEvals", 1);
324
325     flag = CVodeGetNumGEvals(cvode_mem, &nge);
326     check_flag(&flag, "CVodeGetNumGEvals", 1);
327
328     printf("\nFinal␣Statistics:\n");
329     printf("nst␣=␣%-6ld␣nfe␣␣=␣%-6ld␣nsetups␣=␣%-6ld␣nfeLS␣=␣%-6ld␣nje␣=␣%ld\n",
330            nst, nfe, nsetups, nfeLS, nje);
331     printf("nni␣=␣%-6ld␣ncfn␣=␣%-6ld␣netf␣=␣%-6ld␣nge␣=␣%ld\n␣\n",
332            nni, ncfn, netf, nge);
333   }
334
335   /*
336    * Check function return value...
337    *   opt == 0 means SUNDIALS function allocates memory so check if
338    *            returned NULL pointer
339    *   opt == 1 means SUNDIALS function returns a flag so check if
340    *            flag >= 0
341    *   opt == 2 means function allocates memory so check if returned
342    *            NULL pointer
343    */
344
345   static int check_flag(void *flagvalue, char *funcname, int opt)
346   {
347     int *errflag;
348
349     /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
350     if (opt == 0 && flagvalue == NULL) {
351       fprintf(stderr, "\nSUNDIALS_ERROR:␣%s()␣failed␣-␣returned␣NULL␣pointer\n\n",
352               funcname);
```

```
353       return(1); }
354
355     /* Check if flag < 0 */
356     else if (opt == 1) {
357       errflag = (int *) flagvalue;
358       if (*errflag < 0) {
359         fprintf(stderr, "\nSUNDIALS_ERROR: %s() failed with flag = %d\n\n",
360                 funcname, *errflag);
361         return(1); }}
362
363     /* Check if function returned NULL pointer - no memory allocated */
364     else if (opt == 2 && flagvalue == NULL) {
365       fprintf(stderr, "\nMEMORY_ERROR: %s() failed - returned NULL pointer\n\n",
366               funcname);
367       return(1); }
368
369     return(0);
370   }
```

B Listing of cvbanx.c

```
/*
 * -----------------------------------------------------------------
 * $Revision: 1.1 $
 * $Date: 2006/07/05 15:50:05 $
 * -----------------------------------------------------------------
 * Programmer(s): Scott D. Cohen, Alan C. Hindmarsh and
 *                Radu Serban @ LLNL
 * -----------------------------------------------------------------
 * Example problem:
 *
 * The following is a simple example problem with a banded Jacobian,
 * with the program for its solution by CVODE.
 * The problem is the semi-discrete form of the advection-diffusion
 * equation in 2-D:
 *   du/dt = d^2 u / dx^2 + .5 du/dx + d^2 u / dy^2
 * on the rectangle 0 <= x <= 2, 0 <= y <= 1, and the time
 * interval 0 <= t <= 1. Homogeneous Dirichlet boundary conditions
 * are posed, and the initial condition is
 *   u(x,y,t=0) = x(2-x)y(1-y)exp(5xy).
 * The PDE is discretized on a uniform MX+2 by MY+2 grid with
 * central differencing, and with boundary values eliminated,
 * leaving an ODE system of size NEQ = MX*MY.
 * This program solves the problem with the BDF method, Newton
 * iteration with the CVBAND band linear solver, and a user-supplied
 * Jacobian routine.
 * It uses scalar relative and absolute tolerances.
 * Output is printed at t = .1, .2, ..., 1.
 * Run statistics (optional outputs) are printed at the end.
 * -----------------------------------------------------------------
 */

#include <stdio.h>
#include <stdlib.h>
#include <math.h>

/* Header files with a description of contents used in cvbanx.c */

#include <cvode/cvode.h>             /* prototypes for CVODE fcts. and consts. */
#include <cvode/cvode_band.h>        /* prototype for CVBand */
#include <nvector/nvector_serial.h>  /* serial N_Vector types, fcts., and macros */
#include <sundials/sundials_band.h>  /* definitions of type BandMat and macros */
#include <sundials/sundials_types.h> /* definition of type realtype */
#include <sundials/sundials_math.h>  /* definition of ABS and EXP */

/* Problem Constants */

#define XMAX   RCONST(2.0)     /* domain boundaries         */
#define YMAX   RCONST(1.0)
#define MX     10              /* mesh dimensions           */
#define MY     5
#define NEQ    MX*MY           /* number of equations       */
#define ATOL   RCONST(1.0e-5) /* scalar absolute tolerance */
#define T0     RCONST(0.0)     /* initial time              */
#define T1     RCONST(0.1)     /* first output time         */
#define DTOUT  RCONST(0.1)     /* output time increment     */
#define NOUT   10              /* number of output times    */

```

```c
#define ZERO RCONST(0.0)
#define HALF RCONST(0.5)
#define ONE  RCONST(1.0)
#define TWO  RCONST(2.0)
#define FIVE RCONST(5.0)

/* User-defined vector access macro IJth */

/* IJth is defined in order to isolate the translation from the
   mathematical 2-dimensional structure of the dependent variable vector
   to the underlying 1-dimensional storage.
   IJth(vdata,i,j) references the element in the vdata array for
   u at mesh point (i,j), where 1 <= i <= MX, 1 <= j <= MY.
   The vdata array is obtained via the macro call vdata = NV_DATA_S(v),
   where v is an N_Vector.
   The variables are ordered by the y index j, then by the x index i. */

#define IJth(vdata,i,j) (vdata[(j-1) + (i-1)*MY])

/* Type : UserData (contains grid constants) */

typedef struct {
  realtype dx, dy, hdcoef, hacoef, vdcoef;
} *UserData;

/* Private Helper Functions */

static void SetIC(N_Vector u, UserData data);
static void PrintHeader(realtype reltol, realtype abstol, realtype umax);
static void PrintOutput(realtype t, realtype umax, long int nst);
static void PrintFinalStats(void *cvode_mem);

/* Private function to check function return values */

static int check_flag(void *flagvalue, char *funcname, int opt);

/* Functions Called by the Solver */

static int f(realtype t, N_Vector u, N_Vector udot, void *f_data);
static int Jac(long int N, long int mu, long int ml, BandMat J,
               realtype t, N_Vector u, N_Vector fu, void *jac_data,
               N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);

/*
 *--------------------------------
 * Main Program
 *--------------------------------
 */

int main(void)
{
  realtype dx, dy, reltol, abstol, t, tout, umax;
  N_Vector u;
  UserData data;
  void *cvode_mem;
  int iout, flag;
  long int nst;

  u = NULL;
```

```
117     data = NULL;
118     cvode_mem = NULL;
119
120     /* Create a serial vector */
121
122     u = N_VNew_Serial(NEQ);  /* Allocate u vector */
123     if(check_flag((void*)u, "N_VNew_Serial", 0)) return(1);
124
125     reltol = ZERO;  /* Set the tolerances */
126     abstol = ATOL;
127
128     data = (UserData) malloc(sizeof *data);  /* Allocate data memory */
129     if(check_flag((void *)data, "malloc", 2)) return(1);
130     dx = data->dx = XMAX/(MX+1);  /* Set grid coefficients in data */
131     dy = data->dy = YMAX/(MY+1);
132     data->hdcoef = ONE/(dx*dx);
133     data->hacoef = HALF/(TWO*dx);
134     data->vdcoef = ONE/(dy*dy);
135
136     SetIC(u, data);  /* Initialize u vector */
137
138     /*
139        Call CvodeCreate to create integrator memory
140
141        CV_BDF     specifies the Backward Differentiation Formula
142        CV_NEWTON  specifies a Newton iteration
143
144        A pointer to the integrator problem memory is returned and
145        stored in cvode_mem.
146     */
147
148     cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
149     if(check_flag((void *)cvode_mem, "CVodeCreate", 0)) return(1);
150
151     /*
152        Call CVodeMalloc to initialize the integrator memory:
153
154        cvode_mem is the pointer to the integrator memory returned by CVodeCreate
155        f       is the user's right hand side function in y'=f(t,y)
156        T0      is the initial time
157        u       is the initial dependent variable vector
158        CV_SS   specifies scalar relative and absolute tolerances
159        reltol  is the scalar relative tolerance
160        &abstol is a pointer to the scalar absolute tolerance
161     */
162
163     flag = CVodeMalloc(cvode_mem, f, T0, u, CV_SS, reltol, &abstol);
164     if(check_flag(&flag, "CVodeMalloc", 1)) return(1);
165
166     /* Set the pointer to user-defined data */
167
168     flag = CVodeSetFdata(cvode_mem, data);
169     if(check_flag(&flag, "CVodeSetFdata", 1)) return(1);
170
171     /* Call CVBand to specify the CVBAND band linear solver */
172
173     flag = CVBand(cvode_mem, NEQ, MY, MY);
174     if(check_flag(&flag, "CVBand", 1)) return(1);
175
```

```
176     /* Set the user-supplied Jacobian routine Jac and
177        the pointer to the user-defined block data. */
178
179     flag = CVBandSetJacFn(cvode_mem, Jac, data);
180     if(check_flag(&flag, "CVBandSetJacFn", 1)) return(1);
181
182     /* In loop over output points: call CVode, print results, test for errors */
183
184     umax = N_VMaxNorm(u);
185     PrintHeader(reltol, abstol, umax);
186     for(iout=1, tout=T1; iout <= NOUT; iout++, tout += DTOUT) {
187       flag = CVode(cvode_mem, tout, u, &t, CV_NORMAL);
188       if(check_flag(&flag, "CVode", 1)) break;
189       umax = N_VMaxNorm(u);
190       flag = CVodeGetNumSteps(cvode_mem, &nst);
191       check_flag(&flag, "CVodeGetNumSteps", 1);
192       PrintOutput(t, umax, nst);
193     }
194
195     PrintFinalStats(cvode_mem);  /* Print some final statistics   */
196
197     N_VDestroy_Serial(u);   /* Free the u vector */
198     CVodeFree(&cvode_mem);  /* Free the integrator memory */
199     free(data);             /* Free the user data */
200
201     return(0);
202   }
203
204   /*
205    *-------------------------------
206    * Functions called by the solver
207    *-------------------------------
208    */
209
210   /* f routine. Compute f(t,u). */
211
212   static int f(realtype t, N_Vector u,N_Vector udot, void *f_data)
213   {
214     realtype uij, udn, uup, ult, urt, hordc, horac, verdc, hdiff, hadv, vdiff;
215     realtype *udata, *dudata;
216     int i, j;
217     UserData data;
218
219     udata = NV_DATA_S(u);
220     dudata = NV_DATA_S(udot);
221
222     /* Extract needed constants from data */
223
224     data = (UserData) f_data;
225     hordc = data->hdcoef;
226     horac = data->hacoef;
227     verdc = data->vdcoef;
228
229     /* Loop over all grid points. */
230
231     for (j=1; j <= MY; j++) {
232
233       for (i=1; i <= MX; i++) {
234
```

```
235         /* Extract u at x_i, y_j and four neighboring points */
236
237         uij = IJth(udata, i, j);
238         udn = (j == 1)  ? ZERO : IJth(udata, i, j-1);
239         uup = (j == MY) ? ZERO : IJth(udata, i, j+1);
240         ult = (i == 1)  ? ZERO : IJth(udata, i-1, j);
241         urt = (i == MX) ? ZERO : IJth(udata, i+1, j);
242
243         /* Set diffusion and advection terms and load into udot */
244
245         hdiff = hordc*(ult - TWO*uij + urt);
246         hadv = horac*(urt - ult);
247         vdiff = verdc*(uup - TWO*uij + udn);
248         IJth(dudata, i, j) = hdiff + hadv + vdiff;
249       }
250     }
251
252     return(0);
253   }
254
255   /* Jacobian routine. Compute J(t,u). */
256
257   static int Jac(long int N, long int mu, long int ml, BandMat J,
258                  realtype t, N_Vector u, N_Vector fu, void *jac_data,
259                  N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
260   {
261     long int i, j, k;
262     realtype *kthCol, hordc, horac, verdc;
263     UserData data;
264
265     /*
266       The components of f = udot that depend on u(i,j) are
267       f(i,j), f(i-1,j), f(i+1,j), f(i,j-1), f(i,j+1), with
268         df(i,j)/du(i,j) = -2 (1/dx^2 + 1/dy^2)
269         df(i-1,j)/du(i,j) = 1/dx^2 + .25/dx  (if i > 1)
270         df(i+1,j)/du(i,j) = 1/dx^2 - .25/dx  (if i < MX)
271         df(i,j-1)/du(i,j) = 1/dy^2           (if j > 1)
272         df(i,j+1)/du(i,j) = 1/dy^2           (if j < MY)
273     */
274
275     data = (UserData) jac_data;
276     hordc = data->hdcoef;
277     horac = data->hacoef;
278     verdc = data->vdcoef;
279
280     for (j=1; j <= MY; j++) {
281       for (i=1; i <= MX; i++) {
282         k = j-1 + (i-1)*MY;
283         kthCol = BAND_COL(J,k);
284
285         /* set the kth column of J */
286
287         BAND_COL_ELEM(kthCol,k,k) = -TWO*(verdc+hordc);
288         if (i != 1)  BAND_COL_ELEM(kthCol,k-MY,k) = hordc + horac;
289         if (i != MX) BAND_COL_ELEM(kthCol,k+MY,k) = hordc - horac;
290         if (j != 1)  BAND_COL_ELEM(kthCol,k-1,k)  = verdc;
291         if (j != MY) BAND_COL_ELEM(kthCol,k+1,k)  = verdc;
292       }
293     }
```

```
294
295   return(0);
296 }
297
298 /*
299  *------------------------------
300  * Private helper functions
301  *------------------------------
302  */
303
304 /* Set initial conditions in u vector */
305
306 static void SetIC(N_Vector u, UserData data)
307 {
308   int i, j;
309   realtype x, y, dx, dy;
310   realtype *udata;
311
312   /* Extract needed constants from data */
313
314   dx = data->dx;
315   dy = data->dy;
316
317   /* Set pointer to data array in vector u. */
318
319   udata = NV_DATA_S(u);
320
321   /* Load initial profile into u vector */
322
323   for (j=1; j <= MY; j++) {
324     y = j*dy;
325     for (i=1; i <= MX; i++) {
326       x = i*dx;
327       IJth(udata,i,j) = x*(XMAX - x)*y*(YMAX - y)*EXP(FIVE*x*y);
328     }
329   }
330 }
331
332 /* Print first lines of output (problem description) */
333
334 static void PrintHeader(realtype reltol, realtype abstol, realtype umax)
335 {
336   printf("\n2-D␣Advection-Diffusion␣Equation\n");
337   printf("Mesh␣dimensions␣=␣%d␣X␣%d\n", MX, MY);
338   printf("Total␣system␣size␣=␣%d\n", NEQ);
339 #if defined(SUNDIALS_EXTENDED_PRECISION)
340   printf("Tolerance␣parameters:␣reltol␣=␣%Lg␣␣␣abstol␣=␣%Lg\n\n", reltol, abstol);
341   printf("At␣t␣=␣%Lg␣␣␣␣␣␣max.norm(u)␣=%14.6Le␣\n", T0, umax);
342 #elif defined(SUNDIALS_DOUBLE_PRECISION)
343   printf("Tolerance␣parameters:␣reltol␣=␣%lg␣␣␣abstol␣=␣%lg\n\n", reltol, abstol);
344   printf("At␣t␣=␣%lg␣␣␣␣␣␣max.norm(u)␣=%14.6le␣\n", T0, umax);
345 #else
346   printf("Tolerance␣parameters:␣reltol␣=␣%g␣␣␣abstol␣=␣%g\n\n", reltol, abstol);
347   printf("At␣t␣=␣%g␣␣␣␣␣␣max.norm(u)␣=%14.6e␣\n", T0, umax);
348 #endif
349
350   return;
351 }
352
```

```
353  /* Print current value */
354
355  static void PrintOutput(realtype t, realtype umax, long int nst)
356  {
357  #if defined(SUNDIALS_EXTENDED_PRECISION)
358    printf("At␣t␣=␣%4.2Lf␣␣␣max.norm(u)␣=%14.6Le␣␣␣nst␣=␣%4ld\n", t, umax, nst);
359  #elif defined(SUNDIALS_DOUBLE_PRECISION)
360    printf("At␣t␣=␣%4.2f␣␣␣max.norm(u)␣=%14.6le␣␣␣nst␣=␣%4ld\n", t, umax, nst);
361  #else
362    printf("At␣t␣=␣%4.2f␣␣␣max.norm(u)␣=%14.6e␣␣␣nst␣=␣%4ld\n", t, umax, nst);
363  #endif
364
365    return;
366  }
367
368  /* Get and print some final statistics */
369
370  static void PrintFinalStats(void *cvode_mem)
371  {
372    int flag;
373    long int nst, nfe, nsetups, netf, nni, ncfn, nje, nfeLS;
374
375    flag = CVodeGetNumSteps(cvode_mem, &nst);
376    check_flag(&flag, "CVodeGetNumSteps", 1);
377    flag = CVodeGetNumRhsEvals(cvode_mem, &nfe);
378    check_flag(&flag, "CVodeGetNumRhsEvals", 1);
379    flag = CVodeGetNumLinSolvSetups(cvode_mem, &nsetups);
380    check_flag(&flag, "CVodeGetNumLinSolvSetups", 1);
381    flag = CVodeGetNumErrTestFails(cvode_mem, &netf);
382    check_flag(&flag, "CVodeGetNumErrTestFails", 1);
383    flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
384    check_flag(&flag, "CVodeGetNumNonlinSolvIters", 1);
385    flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);
386    check_flag(&flag, "CVodeGetNumNonlinSolvConvFails", 1);
387
388    flag = CVBandGetNumJacEvals(cvode_mem, &nje);
389    check_flag(&flag, "CVBandGetNumJacEvals", 1);
390    flag = CVBandGetNumRhsEvals(cvode_mem, &nfeLS);
391    check_flag(&flag, "CVBandGetNumRhsEvals", 1);
392
393    printf("\nFinal␣Statistics:\n");
394    printf("nst␣=␣%-6ld␣nfe␣␣=␣%-6ld␣nsetups␣=␣%-6ld␣nfeLS␣=␣%-6ld␣nje␣=␣%ld\n",
395           nst, nfe, nsetups, nfeLS, nje);
396    printf("nni␣=␣%-6ld␣ncfn␣=␣%-6ld␣netf␣=␣%ld\n␣\n",
397           nni, ncfn, netf);
398
399    return;
400  }
401
402  /* Check function return value...
403       opt == 0 means SUNDIALS function allocates memory so check if
404                returned NULL pointer
405       opt == 1 means SUNDIALS function returns a flag so check if
406                flag >= 0
407       opt == 2 means function allocates memory so check if returned
408                NULL pointer */
409
410  static int check_flag(void *flagvalue, char *funcname, int opt)
411  {
```

```
412   int *errflag;
413
414   /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
415
416   if (opt == 0 && flagvalue == NULL) {
417     fprintf(stderr, "\nSUNDIALS_ERROR: %s() failed - returned NULL pointer\n\n",
418             funcname);
419     return(1); }
420
421   /* Check if flag < 0 */
422
423   else if (opt == 1) {
424     errflag = (int *) flagvalue;
425     if (*errflag < 0) {
426       fprintf(stderr, "\nSUNDIALS_ERROR: %s() failed with flag = %d\n\n",
427               funcname, *errflag);
428       return(1); }}
429
430   /* Check if function returned NULL pointer - no memory allocated */
431
432   else if (opt == 2 && flagvalue == NULL) {
433     fprintf(stderr, "\nMEMORY_ERROR: %s() failed - returned NULL pointer\n\n",
434             funcname);
435     return(1); }
436
437   return(0);
438 }
```

C Listing of cvkryx.c

```
/*
 * -----------------------------------------------------------------
 * $Revision: 1.2 $
 * $Date: 2006/10/11 16:33:56 $
 * -----------------------------------------------------------------
 * Programmer(s): Scott D. Cohen, Alan C. Hindmarsh and
 *                Radu Serban @ LLNL
 * -----------------------------------------------------------------
 * Example problem:
 *
 * An ODE system is generated from the following 2-species diurnal
 * kinetics advection-diffusion PDE system in 2 space dimensions:
 *
 * dc(i)/dt = Kh*(d/dx)^2 c(i) + V*dc(i)/dx + (d/dy)(Kv(y)*dc(i)/dy)
 *                 + Ri(c1,c2,t)      for i = 1,2,   where
 *   R1(c1,c2,t) = -q1*c1*c3 - q2*c1*c2 + 2*q3(t)*c3 + q4(t)*c2 ,
 *   R2(c1,c2,t) =  q1*c1*c3 - q2*c1*c2 - q4(t)*c2 ,
 *   Kv(y) = Kv0*exp(y/5) ,
 * Kh, V, Kv0, q1, q2, and c3 are constants, and q3(t) and q4(t)
 * vary diurnally. The problem is posed on the square
 *   0 <= x <= 20,    30 <= y <= 50   (all in km),
 * with homogeneous Neumann boundary conditions, and for time t in
 *   0 <= t <= 86400 sec (1 day).
 * The PDE system is treated by central differences on a uniform
 * 10 x 10 mesh, with simple polynomial initial profiles.
 * The problem is solved with CVODE, with the BDF/GMRES
 * method (i.e. using the CVSPGMR linear solver) and the
 * block-diagonal part of the Newton matrix as a left
 * preconditioner. A copy of the block-diagonal part of the
 * Jacobian is saved and conditionally reused within the Precond
 * routine.
 * -----------------------------------------------------------------
 */

#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include <cvode/cvode.h>                 /* main integrator header file */
#include <cvode/cvode_spgmr.h>           /* prototypes & constants for CVSPGMR solver */
#include <nvector/nvector_serial.h>      /* serial N_Vector types, fct. and macros */
#include <sundials/sundials_smalldense.h> /* use generic DENSE solver in preconditioning */
#include <sundials/sundials_types.h>     /* definition of realtype */
#include <sundials/sundials_math.h>      /* contains the macros ABS, SQR, and EXP */

/* Problem Constants */

#define ZERO RCONST(0.0)
#define ONE  RCONST(1.0)
#define TWO  RCONST(2.0)

#define NUM_SPECIES  2                /* number of species         */
#define KH           RCONST(4.0e-6)   /* horizontal diffusivity Kh */
#define VEL          RCONST(0.001)    /* advection velocity V      */
#define KV0          RCONST(1.0e-8)   /* coefficient in Kv(y)      */
#define Q1           RCONST(1.63e-16) /* coefficients q1, q2, c3   */
#define Q2           RCONST(4.66e-16)
```

```
#define C3            RCONST(3.7e16)
#define A3            RCONST(22.62)     /* coefficient in expression for q3(t) */
#define A4            RCONST(7.601)     /* coefficient in expression for q4(t) */
#define C1_SCALE      RCONST(1.0e6)     /* coefficients in initial profiles
*/
#define C2_SCALE      RCONST(1.0e12)

#define T0            ZERO                 /* initial time */
#define NOUT          12                   /* number of output times */
#define TWOHR         RCONST(7200.0)       /* number of seconds in two hours  */
#define HALFDAY       RCONST(4.32e4)       /* number of seconds in a half day */
#define PI       RCONST(3.1415926535898)   /* pi */

#define XMIN          ZERO                 /* grid boundaries in x  */
#define XMAX          RCONST(20.0)
#define YMIN          RCONST(30.0)         /* grid boundaries in y  */
#define YMAX          RCONST(50.0)
#define XMID          RCONST(10.0)         /* grid midpoints in x,y */
#define YMID          RCONST(40.0)

#define MX            10             /* MX = number of x mesh points */
#define MY            10             /* MY = number of y mesh points */
#define NSMX          20             /* NSMX = NUM_SPECIES*MX */
#define MM            (MX*MY)        /* MM = MX*MY */

/* CVodeMalloc Constants */

#define RTOL    RCONST(1.0e-5)    /* scalar relative tolerance */
#define FLOOR   RCONST(100.0)     /* value of C1 or C2 at which tolerances */
                                  /* change from relative to absolute      */
#define ATOL    (RTOL*FLOOR)      /* scalar absolute tolerance */
#define NEQ     (NUM_SPECIES*MM)  /* NEQ = number of equations */

/* User-defined vector and matrix accessor macros: IJKth, IJth */

/* IJKth is defined in order to isolate the translation from the
   mathematical 3-dimensional structure of the dependent variable vector
   to the underlying 1-dimensional storage. IJth is defined in order to
   write code which indexes into small dense matrices with a (row,column)
   pair, where 1 <= row, column <= NUM_SPECIES.

   IJKth(vdata,i,j,k) references the element in the vdata array for
   species i at mesh point (j,k), where 1 <= i <= NUM_SPECIES,
   0 <= j <= MX-1, 0 <= k <= MY-1. The vdata array is obtained via
   the macro call vdata = NV_DATA_S(v), where v is an N_Vector.
   For each mesh point (j,k), the elements for species i and i+1 are
   contiguous within vdata.

   IJth(a,i,j) references the (i,j)th entry of the small matrix realtype **a,
   where 1 <= i,j <= NUM_SPECIES. The small matrix routines in dense.h
   work with matrices stored by column in a 2-dimensional array. In C,
   arrays are indexed starting at 0, not 1. */

#define IJKth(vdata,i,j,k) (vdata[i-1 + (j)*NUM_SPECIES + (k)*NSMX])
#define IJth(a,i,j)        (a[j-1][i-1])

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

```

```c
typedef struct {
  realtype **P[MX][MY], **Jbd[MX][MY];
  long int *pivot[MX][MY];
  realtype q4, om, dx, dy, hdco, haco, vdco;
} *UserData;

/* Private Helper Functions */

static UserData AllocUserData(void);
static void InitUserData(UserData data);
static void FreeUserData(UserData data);
static void SetInitialProfiles(N_Vector u, realtype dx, realtype dy);
static void PrintOutput(void *cvode_mem, N_Vector u, realtype t);
static void PrintFinalStats(void *cvode_mem);
static int check_flag(void *flagvalue, char *funcname, int opt);

/* Functions Called by the Solver */

static int f(realtype t, N_Vector u, N_Vector udot, void *f_data);

static int Precond(realtype tn, N_Vector u, N_Vector fu,
                   booleantype jok, booleantype *jcurPtr, realtype gamma,
                   void *P_data, N_Vector vtemp1, N_Vector vtemp2,
                   N_Vector vtemp3);

static int PSolve(realtype tn, N_Vector u, N_Vector fu,
                  N_Vector r, N_Vector z,
                  realtype gamma, realtype delta,
                  int lr, void *P_data, N_Vector vtemp);


/*
 *--------------------------------
 * Main Program
 *--------------------------------
 */

int main()
{
  realtype abstol, reltol, t, tout;
  N_Vector u;
  UserData data;
  void *cvode_mem;
  int iout, flag;

  u = NULL;
  data = NULL;
  cvode_mem = NULL;

  /* Allocate memory, and set problem data, initial values, tolerances */
  u = N_VNew_Serial(NEQ);
  if(check_flag((void *)u, "N_VNew_Serial", 0)) return(1);
  data = AllocUserData();
  if(check_flag((void *)data, "AllocUserData", 2)) return(1);
  InitUserData(data);
  SetInitialProfiles(u, data->dx, data->dy);
  abstol=ATOL;
  reltol=RTOL;

```

```
175    /* Call CvodeCreate to create the solver memory
176
177       CV_BDF     specifies the Backward Differentiation Formula
178       CV_NEWTON  specifies a Newton iteration
179
180       A pointer to the integrator memory is returned and stored in cvode_mem. */
181    cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
182    if(check_flag((void *)cvode_mem, "CVodeCreate", 0)) return(1);
183
184    /* Set the pointer to user-defined data */
185    flag = CVodeSetFdata(cvode_mem, data);
186    if(check_flag(&flag, "CVodeSetFdata", 1)) return(1);
187
188    /* Call CVodeMalloc to initialize the integrator memory:
189
190       f       is the user's right hand side function in u'=f(t,u)
191       T0      is the initial time
192       u       is the initial dependent variable vector
193       CV_SS   specifies scalar relative and absolute tolerances
194       reltol  is the relative tolerance
195       &abstol is a pointer to the scalar absolute tolerance      */
196    flag = CVodeMalloc(cvode_mem, f, T0, u, CV_SS, reltol, &abstol);
197    if(check_flag(&flag, "CVodeMalloc", 1)) return(1);
198
199    /* Call CVSpgmr to specify the linear solver CVSPGMR
200       with left preconditioning and the maximum Krylov dimension maxl */
201    flag = CVSpgmr(cvode_mem, PREC_LEFT, 0);
202    if(check_flag(&flag, "CVSpgmr", 1)) return(1);
203
204    /* Set modified Gram-Schmidt orthogonalization, preconditioner
205       setup and solve routines Precond and PSolve, and the pointer
206       to the user-defined block data */
207    flag = CVSpilsSetGSType(cvode_mem, MODIFIED_GS);
208    if(check_flag(&flag, "CVSpilsSetGSType", 1)) return(1);
209
210    flag = CVSpilsSetPreconditioner(cvode_mem, Precond, PSolve, data);
211    if(check_flag(&flag, "CVSpilsSetPreconditioner", 1)) return(1);
212
213    /* In loop over output points, call CVode, print results, test for error */
214    printf("␣\n2-species␣diurnal␣advection-diffusion␣problem\n\n");
215    for (iout=1, tout = TWOHR; iout <= NOUT; iout++, tout += TWOHR) {
216      flag = CVode(cvode_mem, tout, u, &t, CV_NORMAL);
217      PrintOutput(cvode_mem, u, t);
218      if(check_flag(&flag, "CVode", 1)) break;
219    }
220
221    PrintFinalStats(cvode_mem);
222
223    /* Free memory */
224    N_VDestroy_Serial(u);
225    FreeUserData(data);
226    CVodeFree(&cvode_mem);
227
228    return(0);
229  }
230
231  /*
232   *-------------------------------
233   * Private helper functions
```

```
234   *--------------------------------
235   */
236
237  /* Allocate memory for data structure of type UserData */
238
239  static UserData AllocUserData(void)
240  {
241    int jx, jy;
242    UserData data;
243
244    data = (UserData) malloc(sizeof *data);
245
246    for (jx=0; jx < MX; jx++) {
247      for (jy=0; jy < MY; jy++) {
248        (data->P)[jx][jy] = denalloc(NUM_SPECIES, NUM_SPECIES);
249        (data->Jbd)[jx][jy] = denalloc(NUM_SPECIES, NUM_SPECIES);
250        (data->pivot)[jx][jy] = denallocpiv(NUM_SPECIES);
251      }
252    }
253
254    return(data);
255  }
256
257  /* Load problem constants in data */
258
259  static void InitUserData(UserData data)
260  {
261    data->om = PI/HALFDAY;
262    data->dx = (XMAX-XMIN)/(MX-1);
263    data->dy = (YMAX-YMIN)/(MY-1);
264    data->hdco = KH/SQR(data->dx);
265    data->haco = VEL/(TWO*data->dx);
266    data->vdco = (ONE/SQR(data->dy))*KV0;
267  }
268
269  /* Free data memory */
270
271  static void FreeUserData(UserData data)
272  {
273    int jx, jy;
274
275    for (jx=0; jx < MX; jx++) {
276      for (jy=0; jy < MY; jy++) {
277        denfree((data->P)[jx][jy]);
278        denfree((data->Jbd)[jx][jy]);
279        denfreepiv((data->pivot)[jx][jy]);
280      }
281    }
282
283    free(data);
284  }
285
286  /* Set initial conditions in u */
287
288  static void SetInitialProfiles(N_Vector u, realtype dx, realtype dy)
289  {
290    int jx, jy;
291    realtype x, y, cx, cy;
292    realtype *udata;
```

```
293
294   /* Set pointer to data array in vector u. */
295
296   udata = NV_DATA_S(u);
297
298   /* Load initial profiles of c1 and c2 into u vector */
299
300   for (jy=0; jy < MY; jy++) {
301     y = YMIN + jy*dy;
302     cy = SQR(RCONST(0.1)*(y - YMID));
303     cy = ONE - cy + RCONST(0.5)*SQR(cy);
304     for (jx=0; jx < MX; jx++) {
305       x = XMIN + jx*dx;
306       cx = SQR(RCONST(0.1)*(x - XMID));
307       cx = ONE - cx + RCONST(0.5)*SQR(cx);
308       IJKth(udata,1,jx,jy) = C1_SCALE*cx*cy;
309       IJKth(udata,2,jx,jy) = C2_SCALE*cx*cy;
310     }
311   }
312 }
313
314 /* Print current t, step count, order, stepsize, and sampled c1,c2 values */
315
316 static void PrintOutput(void *cvode_mem, N_Vector u, realtype t)
317 {
318   long int nst;
319   int qu, flag;
320   realtype hu, *udata;
321   int mxh = MX/2 - 1, myh = MY/2 - 1, mx1 = MX - 1, my1 = MY - 1;
322
323   udata = NV_DATA_S(u);
324
325   flag = CVodeGetNumSteps(cvode_mem, &nst);
326   check_flag(&flag, "CVodeGetNumSteps", 1);
327   flag = CVodeGetLastOrder(cvode_mem, &qu);
328   check_flag(&flag, "CVodeGetLastOrder", 1);
329   flag = CVodeGetLastStep(cvode_mem, &hu);
330   check_flag(&flag, "CVodeGetLastStep", 1);
331
332 #if defined(SUNDIALS_EXTENDED_PRECISION)
333   printf("t␣=␣%.2Le␣␣␣no.␣steps␣=␣%ld␣␣␣order␣=␣%d␣␣␣stepsize␣=␣%.2Le\n",
334          t, nst, qu, hu);
335   printf("c1␣(bot.left/middle/top␣rt.)␣=␣%12.3Le␣␣%12.3Le␣␣%12.3Le\n",
336          IJKth(udata,1,0,0), IJKth(udata,1,mxh,myh), IJKth(udata,1,mx1,my1));
337   printf("c2␣(bot.left/middle/top␣rt.)␣=␣%12.3Le␣␣%12.3Le␣␣%12.3Le\n\n",
338          IJKth(udata,2,0,0), IJKth(udata,2,mxh,myh), IJKth(udata,2,mx1,my1));
339 #elif defined(SUNDIALS_DOUBLE_PRECISION)
340   printf("t␣=␣%.2le␣␣␣no.␣steps␣=␣%ld␣␣␣order␣=␣%d␣␣␣stepsize␣=␣%.2le\n",
341          t, nst, qu, hu);
342   printf("c1␣(bot.left/middle/top␣rt.)␣=␣%12.3le␣␣%12.3le␣␣%12.3le\n",
343          IJKth(udata,1,0,0), IJKth(udata,1,mxh,myh), IJKth(udata,1,mx1,my1));
344   printf("c2␣(bot.left/middle/top␣rt.)␣=␣%12.3le␣␣%12.3le␣␣%12.3le\n\n",
345          IJKth(udata,2,0,0), IJKth(udata,2,mxh,myh), IJKth(udata,2,mx1,my1));
346 #else
347   printf("t␣=␣%.2e␣␣␣no.␣steps␣=␣%ld␣␣␣order␣=␣%d␣␣␣stepsize␣=␣%.2e\n",
348          t, nst, qu, hu);
349   printf("c1␣(bot.left/middle/top␣rt.)␣=␣%12.3e␣␣%12.3e␣␣%12.3e\n",
350          IJKth(udata,1,0,0), IJKth(udata,1,mxh,myh), IJKth(udata,1,mx1,my1));
351   printf("c2␣(bot.left/middle/top␣rt.)␣=␣%12.3e␣␣%12.3e␣␣%12.3e\n\n",
```

```
352           IJKth(udata,2,0,0), IJKth(udata,2,mxh,myh), IJKth(udata,2,mx1,my1));
353 #endif
354 }
355
356 /* Get and print final statistics */
357
358 static void PrintFinalStats(void *cvode_mem)
359 {
360   long int lenrw, leniw ;
361   long int lenrwLS, leniwLS;
362   long int nst, nfe, nsetups, nni, ncfn, netf;
363   long int nli, npe, nps, ncfl, nfeLS;
364   int flag;
365
366   flag = CVodeGetWorkSpace(cvode_mem, &lenrw, &leniw);
367   check_flag(&flag, "CVodeGetWorkSpace", 1);
368   flag = CVodeGetNumSteps(cvode_mem, &nst);
369   check_flag(&flag, "CVodeGetNumSteps", 1);
370   flag = CVodeGetNumRhsEvals(cvode_mem, &nfe);
371   check_flag(&flag, "CVodeGetNumRhsEvals", 1);
372   flag = CVodeGetNumLinSolvSetups(cvode_mem, &nsetups);
373   check_flag(&flag, "CVodeGetNumLinSolvSetups", 1);
374   flag = CVodeGetNumErrTestFails(cvode_mem, &netf);
375   check_flag(&flag, "CVodeGetNumErrTestFails", 1);
376   flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
377   check_flag(&flag, "CVodeGetNumNonlinSolvIters", 1);
378   flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);
379   check_flag(&flag, "CVodeGetNumNonlinSolvConvFails", 1);
380
381   flag = CVSpilsGetWorkSpace(cvode_mem, &lenrwLS, &leniwLS);
382   check_flag(&flag, "CVSpilsGetWorkSpace", 1);
383   flag = CVSpilsGetNumLinIters(cvode_mem, &nli);
384   check_flag(&flag, "CVSpilsGetNumLinIters", 1);
385   flag = CVSpilsGetNumPrecEvals(cvode_mem, &npe);
386   check_flag(&flag, "CVSpilsGetNumPrecEvals", 1);
387   flag = CVSpilsGetNumPrecSolves(cvode_mem, &nps);
388   check_flag(&flag, "CVSpilsGetNumPrecSolves", 1);
389   flag = CVSpilsGetNumConvFails(cvode_mem, &ncfl);
390   check_flag(&flag, "CVSpilsGetNumConvFails", 1);
391   flag = CVSpilsGetNumRhsEvals(cvode_mem, &nfeLS);
392   check_flag(&flag, "CVSpilsGetNumRhsEvals", 1);
393
394   printf("\nFinal␣Statistics..␣\n\n");
395   printf("lenrw␣␣␣=␣%5ld␣␣␣␣␣leniw␣␣␣=␣%5ld\n", lenrw, leniw);
396   printf("lenrwLS␣=␣%5ld␣␣␣␣␣leniwLS␣=␣%5ld\n", lenrwLS, leniwLS);
397   printf("nst␣␣␣␣␣=␣%5ld\n"                    , nst);
398   printf("nfe␣␣␣␣␣=␣%5ld␣␣␣␣␣nfeLS␣␣␣=␣%5ld\n"  , nfe, nfeLS);
399   printf("nni␣␣␣␣␣=␣%5ld␣␣␣␣␣nli␣␣␣␣␣=␣%5ld\n"  , nni, nli);
400   printf("nsetups␣=␣%5ld␣␣␣␣␣netf␣␣␣␣=␣%5ld\n"  , nsetups, netf);
401   printf("npe␣␣␣␣␣=␣%5ld␣␣␣␣␣nps␣␣␣␣␣=␣%5ld\n"  , npe, nps);
402   printf("ncfn␣␣␣␣=␣%5ld␣␣␣␣␣ncfl␣␣␣␣=␣%5ld\n\n", ncfn, ncfl);
403 }
404
405 /* Check function return value...
406      opt == 0 means SUNDIALS function allocates memory so check if
407              returned NULL pointer
408      opt == 1 means SUNDIALS function returns a flag so check if
409              flag >= 0
410      opt == 2 means function allocates memory so check if returned
```

```
411               NULL pointer */
412
413  static int check_flag(void *flagvalue, char *funcname, int opt)
414  {
415    int *errflag;
416
417    /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
418    if (opt == 0 && flagvalue == NULL) {
419      fprintf(stderr, "\nSUNDIALS_ERROR:␣%s()␣failed␣-␣returned␣NULL␣pointer\n\n",
420              funcname);
421      return(1); }
422
423    /* Check if flag < 0 */
424    else if (opt == 1) {
425      errflag = (int *) flagvalue;
426      if (*errflag < 0) {
427        fprintf(stderr, "\nSUNDIALS_ERROR:␣%s()␣failed␣with␣flag␣=␣%d\n\n",
428                funcname, *errflag);
429        return(1); }}
430
431    /* Check if function returned NULL pointer - no memory allocated */
432    else if (opt == 2 && flagvalue == NULL) {
433      fprintf(stderr, "\nMEMORY_ERROR:␣%s()␣failed␣-␣returned␣NULL␣pointer\n\n",
434              funcname);
435      return(1); }
436
437    return(0);
438  }
439
440  /*
441   *-------------------------------
442   * Functions called by the solver
443   *-------------------------------
444   */
445
446  /* f routine. Compute RHS function f(t,u). */
447
448  static int f(realtype t, N_Vector u, N_Vector udot, void *f_data)
449  {
450    realtype q3, c1, c2, c1dn, c2dn, c1up, c2up, c1lt, c2lt;
451    realtype c1rt, c2rt, cydn, cyup, hord1, hord2, horad1, horad2;
452    realtype qq1, qq2, qq3, qq4, rkin1, rkin2, s, vertd1, vertd2, ydn, yup;
453    realtype q4coef, dely, verdco, hordco, horaco;
454    realtype *udata, *dudata;
455    int jx, jy, idn, iup, ileft, iright;
456    UserData data;
457
458    data = (UserData) f_data;
459    udata = NV_DATA_S(u);
460    dudata = NV_DATA_S(udot);
461
462    /* Set diurnal rate coefficients. */
463
464    s = sin(data->om*t);
465    if (s > ZERO) {
466      q3 = EXP(-A3/s);
467      data->q4 = EXP(-A4/s);
468    } else {
469        q3 = ZERO;
```

```
470         data->q4 = ZERO;
471     }
472
473     /* Make local copies of problem variables, for efficiency. */
474
475     q4coef = data->q4;
476     dely = data->dy;
477     verdco = data->vdco;
478     hordco  = data->hdco;
479     horaco  = data->haco;
480
481     /* Loop over all grid points. */
482
483     for (jy=0; jy < MY; jy++) {
484
485       /* Set vertical diffusion coefficients at jy +- 1/2 */
486
487       ydn = YMIN + (jy - RCONST(0.5))*dely;
488       yup = ydn + dely;
489       cydn = verdco*EXP(RCONST(0.2)*ydn);
490       cyup = verdco*EXP(RCONST(0.2)*yup);
491       idn = (jy == 0) ? 1 : -1;
492       iup = (jy == MY-1) ? -1 : 1;
493       for (jx=0; jx < MX; jx++) {
494
495         /* Extract c1 and c2, and set kinetic rate terms. */
496
497         c1 = IJKth(udata,1,jx,jy);
498         c2 = IJKth(udata,2,jx,jy);
499         qq1 = Q1*c1*C3;
500         qq2 = Q2*c1*c2;
501         qq3 = q3*C3;
502         qq4 = q4coef*c2;
503         rkin1 = -qq1 - qq2 + TWO*qq3 + qq4;
504         rkin2 = qq1 - qq2 - qq4;
505
506         /* Set vertical diffusion terms. */
507
508         c1dn = IJKth(udata,1,jx,jy+idn);
509         c2dn = IJKth(udata,2,jx,jy+idn);
510         c1up = IJKth(udata,1,jx,jy+iup);
511         c2up = IJKth(udata,2,jx,jy+iup);
512         vertd1 = cyup*(c1up - c1) - cydn*(c1 - c1dn);
513         vertd2 = cyup*(c2up - c2) - cydn*(c2 - c2dn);
514
515         /* Set horizontal diffusion and advection terms. */
516
517         ileft = (jx == 0) ? 1 : -1;
518         iright =(jx == MX-1) ? -1 : 1;
519         c1lt = IJKth(udata,1,jx+ileft,jy);
520         c2lt = IJKth(udata,2,jx+ileft,jy);
521         c1rt = IJKth(udata,1,jx+iright,jy);
522         c2rt = IJKth(udata,2,jx+iright,jy);
523         hord1 = hordco*(c1rt - TWO*c1 + c1lt);
524         hord2 = hordco*(c2rt - TWO*c2 + c2lt);
525         horad1 = horaco*(c1rt - c1lt);
526         horad2 = horaco*(c2rt - c2lt);
527
528         /* Load all terms into udot. */
```

```
529
530         IJKth(dudata, 1, jx, jy) = vertd1 + hord1 + horad1 + rkin1;
531         IJKth(dudata, 2, jx, jy) = vertd2 + hord2 + horad2 + rkin2;
532       }
533     }
534
535     return(0);
536   }
537
538   /* Preconditioner setup routine. Generate and preprocess P. */
539
540   static int Precond(realtype tn, N_Vector u, N_Vector fu,
541                      booleantype jok, booleantype *jcurPtr, realtype gamma,
542                      void *P_data, N_Vector vtemp1, N_Vector vtemp2,
543                      N_Vector vtemp3)
544   {
545     realtype c1, c2, cydn, cyup, diag, ydn, yup, q4coef, dely, verdco, hordco;
546     realtype **(*P)[MY], **(*Jbd)[MY];
547     long int *(*pivot)[MY], ier;
548     int jx, jy;
549     realtype *udata, **a, **j;
550     UserData data;
551
552     /* Make local copies of pointers in P_data, and of pointer to u's data */
553
554     data = (UserData) P_data;
555     P = data->P;
556     Jbd = data->Jbd;
557     pivot = data->pivot;
558     udata = NV_DATA_S(u);
559
560     if (jok) {
561
562       /* jok = TRUE: Copy Jbd to P */
563
564       for (jy=0; jy < MY; jy++)
565         for (jx=0; jx < MX; jx++)
566           dencopy(Jbd[jx][jy], P[jx][jy], NUM_SPECIES, NUM_SPECIES);
567
568       *jcurPtr = FALSE;
569
570     }
571
572     else {
573       /* jok = FALSE: Generate Jbd from scratch and copy to P */
574
575       /* Make local copies of problem variables, for efficiency. */
576
577       q4coef = data->q4;
578       dely = data->dy;
579       verdco = data->vdco;
580       hordco  = data->hdco;
581
582       /* Compute 2x2 diagonal Jacobian blocks (using q4 values
583          computed on the last f call).  Load into P. */
584
585       for (jy=0; jy < MY; jy++) {
586         ydn = YMIN + (jy - RCONST(0.5))*dely;
587         yup = ydn + dely;
```

```
588         cydn = verdco*EXP(RCONST(0.2)*ydn);
589         cyup = verdco*EXP(RCONST(0.2)*yup);
590         diag = -(cydn + cyup + TWO*hordco);
591         for (jx=0; jx < MX; jx++) {
592           c1 = IJKth(udata,1,jx,jy);
593           c2 = IJKth(udata,2,jx,jy);
594           j = Jbd[jx][jy];
595           a = P[jx][jy];
596           IJth(j,1,1) = (-Q1*C3 - Q2*c2) + diag;
597           IJth(j,1,2) = -Q2*c1 + q4coef;
598           IJth(j,2,1) = Q1*C3 - Q2*c2;
599           IJth(j,2,2) = (-Q2*c1 - q4coef) + diag;
600           dencopy(j, a, NUM_SPECIES, NUM_SPECIES);
601         }
602       }
603
604       *jcurPtr = TRUE;
605
606     }
607
608     /* Scale by -gamma */
609
610     for (jy=0; jy < MY; jy++)
611       for (jx=0; jx < MX; jx++)
612         denscale(-gamma, P[jx][jy], NUM_SPECIES, NUM_SPECIES);
613
614     /* Add identity matrix and do LU decompositions on blocks in place. */
615
616     for (jx=0; jx < MX; jx++) {
617       for (jy=0; jy < MY; jy++) {
618         denaddI(P[jx][jy], NUM_SPECIES);
619         ier = denGETRF(P[jx][jy], NUM_SPECIES, NUM_SPECIES, pivot[jx][jy]);
620         if (ier != 0) return(1);
621       }
622     }
623
624     return(0);
625   }
626
627   /* Preconditioner solve routine */
628
629   static int PSolve(realtype tn, N_Vector u, N_Vector fu,
630                     N_Vector r, N_Vector z,
631                     realtype gamma, realtype delta,
632                     int lr, void *P_data, N_Vector vtemp)
633   {
634     realtype **(*P)[MY];
635     long int *(*pivot)[MY];
636     int jx, jy;
637     realtype *zdata, *v;
638     UserData data;
639
640     /* Extract the P and pivot arrays from P_data. */
641
642     data = (UserData) P_data;
643     P = data->P;
644     pivot = data->pivot;
645     zdata = NV_DATA_S(z);
646
```

```
647     N_VScale(ONE, r, z);
648
649     /* Solve the block-diagonal system Px = r using LU factors stored
650        in P and pivot data in pivot, and return the solution in z. */
651
652     for (jx=0; jx < MX; jx++) {
653       for (jy=0; jy < MY; jy++) {
654         v = &(IJKth(zdata, 1, jx, jy));
655         denGETRS(P[jx][jy], NUM_SPECIES, pivot[jx][jy], v);
656       }
657     }
658
659     return(0);
660   }
```

D Listing of cvnonx_p.c

```
/*
 * -----------------------------------------------------------------
 * $Revision: 1.1 $
 * $Date: 2006/07/05 15:50:05 $
 * -----------------------------------------------------------------
 * Programmer(s): Scott D. Cohen, Alan C. Hindmarsh, George Byrne,
 *                and Radu Serban @ LLNL
 * -----------------------------------------------------------------
 * Example problem:
 *
 * The following is a simple example problem, with the program for
 * its solution by CVODE. The problem is the semi-discrete
 * form of the advection-diffusion equation in 1-D:
 *   du/dt = d^2 u / dx^2 + .5 du/dx
 * on the interval 0 <= x <= 2, and the time interval 0 <= t <= 5.
 * Homogeneous Dirichlet boundary conditions are posed, and the
 * initial condition is the following:
 *   u(x,t=0) = x(2-x)exp(2x) .
 * The PDE is discretized on a uniform grid of size MX+2 with
 * central differencing, and with boundary values eliminated,
 * leaving an ODE system of size NEQ = MX.
 * This program solves the problem with the option for nonstiff
 * systems: ADAMS method and functional iteration.
 * It uses scalar relative and absolute tolerances.
 * Output is printed at t = .5, 1.0, ..., 5.
 * Run statistics (optional outputs) are printed at the end.
 *
 * This version uses MPI for user routines.
 * Execute with Number of Processors = N,  with 1 <= N <= MX.
 * -----------------------------------------------------------------
 */

#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include <cvode/cvode.h>               /* prototypes for CVODE fcts. */
#include <nvector/nvector_parallel.h> /* definition of N_Vector and macros */
#include <sundials/sundials_types.h>  /* definition of realtype */
#include <sundials/sundials_math.h>   /* definition of EXP */

#include <mpi.h>                       /* MPI constants and types */

/* Problem Constants */

#define ZERO  RCONST(0.0)

#define XMAX  RCONST(2.0)    /* domain boundary           */
#define MX    10             /* mesh dimension            */
#define NEQ   MX             /* number of equations       */
#define ATOL  RCONST(1.0e-5) /* scalar absolute tolerance */
#define T0    ZERO           /* initial time              */
#define T1    RCONST(0.5)    /* first output time         */
#define DTOUT RCONST(0.5)    /* output time increment     */
#define NOUT  10             /* number of output times    */

/* Type : UserData
```

```
58     contains grid constants, parallel machine parameters, work array. */
59
60  typedef struct {
61    realtype dx, hdcoef, hacoef;
62    int npes, my_pe;
63    MPI_Comm comm;
64    realtype z[100];
65  } *UserData;
66
67  /* Private Helper Functions */
68
69  static void SetIC(N_Vector u, realtype dx, long int my_length,
70                    long int my_base);
71
72  static void PrintIntro(int npes);
73
74  static void PrintData(realtype t, realtype umax, long int nst);
75
76  static void PrintFinalStats(void *cvode_mem);
77
78  /* Functions Called by the Solver */
79
80  static int f(realtype t, N_Vector u, N_Vector udot, void *f_data);
81
82  /* Private function to check function return values */
83
84  static int check_flag(void *flagvalue, char *funcname, int opt, int id);
85
86  /***************************** Main Program ****************************/
87
88  int main(int argc, char *argv[])
89  {
90    realtype dx, reltol, abstol, t, tout, umax;
91    N_Vector u;
92    UserData data;
93    void *cvode_mem;
94    int iout, flag, my_pe, npes;
95    long int local_N, nperpe, nrem, my_base, nst;
96
97    MPI_Comm comm;
98
99    u = NULL;
100   data = NULL;
101   cvode_mem = NULL;
102
103   /* Get processor number, total number of pe's, and my_pe. */
104   MPI_Init(&argc, &argv);
105   comm = MPI_COMM_WORLD;
106   MPI_Comm_size(comm, &npes);
107   MPI_Comm_rank(comm, &my_pe);
108
109   /* Set local vector length. */
110   nperpe = NEQ/npes;
111   nrem = NEQ - npes*nperpe;
112   local_N = (my_pe < nrem) ? nperpe+1 : nperpe;
113   my_base = (my_pe < nrem) ? my_pe*local_N : my_pe*nperpe + nrem;
114
115   data = (UserData) malloc(sizeof *data);  /* Allocate data memory */
116   if(check_flag((void *)data, "malloc", 2, my_pe)) MPI_Abort(comm, 1);
```

```
117
118     data->comm = comm;
119     data->npes = npes;
120     data->my_pe = my_pe;
121
122     u = N_VNew_Parallel(comm, local_N, NEQ);  /* Allocate u vector */
123     if(check_flag((void *)u, "N_VNew", 0, my_pe)) MPI_Abort(comm, 1);
124
125     reltol = ZERO;  /* Set the tolerances */
126     abstol = ATOL;
127
128     dx = data->dx = XMAX/((realtype)(MX+1));  /* Set grid coefficients in data */
129     data->hdcoef = RCONST(1.0)/(dx*dx);
130     data->hacoef = RCONST(0.5)/(RCONST(2.0)*dx);
131
132     SetIC(u, dx, local_N, my_base);  /* Initialize u vector */
133
134     /*
135        Call CVodeCreate to create the solver memory:
136
137        CV_ADAMS   specifies the Adams Method
138        CV_FUNCTIONAL  specifies functional iteration
139
140        A pointer to the integrator memory is returned and stored in cvode_mem.
141     */
142
143     cvode_mem = CVodeCreate(CV_ADAMS, CV_FUNCTIONAL);
144     if(check_flag((void *)cvode_mem, "CVodeCreate", 0, my_pe)) MPI_Abort(comm, 1);
145
146     flag = CVodeSetFdata(cvode_mem, data);
147     if(check_flag(&flag, "CVodeSetFdata", 1, my_pe)) MPI_Abort(comm, 1);
148
149     /*
150        Call CVodeMalloc to initialize the integrator memory:
151
152        cvode_mem is the pointer to the integrator memory returned by CVodeCreate
153        f       is the user's right hand side function in y'=f(t,y)
154        T0      is the initial time
155        u       is the initial dependent variable vector
156        CV_SS   specifies scalar relative and absolute tolerances
157        reltol  is the relative tolerance
158        &abstol is a pointer to the scalar absolute tolerance
159     */
160
161     flag = CVodeMalloc(cvode_mem, f, T0, u, CV_SS, reltol, &abstol);
162     if(check_flag(&flag, "CVodeMalloc", 1, my_pe)) MPI_Abort(comm, 1);
163
164     if (my_pe == 0) PrintIntro(npes);
165
166     umax = N_VMaxNorm(u);
167
168     if (my_pe == 0) {
169       t = T0;
170       PrintData(t, umax, 0);
171     }
172
173     /* In loop over output points, call CVode, print results, test for error */
174
175     for (iout=1, tout=T1; iout <= NOUT; iout++, tout += DTOUT) {
```

```
176       flag = CVode(cvode_mem, tout, u, &t, CV_NORMAL);
177       if(check_flag(&flag, "CVode", 1, my_pe)) break;
178       umax = N_VMaxNorm(u);
179       flag = CVodeGetNumSteps(cvode_mem, &nst);
180       check_flag(&flag, "CVodeGetNumSteps", 1, my_pe);
181       if (my_pe == 0) PrintData(t, umax, nst);
182     }
183
184     if (my_pe == 0)
185       PrintFinalStats(cvode_mem);  /* Print some final statistics */
186
187     N_VDestroy_Parallel(u);        /* Free the u vector */
188     CVodeFree(&cvode_mem);         /* Free the integrator memory */
189     free(data);                    /* Free user data */
190
191     MPI_Finalize();
192
193     return(0);
194   }
195
196   /*********************** Private Helper Functions ***********************/
197
198   /* Set initial conditions in u vector */
199
200   static void SetIC(N_Vector u, realtype dx, long int my_length,
201                     long int my_base)
202   {
203     int i;
204     long int iglobal;
205     realtype x;
206     realtype *udata;
207
208     /* Set pointer to data array and get local length of u. */
209     udata = NV_DATA_P(u);
210     my_length = NV_LOCLENGTH_P(u);
211
212     /* Load initial profile into u vector */
213     for (i=1; i<=my_length; i++) {
214       iglobal = my_base + i;
215       x = iglobal*dx;
216       udata[i-1] = x*(XMAX - x)*EXP(RCONST(2.0)*x);
217     }
218   }
219
220   /* Print problem introduction */
221
222   static void PrintIntro(int npes)
223   {
224     printf("\n␣1-D␣advection-diffusion␣equation,␣mesh␣size␣=%3d␣\n", MX);
225     printf("\n␣Number␣of␣PEs␣=␣%3d␣\n\n", npes);
226
227     return;
228   }
229
230   /* Print data */
231
232   static void PrintData(realtype t, realtype umax, long int nst)
233   {
234
```

```
#if defined(SUNDIALS_EXTENDED_PRECISION)
  printf("At t = %4.2Lf  max.norm(u) = %14.6Le  nst = %4ld \n", t, umax, nst);
#elif defined(SUNDIALS_DOUBLE_PRECISION)
  printf("At t = %4.2f  max.norm(u) = %14.6le  nst = %4ld \n", t, umax, nst);
#else
  printf("At t = %4.2f  max.norm(u) = %14.6e  nst = %4ld \n", t, umax, nst);
#endif

  return;
}

/* Print some final statistics located in the iopt array */

static void PrintFinalStats(void *cvode_mem)
{
  long int nst, nfe, nni, ncfn, netf;
  int flag;

  flag = CVodeGetNumSteps(cvode_mem, &nst);
  check_flag(&flag, "CVodeGetNumSteps", 1, 0);
  flag = CVodeGetNumRhsEvals(cvode_mem, &nfe);
  check_flag(&flag, "CVodeGetNumRhsEvals", 1, 0);
  flag = CVodeGetNumErrTestFails(cvode_mem, &netf);
  check_flag(&flag, "CVodeGetNumErrTestFails", 1, 0);
  flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
  check_flag(&flag, "CVodeGetNumNonlinSolvIters", 1, 0);
  flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);
  check_flag(&flag, "CVodeGetNumNonlinSolvConvFails", 1, 0);

  printf("\nFinal Statistics: \n\n");
  printf("nst = %-6ld  nfe  = %-6ld  ", nst, nfe);
  printf("nni = %-6ld  ncfn = %-6ld  netf = %ld \n \n", nni, ncfn, netf);
}

/***************** Function Called by the Solver ***********************/

/* f routine. Compute f(t,u). */

static int f(realtype t, N_Vector u, N_Vector udot, void *f_data)
{
  realtype ui, ult, urt, hordc, horac, hdiff, hadv;
  realtype *udata, *dudata, *z;
  int i;
  int npes, my_pe, my_length, my_pe_m1, my_pe_p1, last_pe, my_last;
  UserData data;
  MPI_Status status;
  MPI_Comm comm;

  udata = NV_DATA_P(u);
  dudata = NV_DATA_P(udot);

  /* Extract needed problem constants from data */
  data = (UserData) f_data;
  hordc = data->hdcoef;
  horac = data->hacoef;

  /* Extract parameters for parallel computation. */
  comm = data->comm;
  npes = data->npes;           /* Number of processes. */
```

```
294   my_pe = data->my_pe;          /* Current process number. */
295   my_length = NV_LOCLENGTH_P(u); /* Number of local elements of u. */
296   z = data->z;
297
298   /* Compute related parameters. */
299   my_pe_m1 = my_pe - 1;
300   my_pe_p1 = my_pe + 1;
301   last_pe = npes - 1;
302   my_last = my_length - 1;
303
304   /* Store local segment of u in the working array z. */
305    for (i = 1; i <= my_length; i++)
306      z[i] = udata[i - 1];
307
308   /* Pass needed data to processes before and after current process. */
309    if (my_pe != 0)
310      MPI_Send(&z[1], 1, PVEC_REAL_MPI_TYPE, my_pe_m1, 0, comm);
311    if (my_pe != last_pe)
312      MPI_Send(&z[my_length], 1, PVEC_REAL_MPI_TYPE, my_pe_p1, 0, comm);
313
314   /* Receive needed data from processes before and after current process. */
315    if (my_pe != 0)
316      MPI_Recv(&z[0], 1, PVEC_REAL_MPI_TYPE, my_pe_m1, 0, comm, &status);
317    else z[0] = ZERO;
318    if (my_pe != last_pe)
319      MPI_Recv(&z[my_length+1], 1, PVEC_REAL_MPI_TYPE, my_pe_p1, 0, comm,
320               &status);
321    else z[my_length + 1] = ZERO;
322
323   /* Loop over all grid points in current process. */
324   for (i=1; i<=my_length; i++) {
325
326     /* Extract u at x_i and two neighboring points */
327     ui = z[i];
328     ult = z[i-1];
329     urt = z[i+1];
330
331     /* Set diffusion and advection terms and load into udot */
332     hdiff = hordc*(ult - RCONST(2.0)*ui + urt);
333     hadv = horac*(urt - ult);
334     dudata[i-1] = hdiff + hadv;
335   }
336
337   return(0);
338 }
339
340 /* Check function return value...
341      opt == 0 means SUNDIALS function allocates memory so check if
342               returned NULL pointer
343      opt == 1 means SUNDIALS function returns a flag so check if
344               flag >= 0
345      opt == 2 means function allocates memory so check if returned
346               NULL pointer */
347
348 static int check_flag(void *flagvalue, char *funcname, int opt, int id)
349 {
350   int *errflag;
351
352   /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
```

```
353   if (opt == 0 && flagvalue == NULL) {
354     fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n",
355             id, funcname);
356     return(1); }
357
358   /* Check if flag < 0 */
359   else if (opt == 1) {
360     errflag = (int *) flagvalue;
361     if (*errflag < 0) {
362       fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with flag = %d\n\n",
363               id, funcname, *errflag);
364       return(1); }}
365
366   /* Check if function returned NULL pointer - no memory allocated */
367   else if (opt == 2 && flagvalue == NULL) {
368     fprintf(stderr, "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n",
369             id, funcname);
370     return(1); }
371
372   return(0);
373 }
```

E Listing of cvkryx_p.c

```
/*
 * -----------------------------------------------------------------
 * $Revision: 1.2 $
 * $Date: 2006/10/11 16:33:55 $
 * -----------------------------------------------------------------
 * Programmer(s): S. D. Cohen, A. C. Hindmarsh, M. R. Wittman, and
 *                Radu Serban  @ LLNL
 * -----------------------------------------------------------------
 * Example problem:
 *
 * An ODE system is generated from the following 2-species diurnal
 * kinetics advection-diffusion PDE system in 2 space dimensions:
 *
 * dc(i)/dt = Kh*(d/dx)^2 c(i) + V*dc(i)/dx + (d/dy)(Kv(y)*dc(i)/dy)
 *                 + Ri(c1,c2,t)      for i = 1,2,   where
 *   R1(c1,c2,t) = -q1*c1*c3 - q2*c1*c2 + 2*q3(t)*c3 + q4(t)*c2 ,
 *   R2(c1,c2,t) =  q1*c1*c3 - q2*c1*c2 - q4(t)*c2 ,
 *   Kv(y) = Kv0*exp(y/5) ,
 * Kh, V, Kv0, q1, q2, and c3 are constants, and q3(t) and q4(t)
 * vary diurnally. The problem is posed on the square
 *   0 <= x <= 20,    30 <= y <= 50   (all in km),
 * with homogeneous Neumann boundary conditions, and for time t in
 *   0 <= t <= 86400 sec (1 day).
 * The PDE system is treated by central differences on a uniform
 * mesh, with simple polynomial initial profiles.
 *
 * The problem is solved by CVODE on NPE processors, treated
 * as a rectangular process grid of size NPEX by NPEY, with
 * NPE = NPEX*NPEY. Each processor contains a subgrid of size MXSUB
 * by MYSUB of the (x,y) mesh.  Thus the actual mesh sizes are
 * MX = MXSUB*NPEX and MY = MYSUB*NPEY, and the ODE system size is
 * neq = 2*MX*MY.
 *
 * The solution is done with the BDF/GMRES method (i.e. using the
 * CVSPGMR linear solver) and the block-diagonal part of the
 * Newton matrix as a left preconditioner. A copy of the
 * block-diagonal part of the Jacobian is saved and conditionally
 * reused within the preconditioner routine.
 *
 * Performance data and sampled solution values are printed at
 * selected output times, and all performance counters are printed
 * on completion.
 *
 * This version uses MPI for user routines.
 *
 * Execution: mpirun -np N cvkryx_p   with N = NPEX*NPEY (see
 * constants below).
 * -----------------------------------------------------------------
 */

#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include <cvode/cvode.h>                /* prototypes for CVODE fcts. */
#include <cvode/cvode_spgmr.h>          /* prototypes and constants for CVSPGMR solver */
```

```
#include <nvector/nvector_parallel.h>     /* definition N_Vector and macro NV_DATA_P
*/
#include <sundials/sundials_smalldense.h> /* prototypes for small dense matrix fcts. */
#include <sundials/sundials_types.h>      /* definitions of realtype, booleantype */
#include <sundials/sundials_math.h>       /* definition of macros SQR and EXP */

#include <mpi.h>                          /* MPI constants and types */

/* Problem Constants */

#define NVARS        2                    /* number of species         */
#define KH           RCONST(4.0e-6)       /* horizontal diffusivity Kh */
#define VEL          RCONST(0.001)        /* advection velocity V      */
#define KV0          RCONST(1.0e-8)       /* coefficient in Kv(y)      */
#define Q1           RCONST(1.63e-16)     /* coefficients q1, q2, c3   */
#define Q2           RCONST(4.66e-16)
#define C3           RCONST(3.7e16)
#define A3           RCONST(22.62)     /* coefficient in expression for q3(t) */
#define A4           RCONST(7.601)     /* coefficient in expression for q4(t) */
#define C1_SCALE     RCONST(1.0e6)     /* coefficients in initial profiles
*/
#define C2_SCALE     RCONST(1.0e12)

#define T0           RCONST(0.0)          /* initial time */
#define NOUT         12                   /* number of output times */
#define TWOHR        RCONST(7200.0)       /* number of seconds in two hours  */
#define HALFDAY      RCONST(4.32e4)       /* number of seconds in a half day */
#define PI       RCONST(3.1415926535898)  /* pi */

#define XMIN         RCONST(0.0)          /* grid boundaries in x  */
#define XMAX         RCONST(20.0)
#define YMIN         RCONST(30.0)         /* grid boundaries in y  */
#define YMAX         RCONST(50.0)

#define NPEX         2              /* no. PEs in x direction of PE array */
#define NPEY         2              /* no. PEs in y direction of PE array */
                                    /* Total no. PEs = NPEX*NPEY */
#define MXSUB        5              /* no. x points per subgrid */
#define MYSUB        5              /* no. y points per subgrid */

#define MX           (NPEX*MXSUB)   /* MX = number of x mesh points */
#define MY           (NPEY*MYSUB)   /* MY = number of y mesh points */
                                    /* Spatial mesh is MX by MY */
/* CVodeMalloc Constants */

#define RTOL    RCONST(1.0e-5)    /* scalar relative tolerance */
#define FLOOR   RCONST(100.0)     /* value of C1 or C2 at which tolerances */
                                  /* change from relative to absolute      */
#define ATOL    (RTOL*FLOOR)      /* scalar absolute tolerance */


/* User-defined matrix accessor macro: IJth */

/* IJth is defined in order to write code which indexes into small dense
   matrices with a (row,column) pair, where 1 <= row,column <= NVARS.

   IJth(a,i,j) references the (i,j)th entry of the small matrix realtype **a,
   where 1 <= i,j <= NVARS. The small matrix routines in dense.h
   work with matrices stored by column in a 2-dimensional array. In C,
```

```
114     arrays are indexed starting at 0, not 1. */
115
116  #define IJth(a,i,j) (a[j-1][i-1])
117
118  /* Type : UserData
119     contains problem constants, preconditioner blocks, pivot arrays,
120     grid constants, and processor indices */
121
122  typedef struct {
123    realtype q4, om, dx, dy, hdco, haco, vdco;
124    realtype uext[NVARS*(MXSUB+2)*(MYSUB+2)];
125    int my_pe, isubx, isuby;
126    long int nvmxsub, nvmxsub2;
127    MPI_Comm comm;
128  } *UserData;
129
130  typedef struct {
131    void *f_data;
132    realtype **P[MXSUB][MYSUB], **Jbd[MXSUB][MYSUB];
133    long int *pivot[MXSUB][MYSUB];
134  } *PreconData;
135
136
137  /* Private Helper Functions */
138
139  static PreconData AllocPreconData(UserData data);
140  static void InitUserData(int my_pe, MPI_Comm comm, UserData data);
141  static void FreePreconData(PreconData pdata);
142  static void SetInitialProfiles(N_Vector u, UserData data);
143  static void PrintOutput(void *cvode_mem, int my_pe, MPI_Comm comm,
144                          N_Vector u, realtype t);
145  static void PrintFinalStats(void *cvode_mem);
146  static void BSend(MPI_Comm comm,
147                    int my_pe, int isubx, int isuby,
148                    long int dsizex, long int dsizey,
149                    realtype udata[]);
150  static void BRecvPost(MPI_Comm comm, MPI_Request request[],
151                        int my_pe, int isubx, int isuby,
152                        long int dsizex, long int dsizey,
153                        realtype uext[], realtype buffer[]);
154  static void BRecvWait(MPI_Request request[],
155                        int isubx, int isuby,
156                        long int dsizex, realtype uext[],
157                        realtype buffer[]);
158  static void ucomm(realtype t, N_Vector u, UserData data);
159  static void fcalc(realtype t, realtype udata[], realtype dudata[],
160                    UserData data);
161
162
163  /* Functions Called by the Solver */
164
165  static int f(realtype t, N_Vector u, N_Vector udot, void *f_data);
166
167  static int Precond(realtype tn, N_Vector u, N_Vector fu,
168                     booleantype jok, booleantype *jcurPtr,
169                     realtype gamma, void *P_data,
170                     N_Vector vtemp1, N_Vector vtemp2, N_Vector vtemp3);
171
172  static int PSolve(realtype tn, N_Vector u, N_Vector fu,
```

```
                   N_Vector r, N_Vector z,
                   realtype gamma, realtype delta,
                   int lr, void *P_data, N_Vector vtemp);


/* Private function to check function return values */

static int check_flag(void *flagvalue, char *funcname, int opt, int id);


/***************************** Main Program ******************************/

int main(int argc, char *argv[])
{
  realtype abstol, reltol, t, tout;
  N_Vector u;
  UserData data;
  PreconData predata;
  void *cvode_mem;
  int iout, flag, my_pe, npes;
  long int neq, local_N;
  MPI_Comm comm;

  u = NULL;
  data = NULL;
  predata = NULL;
  cvode_mem = NULL;

  /* Set problem size neq */
  neq = NVARS*MX*MY;

  /* 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);

  if (npes != NPEX*NPEY) {
    if (my_pe == 0)
      fprintf(stderr, "\nMPI_ERROR(0): npes = %d is not equal to NPEX*NPEY = %d\n\n",
              npes,NPEX*NPEY);
    MPI_Finalize();
    return(1);
  }

  /* Set local length */
  local_N = NVARS*MXSUB*MYSUB;

  /* Allocate and load user data block; allocate preconditioner block */
  data = (UserData) malloc(sizeof *data);
  if (check_flag((void *)data, "malloc", 2, my_pe)) MPI_Abort(comm, 1);
  InitUserData(my_pe, comm, data);
  predata = AllocPreconData (data);

  /* Allocate u, and set initial values and tolerances */
  u = N_VNew_Parallel(comm, local_N, neq);
  if (check_flag((void *)u, "N_VNew", 0, my_pe)) MPI_Abort(comm, 1);
  SetInitialProfiles(u, data);
  abstol = ATOL; reltol = RTOL;
```

```
232
233     /*
234        Call CVodeCreate to create the solver memory:
235
236        CV_BDF     specifies the Backward Differentiation Formula
237        CV_NEWTON  specifies a Newton iteration
238
239        A pointer to the integrator memory is returned and stored in cvode_mem.
240     */
241     cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
242     if (check_flag((void *)cvode_mem, "CVodeCreate", 0, my_pe)) MPI_Abort(comm, 1);
243
244     /* Set the pointer to user-defined data */
245     flag = CVodeSetFdata(cvode_mem, data);
246     if (check_flag(&flag, "CVodeSetFdata", 1, my_pe)) MPI_Abort(comm, 1);
247
248     /*
249        Call CVodeMalloc to initialize the integrator memory:
250
251        cvode_mem is the pointer to the integrator memory returned by CVodeCreate
252        f       is the user's right hand side function in y'=f(t,y)
253        T0      is the initial time
254        u       is the initial dependent variable vector
255        CV_SS   specifies scalar relative and absolute tolerances
256        reltol  is the relative tolerance
257        &abstol is a pointer to the scalar absolute tolerance
258     */
259     flag = CVodeMalloc(cvode_mem, f, T0, u, CV_SS, reltol, &abstol);
260     if (check_flag(&flag, "CVodeMalloc", 1, my_pe)) MPI_Abort(comm, 1);
261
262     /* Call CVSpgmr to specify the linear solver CVSPGMR
263        with left preconditioning and the maximum Krylov dimension maxl */
264     flag = CVSpgmr(cvode_mem, PREC_LEFT, 0);
265     if (check_flag(&flag, "CVSpgmr", 1, my_pe)) MPI_Abort(comm, 1);
266
267     /* Set preconditioner setup and solve routines Precond and PSolve,
268        and the pointer to the user-defined block data */
269     flag = CVSpilsSetPreconditioner(cvode_mem, Precond, PSolve, predata);
270     if (check_flag(&flag, "CVSpilsSetPreconditioner", 1, my_pe)) MPI_Abort(comm, 1);
271
272     if (my_pe == 0)
273       printf("\n2-species␣diurnal␣advection-diffusion␣problem\n\n");
274
275     /* In loop over output points, call CVode, print results, test for error */
276     for (iout=1, tout = TWOHR; iout <= NOUT; iout++, tout += TWOHR) {
277       flag = CVode(cvode_mem, tout, u, &t, CV_NORMAL);
278       if (check_flag(&flag, "CVode", 1, my_pe)) break;
279       PrintOutput(cvode_mem, my_pe, comm, u, t);
280     }
281
282     /* Print final statistics */
283     if (my_pe == 0) PrintFinalStats(cvode_mem);
284
285     /* Free memory */
286     N_VDestroy_Parallel(u);
287     free(data);
288     FreePreconData(predata);
289     CVodeFree(&cvode_mem);
290
```

```
291   MPI_Finalize();
292
293   return(0);
294 }
295
296
297 /********************** Private Helper Functions ***********************/
298
299 /* Allocate memory for data structure of type UserData */
300
301 static PreconData AllocPreconData(UserData fdata)
302 {
303   int lx, ly;
304   PreconData pdata;
305
306   pdata = (PreconData) malloc(sizeof *pdata);
307
308   pdata->f_data = fdata;
309
310   for (lx = 0; lx < MXSUB; lx++) {
311     for (ly = 0; ly < MYSUB; ly++) {
312       (pdata->P)[lx][ly] = denalloc(NVARS, NVARS);
313       (pdata->Jbd)[lx][ly] = denalloc(NVARS, NVARS);
314       (pdata->pivot)[lx][ly] = denallocpiv(NVARS);
315     }
316   }
317
318   return(pdata);
319 }
320
321 /* Load constants in data */
322
323 static void InitUserData(int my_pe, MPI_Comm comm, UserData data)
324 {
325   int isubx, isuby;
326
327   /* Set problem constants */
328   data->om = PI/HALFDAY;
329   data->dx = (XMAX-XMIN)/((realtype)(MX-1));
330   data->dy = (YMAX-YMIN)/((realtype)(MY-1));
331   data->hdco = KH/SQR(data->dx);
332   data->haco = VEL/(RCONST(2.0)*data->dx);
333   data->vdco = (RCONST(1.0)/SQR(data->dy))*KV0;
334
335   /* Set machine-related constants */
336   data->comm = comm;
337   data->my_pe = my_pe;
338
339   /* isubx and isuby are the PE grid indices corresponding to my_pe */
340   isuby = my_pe/NPEX;
341   isubx = my_pe - isuby*NPEX;
342   data->isubx = isubx;
343   data->isuby = isuby;
344
345   /* Set the sizes of a boundary x-line in u and uext */
346   data->nvmxsub = NVARS*MXSUB;
347   data->nvmxsub2 = NVARS*(MXSUB+2);
348 }
349
```

```
350  /* Free preconditioner data memory */
351
352  static void FreePreconData(PreconData pdata)
353  {
354    int lx, ly;
355
356    for (lx = 0; lx < MXSUB; lx++) {
357      for (ly = 0; ly < MYSUB; ly++) {
358        denfree((pdata->P)[lx][ly]);
359        denfree((pdata->Jbd)[lx][ly]);
360        denfreepiv((pdata->pivot)[lx][ly]);
361      }
362    }
363
364    free(pdata);
365  }
366
367  /* Set initial conditions in u */
368
369  static void SetInitialProfiles(N_Vector u, UserData data)
370  {
371    int isubx, isuby, lx, ly, jx, jy;
372    long int offset;
373    realtype dx, dy, x, y, cx, cy, xmid, ymid;
374    realtype *udata;
375
376    /* Set pointer to data array in vector u */
377    udata = NV_DATA_P(u);
378
379    /* Get mesh spacings, and subgrid indices for this PE */
380    dx = data->dx;          dy = data->dy;
381    isubx = data->isubx;    isuby = data->isuby;
382
383    /* Load initial profiles of c1 and c2 into local u vector.
384    Here lx and ly are local mesh point indices on the local subgrid,
385    and jx and jy are the global mesh point indices. */
386    offset = 0;
387    xmid = RCONST(0.5)*(XMIN + XMAX);
388    ymid = RCONST(0.5)*(YMIN + YMAX);
389    for (ly = 0; ly < MYSUB; ly++) {
390      jy = ly + isuby*MYSUB;
391      y = YMIN + jy*dy;
392      cy = SQR(RCONST(0.1)*(y - ymid));
393      cy = RCONST(1.0) - cy + RCONST(0.5)*SQR(cy);
394      for (lx = 0; lx < MXSUB; lx++) {
395        jx = lx + isubx*MXSUB;
396        x = XMIN + jx*dx;
397        cx = SQR(RCONST(0.1)*(x - xmid));
398        cx = RCONST(1.0) - cx + RCONST(0.5)*SQR(cx);
399        udata[offset  ] = C1_SCALE*cx*cy;
400        udata[offset+1] = C2_SCALE*cx*cy;
401        offset = offset + 2;
402      }
403    }
404  }
405
406  /* Print current t, step count, order, stepsize, and sampled c1,c2 values */
407
408  static void PrintOutput(void *cvode_mem, int my_pe, MPI_Comm comm,
```

```
409                           N_Vector u, realtype t)
410 {
411   int qu, flag;
412   realtype hu, *udata, tempu[2];
413   int npelast;
414   long int i0, i1, nst;
415   MPI_Status status;
416 
417   npelast = NPEX*NPEY - 1;
418   udata = NV_DATA_P(u);
419 
420   /* Send c1,c2 at top right mesh point to PE 0 */
421   if (my_pe == npelast) {
422     i0 = NVARS*MXSUB*MYSUB - 2;
423     i1 = i0 + 1;
424     if (npelast != 0)
425       MPI_Send(&udata[i0], 2, PVEC_REAL_MPI_TYPE, 0, 0, comm);
426     else {
427       tempu[0] = udata[i0];
428       tempu[1] = udata[i1];
429     }
430   }
431 
432   /* On PE 0, receive c1,c2 at top right, then print performance data
433      and sampled solution values */
434   if (my_pe == 0) {
435     if (npelast != 0)
436       MPI_Recv(&tempu[0], 2, PVEC_REAL_MPI_TYPE, npelast, 0, comm, &status);
437     flag = CVodeGetNumSteps(cvode_mem, &nst);
438     check_flag(&flag, "CVodeGetNumSteps", 1, my_pe);
439     flag = CVodeGetLastOrder(cvode_mem, &qu);
440     check_flag(&flag, "CVodeGetLastOrder", 1, my_pe);
441     flag = CVodeGetLastStep(cvode_mem, &hu);
442     check_flag(&flag, "CVodeGetLastStep", 1, my_pe);
443 
444 #if defined(SUNDIALS_EXTENDED_PRECISION)
445     printf("t␣=␣%.2Le␣␣␣no.␣steps␣=␣%ld␣␣␣order␣=␣%d␣␣␣stepsize␣=␣%.2Le\n",
446            t, nst, qu, hu);
447     printf("At␣bottom␣left:␣␣c1,␣c2␣=␣%12.3Le␣%12.3Le␣\n", udata[0], udata[1]);
448     printf("At␣top␣right:␣␣␣␣c1,␣c2␣=␣%12.3Le␣%12.3Le␣\n\n", tempu[0], tempu[1]);
449 #elif defined(SUNDIALS_DOUBLE_PRECISION)
450     printf("t␣=␣%.2le␣␣␣no.␣steps␣=␣%ld␣␣␣order␣=␣%d␣␣␣stepsize␣=␣%.2le\n",
451            t, nst, qu, hu);
452     printf("At␣bottom␣left:␣␣c1,␣c2␣=␣%12.3le␣%12.3le␣\n", udata[0], udata[1]);
453     printf("At␣top␣right:␣␣␣␣c1,␣c2␣=␣%12.3le␣%12.3le␣\n\n", tempu[0], tempu[1]);
454 #else
455     printf("t␣=␣%.2e␣␣␣no.␣steps␣=␣%ld␣␣␣order␣=␣%d␣␣␣stepsize␣=␣%.2e\n",
456            t, nst, qu, hu);
457     printf("At␣bottom␣left:␣␣c1,␣c2␣=␣%12.3e␣%12.3e␣\n", udata[0], udata[1]);
458     printf("At␣top␣right:␣␣␣␣c1,␣c2␣=␣%12.3e␣%12.3e␣\n\n", tempu[0], tempu[1]);
459 #endif
460   }
461 }
462 
463 /* Print final statistics contained in iopt */
464 
465 static void PrintFinalStats(void *cvode_mem)
466 {
467   long int lenrw, leniw ;
```

```
  long int lenrwLS, leniwLS;
  long int nst, nfe, nsetups, nni, ncfn, netf;
  long int nli, npe, nps, ncfl, nfeLS;
  int flag;

  flag = CVodeGetWorkSpace(cvode_mem, &lenrw, &leniw);
  check_flag(&flag, "CVodeGetWorkSpace", 1, 0);
  flag = CVodeGetNumSteps(cvode_mem, &nst);
  check_flag(&flag, "CVodeGetNumSteps", 1, 0);
  flag = CVodeGetNumRhsEvals(cvode_mem, &nfe);
  check_flag(&flag, "CVodeGetNumRhsEvals", 1, 0);
  flag = CVodeGetNumLinSolvSetups(cvode_mem, &nsetups);
  check_flag(&flag, "CVodeGetNumLinSolvSetups", 1, 0);
  flag = CVodeGetNumErrTestFails(cvode_mem, &netf);
  check_flag(&flag, "CVodeGetNumErrTestFails", 1, 0);
  flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
  check_flag(&flag, "CVodeGetNumNonlinSolvIters", 1, 0);
  flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);
  check_flag(&flag, "CVodeGetNumNonlinSolvConvFails", 1, 0);

  flag = CVSpilsGetWorkSpace(cvode_mem, &lenrwLS, &leniwLS);
  check_flag(&flag, "CVSpilsGetWorkSpace", 1, 0);
  flag = CVSpilsGetNumLinIters(cvode_mem, &nli);
  check_flag(&flag, "CVSpilsGetNumLinIters", 1, 0);
  flag = CVSpilsGetNumPrecEvals(cvode_mem, &npe);
  check_flag(&flag, "CVSpilsGetNumPrecEvals", 1, 0);
  flag = CVSpilsGetNumPrecSolves(cvode_mem, &nps);
  check_flag(&flag, "CVSpilsGetNumPrecSolves", 1, 0);
  flag = CVSpilsGetNumConvFails(cvode_mem, &ncfl);
  check_flag(&flag, "CVSpilsGetNumConvFails", 1, 0);
  flag = CVSpilsGetNumRhsEvals(cvode_mem, &nfeLS);
  check_flag(&flag, "CVSpilsGetNumRhsEvals", 1, 0);

  printf("\nFinal␣Statistics:␣\n\n");
  printf("lenrw␣␣␣=␣%5ld␣␣␣␣␣␣leniw␣␣␣=␣%5ld\n", lenrw, leniw);
  printf("lenrwls␣=␣%5ld␣␣␣␣␣␣leniwls␣=␣%5ld\n", lenrwLS, leniwLS);
  printf("nst␣␣␣␣␣␣=␣%5ld\n"                    , nst);
  printf("nfe␣␣␣␣␣␣=␣%5ld␣␣␣␣␣␣nfels␣␣␣=␣%5ld\n"  , nfe, nfeLS);
  printf("nni␣␣␣␣␣␣=␣%5ld␣␣␣␣␣␣nli␣␣␣␣␣␣=␣%5ld\n"  , nni, nli);
  printf("nsetups␣=␣%5ld␣␣␣␣␣␣netf␣␣␣␣=␣%5ld\n"  , nsetups, netf);
  printf("npe␣␣␣␣␣␣=␣%5ld␣␣␣␣␣␣nps␣␣␣␣␣␣=␣%5ld\n"  , npe, nps);
  printf("ncfn␣␣␣␣=␣%5ld␣␣␣␣␣␣ncfl␣␣␣␣=␣%5ld\n\n", ncfn, ncfl);
}

/* Routine to send boundary data to neighboring PEs */

static void BSend(MPI_Comm comm,
                  int my_pe, int isubx, int isuby,
                  long int dsizex, long int dsizey,
                  realtype udata[])
{
  int i, ly;
  long int offsetu, offsetbuf;
  realtype bufleft[NVARS*MYSUB], bufright[NVARS*MYSUB];

  /* If isuby > 0, send data from bottom x-line of u */
  if (isuby != 0)
    MPI_Send(&udata[0], dsizex, PVEC_REAL_MPI_TYPE, my_pe-NPEX, 0, comm);

```

```
527     /* If isuby < NPEY-1, send data from top x-line of u */
528     if (isuby != NPEY-1) {
529       offsetu = (MYSUB-1)*dsizex;
530       MPI_Send(&udata[offsetu], dsizex, PVEC_REAL_MPI_TYPE, my_pe+NPEX, 0, comm);
531     }
532
533     /* If isubx > 0, send data from left y-line of u (via bufleft) */
534     if (isubx != 0) {
535       for (ly = 0; ly < MYSUB; ly++) {
536         offsetbuf = ly*NVARS;
537         offsetu = ly*dsizex;
538         for (i = 0; i < NVARS; i++)
539           bufleft[offsetbuf+i] = udata[offsetu+i];
540       }
541       MPI_Send(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE, my_pe-1, 0, comm);
542     }
543
544     /* If isubx < NPEX-1, send data from right y-line of u (via bufright) */
545     if (isubx != NPEX-1) {
546       for (ly = 0; ly < MYSUB; ly++) {
547         offsetbuf = ly*NVARS;
548         offsetu = offsetbuf*MXSUB + (MXSUB-1)*NVARS;
549         for (i = 0; i < NVARS; i++)
550           bufright[offsetbuf+i] = udata[offsetu+i];
551       }
552       MPI_Send(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE, my_pe+1, 0, comm);
553     }
554   }
555
556   /* Routine to start receiving boundary data from neighboring PEs.
557      Notes:
558      1) buffer should be able to hold 2*NVARS*MYSUB realtype entries, should be
559      passed to both the BRecvPost and BRecvWait functions, and should not
560      be manipulated between the two calls.
561      2) request should have 4 entries, and should be passed in both calls also. */
562
563   static void BRecvPost(MPI_Comm comm, MPI_Request request[],
564                         int my_pe, int isubx, int isuby,
565                         long int dsizex, long int dsizey,
566                         realtype uext[], realtype buffer[])
567   {
568     long int offsetue;
569     /* Have bufleft and bufright use the same buffer */
570     realtype *bufleft = buffer, *bufright = buffer+NVARS*MYSUB;
571
572     /* If isuby > 0, receive data for bottom x-line of uext */
573     if (isuby != 0)
574       MPI_Irecv(&uext[NVARS], dsizex, PVEC_REAL_MPI_TYPE,
575                                         my_pe-NPEX, 0, comm, &request[0]);
576
577     /* If isuby < NPEY-1, receive data for top x-line of uext */
578     if (isuby != NPEY-1) {
579       offsetue = NVARS*(1 + (MYSUB+1)*(MXSUB+2));
580       MPI_Irecv(&uext[offsetue], dsizex, PVEC_REAL_MPI_TYPE,
581                                         my_pe+NPEX, 0, comm, &request[1]);
582     }
583
584     /* If isubx > 0, receive data for left y-line of uext (via bufleft) */
585     if (isubx != 0) {
```

```
586       MPI_Irecv(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE,
587                                              my_pe-1, 0, comm, &request[2]);
588     }
589
590     /* If isubx < NPEX-1, receive data for right y-line of uext (via bufright) */
591     if (isubx != NPEX-1) {
592       MPI_Irecv(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE,
593                                              my_pe+1, 0, comm, &request[3]);
594     }
595   }
596
597   /* Routine to finish receiving boundary data from neighboring PEs.
598      Notes:
599      1) buffer should be able to hold 2*NVARS*MYSUB realtype entries, should be
600      passed to both the BRecvPost and BRecvWait functions, and should not
601      be manipulated between the two calls.
602      2) request should have 4 entries, and should be passed in both calls also. */
603
604   static void BRecvWait(MPI_Request request[],
605                         int isubx, int isuby,
606                         long int dsizex, realtype uext[],
607                         realtype buffer[])
608   {
609     int i, ly;
610     long int dsizex2, offsetue, offsetbuf;
611     realtype *bufleft = buffer, *bufright = buffer+NVARS*MYSUB;
612     MPI_Status status;
613
614     dsizex2 = dsizex + 2*NVARS;
615
616     /* If isuby > 0, receive data for bottom x-line of uext */
617     if (isuby != 0)
618       MPI_Wait(&request[0],&status);
619
620     /* If isuby < NPEY-1, receive data for top x-line of uext */
621     if (isuby != NPEY-1)
622       MPI_Wait(&request[1],&status);
623
624     /* If isubx > 0, receive data for left y-line of uext (via bufleft) */
625     if (isubx != 0) {
626       MPI_Wait(&request[2],&status);
627
628       /* Copy the buffer to uext */
629       for (ly = 0; ly < MYSUB; ly++) {
630         offsetbuf = ly*NVARS;
631         offsetue = (ly+1)*dsizex2;
632         for (i = 0; i < NVARS; i++)
633           uext[offsetue+i] = bufleft[offsetbuf+i];
634       }
635     }
636
637     /* If isubx < NPEX-1, receive data for right y-line of uext (via bufright) */
638     if (isubx != NPEX-1) {
639       MPI_Wait(&request[3],&status);
640
641       /* Copy the buffer to uext */
642       for (ly = 0; ly < MYSUB; ly++) {
643         offsetbuf = ly*NVARS;
644         offsetue = (ly+2)*dsizex2 - NVARS;
```

```
645         for (i = 0; i < NVARS; i++)
646           uext[offsetue+i] = bufright[offsetbuf+i];
647       }
648     }
649   }
650
651   /* ucomm routine.  This routine performs all communication
652      between processors of data needed to calculate f. */
653
654   static void ucomm(realtype t, N_Vector u, UserData data)
655   {
656
657     realtype *udata, *uext, buffer[2*NVARS*MYSUB];
658     MPI_Comm comm;
659     int my_pe, isubx, isuby;
660     long int nvmxsub, nvmysub;
661     MPI_Request request[4];
662
663     udata = NV_DATA_P(u);
664
665     /* Get comm, my_pe, subgrid indices, data sizes, extended array uext */
666     comm = data->comm;  my_pe = data->my_pe;
667     isubx = data->isubx;   isuby = data->isuby;
668     nvmxsub = data->nvmxsub;
669     nvmysub = NVARS*MYSUB;
670     uext = data->uext;
671
672     /* Start receiving boundary data from neighboring PEs */
673     BRecvPost(comm, request, my_pe, isubx, isuby, nvmxsub, nvmysub, uext, buffer);
674
675     /* Send data from boundary of local grid to neighboring PEs */
676     BSend(comm, my_pe, isubx, isuby, nvmxsub, nvmysub, udata);
677
678     /* Finish receiving boundary data from neighboring PEs */
679     BRecvWait(request, isubx, isuby, nvmxsub, uext, buffer);
680   }
681
682   /* fcalc routine. Compute f(t,y).  This routine assumes that communication
683      between processors of data needed to calculate f has already been done,
684      and this data is in the work array uext. */
685
686   static void fcalc(realtype t, realtype udata[],
687                     realtype dudata[], UserData data)
688   {
689     realtype *uext;
690     realtype q3, c1, c2, c1dn, c2dn, c1up, c2up, c1lt, c2lt;
691     realtype c1rt, c2rt, cydn, cyup, hord1, hord2, horad1, horad2;
692     realtype qq1, qq2, qq3, qq4, rkin1, rkin2, s, vertd1, vertd2, ydn, yup;
693     realtype q4coef, dely, verdco, hordco, horaco;
694     int i, lx, ly, jx, jy;
695     int isubx, isuby;
696     long int nvmxsub, nvmxsub2, offsetu, offsetue;
697
698     /* Get subgrid indices, data sizes, extended work array uext */
699     isubx = data->isubx;   isuby = data->isuby;
700     nvmxsub = data->nvmxsub; nvmxsub2 = data->nvmxsub2;
701     uext = data->uext;
702
703     /* Copy local segment of u vector into the working extended array uext */
```

```
704     offsetu = 0;
705     offsetue = nvmxsub2 + NVARS;
706     for (ly = 0; ly < MYSUB; ly++) {
707       for (i = 0; i < nvmxsub; i++) uext[offsetue+i] = udata[offsetu+i];
708       offsetu = offsetu + nvmxsub;
709       offsetue = offsetue + nvmxsub2;
710     }
711
712     /* To facilitate homogeneous Neumann boundary conditions, when this is
713     a boundary PE, copy data from the first interior mesh line of u to uext */
714
715     /* If isuby = 0, copy x-line 2 of u to uext */
716     if (isuby == 0) {
717       for (i = 0; i < nvmxsub; i++) uext[NVARS+i] = udata[nvmxsub+i];
718     }
719
720     /* If isuby = NPEY-1, copy x-line MYSUB-1 of u to uext */
721     if (isuby == NPEY-1) {
722       offsetu = (MYSUB-2)*nvmxsub;
723       offsetue = (MYSUB+1)*nvmxsub2 + NVARS;
724       for (i = 0; i < nvmxsub; i++) uext[offsetue+i] = udata[offsetu+i];
725     }
726
727     /* If isubx = 0, copy y-line 2 of u to uext */
728     if (isubx == 0) {
729       for (ly = 0; ly < MYSUB; ly++) {
730         offsetu = ly*nvmxsub + NVARS;
731         offsetue = (ly+1)*nvmxsub2;
732         for (i = 0; i < NVARS; i++) uext[offsetue+i] = udata[offsetu+i];
733       }
734     }
735
736     /* If isubx = NPEX-1, copy y-line MXSUB-1 of u to uext */
737     if (isubx == NPEX-1) {
738       for (ly = 0; ly < MYSUB; ly++) {
739         offsetu = (ly+1)*nvmxsub - 2*NVARS;
740         offsetue = (ly+2)*nvmxsub2 - NVARS;
741         for (i = 0; i < NVARS; i++) uext[offsetue+i] = udata[offsetu+i];
742       }
743     }
744
745     /* Make local copies of problem variables, for efficiency */
746     dely = data->dy;
747     verdco = data->vdco;
748     hordco  = data->hdco;
749     horaco  = data->haco;
750
751     /* Set diurnal rate coefficients as functions of t, and save q4 in
752     data block for use by preconditioner evaluation routine */
753     s = sin((data->om)*t);
754     if (s > RCONST(0.0)) {
755       q3 = EXP(-A3/s);
756       q4coef = EXP(-A4/s);
757     } else {
758       q3 = RCONST(0.0);
759       q4coef = RCONST(0.0);
760     }
761     data->q4 = q4coef;
762
```

```
763     /* Loop over all grid points in local subgrid */
764     for (ly = 0; ly < MYSUB; ly++) {
765
766       jy = ly + isuby*MYSUB;
767
768       /* Set vertical diffusion coefficients at jy +- 1/2 */
769       ydn = YMIN + (jy - RCONST(0.5))*dely;
770       yup = ydn + dely;
771       cydn = verdco*EXP(RCONST(0.2)*ydn);
772       cyup = verdco*EXP(RCONST(0.2)*yup);
773       for (lx = 0; lx < MXSUB; lx++) {
774
775         jx = lx + isubx*MXSUB;
776
777         /* Extract c1 and c2, and set kinetic rate terms */
778         offsetue = (lx+1)*NVARS + (ly+1)*nvmxsub2;
779         c1 = uext[offsetue];
780         c2 = uext[offsetue+1];
781         qq1 = Q1*c1*C3;
782         qq2 = Q2*c1*c2;
783         qq3 = q3*C3;
784         qq4 = q4coef*c2;
785         rkin1 = -qq1 - qq2 + RCONST(2.0)*qq3 + qq4;
786         rkin2 = qq1 - qq2 - qq4;
787
788         /* Set vertical diffusion terms */
789         c1dn = uext[offsetue-nvmxsub2];
790         c2dn = uext[offsetue-nvmxsub2+1];
791         c1up = uext[offsetue+nvmxsub2];
792         c2up = uext[offsetue+nvmxsub2+1];
793         vertd1 = cyup*(c1up - c1) - cydn*(c1 - c1dn);
794         vertd2 = cyup*(c2up - c2) - cydn*(c2 - c2dn);
795
796         /* Set horizontal diffusion and advection terms */
797         c1lt = uext[offsetue-2];
798         c2lt = uext[offsetue-1];
799         c1rt = uext[offsetue+2];
800         c2rt = uext[offsetue+3];
801         hord1 = hordco*(c1rt - RCONST(2.0)*c1 + c1lt);
802         hord2 = hordco*(c2rt - RCONST(2.0)*c2 + c2lt);
803         horad1 = horaco*(c1rt - c1lt);
804         horad2 = horaco*(c2rt - c2lt);
805
806         /* Load all terms into dudata */
807         offsetu = lx*NVARS + ly*nvmxsub;
808         dudata[offsetu]   = vertd1 + hord1 + horad1 + rkin1;
809         dudata[offsetu+1] = vertd2 + hord2 + horad2 + rkin2;
810       }
811     }
812   }
813
814
815   /****************** Functions Called by the Solver ************************/
816
817   /* f routine.  Evaluate f(t,y).  First call ucomm to do communication of
818      subgrid boundary data into uext.  Then calculate f by a call to fcalc. */
819
820   static int f(realtype t, N_Vector u, N_Vector udot, void *f_data)
821   {
```

```
822     realtype *udata, *dudata;
823     UserData data;
824
825     udata = NV_DATA_P(u);
826     dudata = NV_DATA_P(udot);
827     data = (UserData) f_data;
828
829     /* Call ucomm to do inter-processor communication */
830     ucomm(t, u, data);
831
832     /* Call fcalc to calculate all right-hand sides */
833     fcalc(t, udata, dudata, data);
834
835     return(0);
836   }
837
838   /* Preconditioner setup routine. Generate and preprocess P. */
839   static int Precond(realtype tn, N_Vector u, N_Vector fu,
840                      booleantype jok, booleantype *jcurPtr,
841                      realtype gamma, void *P_data,
842                      N_Vector vtemp1, N_Vector vtemp2, N_Vector vtemp3)
843   {
844     realtype c1, c2, cydn, cyup, diag, ydn, yup, q4coef, dely, verdco, hordco;
845     realtype **(*P)[MYSUB], **(*Jbd)[MYSUB];
846     long int nvmxsub, *(*pivot)[MYSUB], ier, offset;
847     int lx, ly, jx, jy, isubx, isuby;
848     realtype *udata, **a, **j;
849     PreconData predata;
850     UserData data;
851
852     /* Make local copies of pointers in P_data, pointer to u's data,
853        and PE index pair */
854     predata = (PreconData) P_data;
855     data = (UserData) (predata->f_data);
856     P = predata->P;
857     Jbd = predata->Jbd;
858     pivot = predata->pivot;
859     udata = NV_DATA_P(u);
860     isubx = data->isubx;   isuby = data->isuby;
861     nvmxsub = data->nvmxsub;
862
863     if (jok) {
864
865     /* jok = TRUE: Copy Jbd to P */
866       for (ly = 0; ly < MYSUB; ly++)
867         for (lx = 0; lx < MXSUB; lx++)
868           dencopy(Jbd[lx][ly], P[lx][ly], NVARS, NVARS);
869
870     *jcurPtr = FALSE;
871
872     }
873
874     else {
875
876     /* jok = FALSE: Generate Jbd from scratch and copy to P */
877
878     /* Make local copies of problem variables, for efficiency */
879     q4coef = data->q4;
880     dely = data->dy;
```

```
881     verdco = data->vdco;
882     hordco  = data->hdco;
883
884     /* Compute 2x2 diagonal Jacobian blocks (using q4 values
885        computed on the last f call).  Load into P. */
886       for (ly = 0; ly < MYSUB; ly++) {
887         jy = ly + isuby*MYSUB;
888         ydn = YMIN + (jy - RCONST(0.5))*dely;
889         yup = ydn + dely;
890         cydn = verdco*EXP(RCONST(0.2)*ydn);
891         cyup = verdco*EXP(RCONST(0.2)*yup);
892         diag = -(cydn + cyup + RCONST(2.0)*hordco);
893         for (lx = 0; lx < MXSUB; lx++) {
894           jx = lx + isubx*MXSUB;
895           offset = lx*NVARS + ly*nvmxsub;
896           c1 = udata[offset];
897           c2 = udata[offset+1];
898           j = Jbd[lx][ly];
899           a = P[lx][ly];
900           IJth(j,1,1) = (-Q1*C3 - Q2*c2) + diag;
901           IJth(j,1,2) = -Q2*c1 + q4coef;
902           IJth(j,2,1) = Q1*C3 - Q2*c2;
903           IJth(j,2,2) = (-Q2*c1 - q4coef) + diag;
904           dencopy(j, a, NVARS, NVARS);
905         }
906       }
907
908     *jcurPtr = TRUE;
909
910     }
911
912     /* Scale by -gamma */
913       for (ly = 0; ly < MYSUB; ly++)
914         for (lx = 0; lx < MXSUB; lx++)
915           denscale(-gamma, P[lx][ly], NVARS, NVARS);
916
917     /* Add identity matrix and do LU decompositions on blocks in place */
918     for (lx = 0; lx < MXSUB; lx++) {
919       for (ly = 0; ly < MYSUB; ly++) {
920         denaddI(P[lx][ly], NVARS);
921         ier = denGETRF(P[lx][ly], NVARS, NVARS, pivot[lx][ly]);
922         if (ier != 0) return(1);
923       }
924     }
925
926     return(0);
927   }
928
929   /* Preconditioner solve routine */
930   static int PSolve(realtype tn, N_Vector u, N_Vector fu,
931                     N_Vector r, N_Vector z,
932                     realtype gamma, realtype delta,
933                     int lr, void *P_data, N_Vector vtemp)
934   {
935     realtype **(*P)[MYSUB];
936     long int nvmxsub, *(*pivot)[MYSUB];
937     int lx, ly;
938     realtype *zdata, *v;
939     PreconData predata;
```

```
940   UserData data;
941
942   /* Extract the P and pivot arrays from P_data */
943   predata = (PreconData) P_data;
944   data = (UserData) (predata->f_data);
945   P = predata->P;
946   pivot = predata->pivot;
947
948   /* Solve the block-diagonal system Px = r using LU factors stored
949      in P and pivot data in pivot, and return the solution in z.
950      First copy vector r to z. */
951   N_VScale(RCONST(1.0), r, z);
952
953   nvmxsub = data->nvmxsub;
954   zdata = NV_DATA_P(z);
955
956   for (lx = 0; lx < MXSUB; lx++) {
957     for (ly = 0; ly < MYSUB; ly++) {
958       v = &(zdata[lx*NVARS + ly*nvmxsub]);
959       denGETRS(P[lx][ly], NVARS, pivot[lx][ly], v);
960     }
961   }
962
963   return(0);
964 }
965
966
967 /*********************** Private Helper Function ************************/
968
969 /* Check function return value...
970      opt == 0 means SUNDIALS function allocates memory so check if
971               returned NULL pointer
972      opt == 1 means SUNDIALS function returns a flag so check if
973               flag >= 0
974      opt == 2 means function allocates memory so check if returned
975               NULL pointer */
976
977 static int check_flag(void *flagvalue, char *funcname, int opt, int id)
978 {
979   int *errflag;
980
981   /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
982   if (opt == 0 && flagvalue == NULL) {
983     fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n",
984             id, funcname);
985     return(1); }
986
987   /* Check if flag < 0 */
988   else if (opt == 1) {
989     errflag = (int *) flagvalue;
990     if (*errflag < 0) {
991       fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with flag = %d\n\n",
992               id, funcname, *errflag);
993       return(1); }}
994
995   /* Check if function returned NULL pointer - no memory allocated */
996   else if (opt == 2 && flagvalue == NULL) {
997     fprintf(stderr, "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n",
998             id, funcname);
```

```
999         return(1); }
1000
1001      return(0);
1002    }
```

F Listing of cvkryx_bbd_p.c

```
/*
 * -----------------------------------------------------------------
 * $Revision: 1.1 $
 * $Date: 2006/07/05 15:50:05 $
 * -----------------------------------------------------------------
 * Programmer(s): S. D. Cohen, A. C. Hindmarsh, M. R. Wittman, and
 *                Radu Serban  @ LLNL
 * -----------------------------------------------------------------
 * Example problem:
 *
 * An ODE system is generated from the following 2-species diurnal
 * kinetics advection-diffusion PDE system in 2 space dimensions:
 *
 * dc(i)/dt = Kh*(d/dx)^2 c(i) + V*dc(i)/dx + (d/dy)(Kv(y)*dc(i)/dy)
 *                 + Ri(c1,c2,t)      for i = 1,2,   where
 *   R1(c1,c2,t) = -q1*c1*c3 - q2*c1*c2 + 2*q3(t)*c3 + q4(t)*c2 ,
 *   R2(c1,c2,t) =  q1*c1*c3 - q2*c1*c2 - q4(t)*c2 ,
 *   Kv(y) = Kv0*exp(y/5) ,
 * Kh, V, Kv0, q1, q2, and c3 are constants, and q3(t) and q4(t)
 * vary diurnally. The problem is posed on the square
 *   0 <= x <= 20,    30 <= y <= 50   (all in km),
 * with homogeneous Neumann boundary conditions, and for time t in
 *   0 <= t <= 86400 sec (1 day).
 * The PDE system is treated by central differences on a uniform
 * mesh, with simple polynomial initial profiles.
 *
 * The problem is solved by CVODE on NPE processors, treated
 * as a rectangular process grid of size NPEX by NPEY, with
 * NPE = NPEX*NPEY. Each processor contains a subgrid of size MXSUB
 * by MYSUB of the (x,y) mesh. Thus the actual mesh sizes are
 * MX = MXSUB*NPEX and MY = MYSUB*NPEY, and the ODE system size is
 * neq = 2*MX*MY.
 *
 * The solution is done with the BDF/GMRES method (i.e. using the
 * CVSPGMR linear solver) and a block-diagonal matrix with banded
 * blocks as a preconditioner, using the CVBBDPRE module.
 * Each block is generated using difference quotients, with
 * half-bandwidths mudq = mldq = 2*MXSUB, but the retained banded
 * blocks have half-bandwidths mukeep = mlkeep = 2.
 * A copy of the approximate Jacobian is saved and conditionally
 * reused within the preconditioner routine.
 *
 * The problem is solved twice -- with left and right preconditioning.
 *
 * Performance data and sampled solution values are printed at
 * selected output times, and all performance counters are printed
 * on completion.
 *
 * This version uses MPI for user routines.
 * Execute with number of processors = NPEX*NPEY (see constants below).
 * -----------------------------------------------------------------
 */

#include <stdio.h>
#include <stdlib.h>
#include <math.h>

```

```
#include <cvode/cvode.h>               /* prototypes for CVODE fcts. */
#include <cvode/cvode_spgmr.h>         /* prototypes and constants for CVSPGMR solver */
#include <cvode/cvode_bbdpre.h>        /* prototypes for CVBBDPRE module */
#include <nvector/nvector_parallel.h> /* definition N_Vector and macro NV_DATA_P */
#include <sundials/sundials_types.h>  /* definitions of realtype, booleantype */
#include <sundials/sundials_math.h>   /* definition of macros SQR and EXP */

#include <mpi.h>                      /* MPI constants and types */


/* Problem Constants */

#define ZERO          RCONST(0.0)

#define NVARS         2                /* number of species         */
#define KH            RCONST(4.0e-6)   /* horizontal diffusivity Kh */
#define VEL           RCONST(0.001)    /* advection velocity V      */
#define KV0           RCONST(1.0e-8)   /* coefficient in Kv(y)      */
#define Q1            RCONST(1.63e-16) /* coefficients q1, q2, c3   */
#define Q2            RCONST(4.66e-16)
#define C3            RCONST(3.7e16)
#define A3            RCONST(22.62)    /* coefficient in expression for q3(t) */
#define A4            RCONST(7.601)    /* coefficient in expression for q4(t) */
#define C1_SCALE      RCONST(1.0e6)    /* coefficients in initial profiles
*/
#define C2_SCALE      RCONST(1.0e12)

#define T0            ZERO               /* initial time */
#define NOUT          12                 /* number of output times */
#define TWOHR         RCONST(7200.0)     /* number of seconds in two hours  */
#define HALFDAY       RCONST(4.32e4)     /* number of seconds in a half day */
#define PI       RCONST(3.1415926535898) /* pi */

#define XMIN          ZERO               /* grid boundaries in x  */
#define XMAX          RCONST(20.0)
#define YMIN          RCONST(30.0)       /* grid boundaries in y  */
#define YMAX          RCONST(50.0)

#define NPEX          2             /* no. PEs in x direction of PE array */
#define NPEY          2             /* no. PEs in y direction of PE array */
                                    /* Total no. PEs = NPEX*NPEY */
#define MXSUB         5             /* no. x points per subgrid */
#define MYSUB         5             /* no. y points per subgrid */

#define MX            (NPEX*MXSUB)  /* MX = number of x mesh points */
#define MY            (NPEY*MYSUB)  /* MY = number of y mesh points */
                                    /* Spatial mesh is MX by MY */
/* CVodeMalloc Constants */

#define RTOL    RCONST(1.0e-5)    /* scalar relative tolerance */
#define FLOOR   RCONST(100.0)     /* value of C1 or C2 at which tolerances */
                                  /* change from relative to absolute      */
#define ATOL    (RTOL*FLOOR)      /* scalar absolute tolerance */

/* Type : UserData
   contains problem constants, extended dependent variable array,
   grid constants, processor indices, MPI communicator */

typedef struct {
```

```
116   realtype q4, om, dx, dy, hdco, haco, vdco;
117   realtype uext[NVARS*(MXSUB+2)*(MYSUB+2)];
118   int my_pe, isubx, isuby;
119   long int nvmxsub, nvmxsub2, Nlocal;
120   MPI_Comm comm;
121 } *UserData;
122 
123 /* Prototypes of private helper functions */
124 
125 static void InitUserData(int my_pe, long int local_N, MPI_Comm comm,
126                          UserData data);
127 static void SetInitialProfiles(N_Vector u, UserData data);
128 static void PrintIntro(int npes, long int mudq, long int mldq,
129                        long int mukeep, long int mlkeep);
130 static void PrintOutput(void *cvode_mem, int my_pe, MPI_Comm comm,
131                         N_Vector u, realtype t);
132 static void PrintFinalStats(void *cvode_mem, void *pdata);
133 static void BSend(MPI_Comm comm,
134                   int my_pe, int isubx, int isuby,
135                   long int dsizex, long int dsizey,
136                   realtype uarray[]);
137 static void BRecvPost(MPI_Comm comm, MPI_Request request[],
138                       int my_pe, int isubx, int isuby,
139                       long int dsizex, long int dsizey,
140                       realtype uext[], realtype buffer[]);
141 static void BRecvWait(MPI_Request request[],
142                       int isubx, int isuby,
143                       long int dsizex, realtype uext[],
144                       realtype buffer[]);
145 
146 static void fucomm(realtype t, N_Vector u, void *f_data);
147 
148 /* Prototype of function called by the solver */
149 
150 static int f(realtype t, N_Vector u, N_Vector udot, void *f_data);
151 
152 /* Prototype of functions called by the CVBBDPRE module */
153 
154 static int flocal(long int Nlocal, realtype t, N_Vector u,
155                   N_Vector udot, void *f_data);
156 
157 /* Private function to check function return values */
158 
159 static int check_flag(void *flagvalue, char *funcname, int opt, int id);
160 
161 /***************************** Main Program ******************************/
162 
163 int main(int argc, char *argv[])
164 {
165   UserData data;
166   void *cvode_mem;
167   void *pdata;
168   realtype abstol, reltol, t, tout;
169   N_Vector u;
170   int iout, my_pe, npes, flag, jpre;
171   long int neq, local_N, mudq, mldq, mukeep, mlkeep;
172   MPI_Comm comm;
173 
174   data = NULL;
```

```
  cvode_mem = pdata = NULL;
  u = NULL;

  /* Set problem size neq */
  neq = NVARS*MX*MY;

  /* 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);

  if (npes != NPEX*NPEY) {
    if (my_pe == 0)
      fprintf(stderr, "\nMPI_ERROR(0): npes = %d is not equal to NPEX*NPEY = %d\n\n",
              npes, NPEX*NPEY);
    MPI_Finalize();
    return(1);
  }

  /* Set local length */
  local_N = NVARS*MXSUB*MYSUB;

  /* Allocate and load user data block */
  data = (UserData) malloc(sizeof *data);
  if(check_flag((void *)data, "malloc", 2, my_pe)) MPI_Abort(comm, 1);
  InitUserData(my_pe, local_N, comm, data);

  /* Allocate and initialize u, and set tolerances */
  u = N_VNew_Parallel(comm, local_N, neq);
  if(check_flag((void *)u, "N_VNew_Parallel", 0, my_pe)) MPI_Abort(comm, 1);
  SetInitialProfiles(u, data);
  abstol = ATOL;
  reltol = RTOL;

  /*
     Call CVodeCreate to create the solver memory:

     CV_BDF     specifies the Backward Differentiation Formula
     CV_NEWTON  specifies a Newton iteration

     A pointer to the integrator memory is returned and stored in cvode_mem.
  */

  cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
  if(check_flag((void *)cvode_mem, "CVodeCreate", 0, my_pe)) MPI_Abort(comm, 1);

  /* Set the pointer to user-defined data */
  flag = CVodeSetFdata(cvode_mem, data);
  if(check_flag(&flag, "CVodeSetFdata", 1, my_pe)) MPI_Abort(comm, 1);

  /*
     Call CVodeMalloc to initialize the integrator memory:

     cvode_mem is the pointer to the integrator memory returned by CVodeCreate
     f       is the user's right hand side function in y'=f(t,y)
     T0      is the initial time
     u       is the initial dependent variable vector
     CV_SS   specifies scalar relative and absolute tolerances
```

```
234       reltol  is the relative tolerance
235       &abstol is a pointer to the scalar absolute tolerance
236    */
237
238    flag = CVodeMalloc(cvode_mem, f, T0, u, CV_SS, reltol, &abstol);
239    if(check_flag(&flag, "CVodeMalloc", 1, my_pe)) MPI_Abort(comm, 1);
240
241    /* Allocate preconditioner block */
242    mudq = mldq = NVARS*MXSUB;
243    mukeep = mlkeep = NVARS;
244    pdata = CVBBDPrecAlloc(cvode_mem, local_N, mudq, mldq,
245                           mukeep, mlkeep, ZERO, flocal, NULL);
246    if(check_flag((void *)pdata, "CVBBDPrecAlloc", 0, my_pe)) MPI_Abort(comm, 1);
247
248    /* Call CVBBDSpgmr to specify the linear solver CVSPGMR using the
249       CVBBDPRE preconditioner, with left preconditioning and the
250       default maximum Krylov dimension maxl  */
251    flag = CVBBDSpgmr(cvode_mem, PREC_LEFT, 0, pdata);
252    if(check_flag(&flag, "CVBBDSpgmr", 1, my_pe)) MPI_Abort(comm, 1);
253
254    /* Print heading */
255    if (my_pe == 0) PrintIntro(npes, mudq, mldq, mukeep, mlkeep);
256
257    /* Loop over jpre (= PREC_LEFT, PREC_RIGHT), and solve the problem */
258    for (jpre = PREC_LEFT; jpre <= PREC_RIGHT; jpre++) {
259
260    /* On second run, re-initialize u, the integrator, CVBBDPRE, and CVSPGMR */
261
262    if (jpre == PREC_RIGHT) {
263
264      SetInitialProfiles(u, data);
265
266      flag = CVodeReInit(cvode_mem, f, T0, u, CV_SS, reltol, &abstol);
267      if(check_flag(&flag, "CVodeReInit", 1, my_pe)) MPI_Abort(comm, 1);
268
269      flag = CVBBDPrecReInit(pdata, mudq, mldq, ZERO, flocal, NULL);
270      if(check_flag(&flag, "CVBBDPrecReInit", 1, my_pe)) MPI_Abort(comm, 1);
271
272      flag = CVSpilsSetPrecType(cvode_mem, PREC_RIGHT);
273      check_flag(&flag, "CVSpilsSetPrecType", 1, my_pe);
274
275      if (my_pe == 0) {
276        printf("\n\n------------------------------------------------------------");
277        printf("------------\n");
278      }
279
280    }
281
282
283    if (my_pe == 0) {
284      printf("\n\nPreconditioner␣type␣is:␣␣jpre␣=␣%s\n\n",
285             (jpre == PREC_LEFT) ? "PREC_LEFT" : "PREC_RIGHT");
286    }
287
288    /* In loop over output points, call CVode, print results, test for error */
289
290    for (iout = 1, tout = TWOHR; iout <= NOUT; iout++, tout += TWOHR) {
291      flag = CVode(cvode_mem, tout, u, &t, CV_NORMAL);
292      if(check_flag(&flag, "CVode", 1, my_pe)) break;
```

```
293       PrintOutput(cvode_mem, my_pe, comm, u, t);
294     }
295
296     /* Print final statistics */
297
298     if (my_pe == 0) PrintFinalStats(cvode_mem, pdata);
299
300     } /* End of jpre loop */
301
302     /* Free memory */
303     N_VDestroy_Parallel(u);
304     CVBBDPrecFree(&pdata);
305     free(data);
306     CVodeFree(&cvode_mem);
307
308     MPI_Finalize();
309
310     return(0);
311   }
312
313   /*********************** Private Helper Functions ***********************/
314
315   /* Load constants in data */
316
317   static void InitUserData(int my_pe, long int local_N, MPI_Comm comm,
318                            UserData data)
319   {
320     int isubx, isuby;
321
322     /* Set problem constants */
323     data->om = PI/HALFDAY;
324     data->dx = (XMAX-XMIN)/((realtype)(MX-1));
325     data->dy = (YMAX-YMIN)/((realtype)(MY-1));
326     data->hdco = KH/SQR(data->dx);
327     data->haco = VEL/(RCONST(2.0)*data->dx);
328     data->vdco = (RCONST(1.0)/SQR(data->dy))*KV0;
329
330     /* Set machine-related constants */
331     data->comm = comm;
332     data->my_pe = my_pe;
333     data->Nlocal = local_N;
334     /* isubx and isuby are the PE grid indices corresponding to my_pe */
335     isuby = my_pe/NPEX;
336     isubx = my_pe - isuby*NPEX;
337     data->isubx = isubx;
338     data->isuby = isuby;
339     /* Set the sizes of a boundary x-line in u and uext */
340     data->nvmxsub = NVARS*MXSUB;
341     data->nvmxsub2 = NVARS*(MXSUB+2);
342   }
343
344   /* Set initial conditions in u */
345
346   static void SetInitialProfiles(N_Vector u, UserData data)
347   {
348     int isubx, isuby;
349     int lx, ly, jx, jy;
350     long int offset;
351     realtype dx, dy, x, y, cx, cy, xmid, ymid;
```

```
352   realtype *uarray;
353
354   /* Set pointer to data array in vector u */
355
356   uarray = NV_DATA_P(u);
357
358   /* Get mesh spacings, and subgrid indices for this PE */
359
360   dx = data->dx;          dy = data->dy;
361   isubx = data->isubx;    isuby = data->isuby;
362
363   /* Load initial profiles of c1 and c2 into local u vector.
364   Here lx and ly are local mesh point indices on the local subgrid,
365   and jx and jy are the global mesh point indices. */
366
367   offset = 0;
368   xmid = RCONST(0.5)*(XMIN + XMAX);
369   ymid = RCONST(0.5)*(YMIN + YMAX);
370   for (ly = 0; ly < MYSUB; ly++) {
371     jy = ly + isuby*MYSUB;
372     y = YMIN + jy*dy;
373     cy = SQR(RCONST(0.1)*(y - ymid));
374     cy = RCONST(1.0) - cy + RCONST(0.5)*SQR(cy);
375     for (lx = 0; lx < MXSUB; lx++) {
376       jx = lx + isubx*MXSUB;
377       x = XMIN + jx*dx;
378       cx = SQR(RCONST(0.1)*(x - xmid));
379       cx = RCONST(1.0) - cx + RCONST(0.5)*SQR(cx);
380       uarray[offset  ] = C1_SCALE*cx*cy;
381       uarray[offset+1] = C2_SCALE*cx*cy;
382       offset = offset + 2;
383     }
384   }
385 }
386
387 /* Print problem introduction */
388
389 static void PrintIntro(int npes, long int mudq, long int mldq,
390                        long int mukeep, long int mlkeep)
391 {
392   printf("\n2-species␣diurnal␣advection-diffusion␣problem\n");
393   printf("␣␣%d␣by␣%d␣mesh␣on␣%d␣processors\n", MX, MY, npes);
394   printf("␣␣Using␣CVBBDPRE␣preconditioner␣module\n");
395   printf("␣␣␣␣Difference-quotient␣half-bandwidths␣are");
396   printf("␣mudq␣=␣%ld,␣␣mldq␣=␣%ld\n", mudq, mldq);
397   printf("␣␣␣␣Retained␣band␣block␣half-bandwidths␣are");
398   printf("␣mukeep␣=␣%ld,␣␣mlkeep␣=␣%ld", mukeep, mlkeep);
399
400   return;
401 }
402
403 /* Print current t, step count, order, stepsize, and sampled c1,c2 values */
404
405 static void PrintOutput(void *cvode_mem, int my_pe, MPI_Comm comm,
406                         N_Vector u, realtype t)
407 {
408   int qu, flag, npelast;
409   long int i0, i1, nst;
410   realtype hu, *uarray, tempu[2];
```

```
  MPI_Status status;

  npelast = NPEX*NPEY - 1;
  uarray = NV_DATA_P(u);

  /* Send c1,c2 at top right mesh point to PE 0 */
  if (my_pe == npelast) {
    i0 = NVARS*MXSUB*MYSUB - 2;
    i1 = i0 + 1;
    if (npelast != 0)
      MPI_Send(&uarray[i0], 2, PVEC_REAL_MPI_TYPE, 0, 0, comm);
    else {
      tempu[0] = uarray[i0];
      tempu[1] = uarray[i1];
    }
  }

  /* On PE 0, receive c1,c2 at top right, then print performance data
     and sampled solution values */
  if (my_pe == 0) {
    if (npelast != 0)
      MPI_Recv(&tempu[0], 2, PVEC_REAL_MPI_TYPE, npelast, 0, comm, &status);
    flag = CVodeGetNumSteps(cvode_mem, &nst);
    check_flag(&flag, "CVodeGetNumSteps", 1, my_pe);
    flag = CVodeGetLastOrder(cvode_mem, &qu);
    check_flag(&flag, "CVodeGetLastOrder", 1, my_pe);
    flag = CVodeGetLastStep(cvode_mem, &hu);
    check_flag(&flag, "CVodeGetLastStep", 1, my_pe);
#if defined(SUNDIALS_EXTENDED_PRECISION)
    printf("t = %.2Le    no. steps = %ld    order = %d    stepsize = %.2Le\n",
           t, nst, qu, hu);
    printf("At bottom left:   c1, c2 = %12.3Le %12.3Le \n", uarray[0], uarray[1]);
    printf("At top right:     c1, c2 = %12.3Le %12.3Le \n\n", tempu[0], tempu[1]);
#elif defined(SUNDIALS_DOUBLE_PRECISION)
    printf("t = %.2le    no. steps = %ld    order = %d    stepsize = %.2le\n",
           t, nst, qu, hu);
    printf("At bottom left:   c1, c2 = %12.3le %12.3le \n", uarray[0], uarray[1]);
    printf("At top right:     c1, c2 = %12.3le %12.3le \n\n", tempu[0], tempu[1]);
#else
    printf("t = %.2e    no. steps = %ld    order = %d    stepsize = %.2e\n",
           t, nst, qu, hu);
    printf("At bottom left:   c1, c2 = %12.3e %12.3e \n", uarray[0], uarray[1]);
    printf("At top right:     c1, c2 = %12.3e %12.3e \n\n", tempu[0], tempu[1]);
#endif
  }
}

/* Print final statistics contained in iopt */

static void PrintFinalStats(void *cvode_mem, void *pdata)
{
  long int lenrw, leniw ;
  long int lenrwLS, leniwLS;
  long int lenrwBBDP, leniwBBDP, ngevalsBBDP;
  long int nst, nfe, nsetups, nni, ncfn, netf;
  long int nli, npe, nps, ncfl, nfeLS;
  int flag;

  flag = CVodeGetWorkSpace(cvode_mem, &lenrw, &leniw);
```

```
470   check_flag(&flag, "CVodeGetWorkSpace", 1, 0);
471   flag = CVodeGetNumSteps(cvode_mem, &nst);
472   check_flag(&flag, "CVodeGetNumSteps", 1, 0);
473   flag = CVodeGetNumRhsEvals(cvode_mem, &nfe);
474   check_flag(&flag, "CVodeGetNumRhsEvals", 1, 0);
475   flag = CVodeGetNumLinSolvSetups(cvode_mem, &nsetups);
476   check_flag(&flag, "CVodeGetNumLinSolvSetups", 1, 0);
477   flag = CVodeGetNumErrTestFails(cvode_mem, &netf);
478   check_flag(&flag, "CVodeGetNumErrTestFails", 1, 0);
479   flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
480   check_flag(&flag, "CVodeGetNumNonlinSolvIters", 1, 0);
481   flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);
482   check_flag(&flag, "CVodeGetNumNonlinSolvConvFails", 1, 0);
483
484   flag = CVSpilsGetWorkSpace(cvode_mem, &lenrwLS, &leniwLS);
485   check_flag(&flag, "CVSpilsGetWorkSpace", 1, 0);
486   flag = CVSpilsGetNumLinIters(cvode_mem, &nli);
487   check_flag(&flag, "CVSpilsGetNumLinIters", 1, 0);
488   flag = CVSpilsGetNumPrecEvals(cvode_mem, &npe);
489   check_flag(&flag, "CVSpilsGetNumPrecEvals", 1, 0);
490   flag = CVSpilsGetNumPrecSolves(cvode_mem, &nps);
491   check_flag(&flag, "CVSpilsGetNumPrecSolves", 1, 0);
492   flag = CVSpilsGetNumConvFails(cvode_mem, &ncfl);
493   check_flag(&flag, "CVSpilsGetNumConvFails", 1, 0);
494   flag = CVSpilsGetNumRhsEvals(cvode_mem, &nfeLS);
495   check_flag(&flag, "CVSpilsGetNumRhsEvals", 1, 0);
496
497   printf("\nFinal␣Statistics:␣\n\n");
498   printf("lenrw␣␣␣=␣%5ld␣␣␣␣␣␣leniw␣␣␣=␣%5ld\n", lenrw, leniw);
499   printf("lenrwls␣=␣%5ld␣␣␣␣␣␣leniwls␣=␣%5ld\n", lenrwLS, leniwLS);
500   printf("nst␣␣␣␣␣␣=␣%5ld\n"                    , nst);
501   printf("nfe␣␣␣␣␣␣=␣%5ld␣␣␣␣␣␣nfels␣␣␣=␣%5ld\n"  , nfe, nfeLS);
502   printf("nni␣␣␣␣␣␣=␣%5ld␣␣␣␣␣␣nli␣␣␣␣␣␣=␣%5ld\n"  , nni, nli);
503   printf("nsetups␣=␣%5ld␣␣␣␣␣␣netf␣␣␣␣=␣%5ld\n"  , nsetups, netf);
504   printf("npe␣␣␣␣␣␣=␣%5ld␣␣␣␣␣␣nps␣␣␣␣␣␣=␣%5ld\n"  , npe, nps);
505   printf("ncfn␣␣␣␣=␣%5ld␣␣␣␣␣␣ncfl␣␣␣␣=␣%5ld\n\n", ncfn, ncfl);
506
507   flag = CVBBDPrecGetWorkSpace(pdata, &lenrwBBDP, &leniwBBDP);
508   check_flag(&flag, "CVBBDPrecGetWorkSpace", 1, 0);
509   flag = CVBBDPrecGetNumGfnEvals(pdata, &ngevalsBBDP);
510   check_flag(&flag, "CVBBDPrecGetNumGfnEvals", 1, 0);
511   printf("In␣CVBBDPRE:␣real/integer␣local␣work␣space␣sizes␣=␣%ld,␣%ld\n",
512          lenrwBBDP, leniwBBDP);
513   printf("␣␣␣␣␣␣␣␣␣␣␣␣␣␣no.␣flocal␣evals.␣=␣%ld\n",ngevalsBBDP);
514 }
515
516 /* Routine to send boundary data to neighboring PEs */
517
518 static void BSend(MPI_Comm comm,
519                   int my_pe, int isubx, int isuby,
520                   long int dsizex, long int dsizey,
521                   realtype uarray[])
522 {
523   int i, ly;
524   long int offsetu, offsetbuf;
525   realtype bufleft[NVARS*MYSUB], bufright[NVARS*MYSUB];
526
527   /* If isuby > 0, send data from bottom x-line of u */
528
```

```
529     if (isuby != 0)
530       MPI_Send(&uarray[0], dsizex, PVEC_REAL_MPI_TYPE, my_pe-NPEX, 0, comm);
531
532     /* If isuby < NPEY-1, send data from top x-line of u */
533
534     if (isuby != NPEY-1) {
535       offsetu = (MYSUB-1)*dsizex;
536       MPI_Send(&uarray[offsetu], dsizex, PVEC_REAL_MPI_TYPE, my_pe+NPEX, 0, comm);
537     }
538
539     /* If isubx > 0, send data from left y-line of u (via bufleft) */
540
541     if (isubx != 0) {
542       for (ly = 0; ly < MYSUB; ly++) {
543         offsetbuf = ly*NVARS;
544         offsetu = ly*dsizex;
545         for (i = 0; i < NVARS; i++)
546           bufleft[offsetbuf+i] = uarray[offsetu+i];
547       }
548       MPI_Send(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE, my_pe-1, 0, comm);
549     }
550
551     /* If isubx < NPEX-1, send data from right y-line of u (via bufright) */
552
553     if (isubx != NPEX-1) {
554       for (ly = 0; ly < MYSUB; ly++) {
555         offsetbuf = ly*NVARS;
556         offsetu = offsetbuf*MXSUB + (MXSUB-1)*NVARS;
557         for (i = 0; i < NVARS; i++)
558           bufright[offsetbuf+i] = uarray[offsetu+i];
559       }
560       MPI_Send(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE, my_pe+1, 0, comm);
561     }
562
563   }
564
565   /* Routine to start receiving boundary data from neighboring PEs.
566      Notes:
567      1) buffer should be able to hold 2*NVARS*MYSUB realtype entries, should be
568      passed to both the BRecvPost and BRecvWait functions, and should not
569      be manipulated between the two calls.
570      2) request should have 4 entries, and should be passed in both calls also. */
571
572   static void BRecvPost(MPI_Comm comm, MPI_Request request[],
573                         int my_pe, int isubx, int isuby,
574                         long int dsizex, long int dsizey,
575                         realtype uext[], realtype buffer[])
576   {
577     long int offsetue;
578     /* Have bufleft and bufright use the same buffer */
579     realtype *bufleft = buffer, *bufright = buffer+NVARS*MYSUB;
580
581     /* If isuby > 0, receive data for bottom x-line of uext */
582     if (isuby != 0)
583       MPI_Irecv(&uext[NVARS], dsizex, PVEC_REAL_MPI_TYPE,
584                                           my_pe-NPEX, 0, comm, &request[0]);
585
586     /* If isuby < NPEY-1, receive data for top x-line of uext */
587     if (isuby != NPEY-1) {
```

```
588       offsetue = NVARS*(1 + (MYSUB+1)*(MXSUB+2));
589       MPI_Irecv(&uext[offsetue], dsizex, PVEC_REAL_MPI_TYPE,
590                                           my_pe+NPEX, 0, comm, &request[1]);
591     }
592
593     /* If isubx > 0, receive data for left y-line of uext (via bufleft) */
594     if (isubx != 0) {
595       MPI_Irecv(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE,
596                                           my_pe-1, 0, comm, &request[2]);
597     }
598
599     /* If isubx < NPEX-1, receive data for right y-line of uext (via bufright) */
600     if (isubx != NPEX-1) {
601       MPI_Irecv(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE,
602                                           my_pe+1, 0, comm, &request[3]);
603     }
604
605   }
606
607   /* Routine to finish receiving boundary data from neighboring PEs.
608      Notes:
609      1) buffer should be able to hold 2*NVARS*MYSUB realtype entries, should be
610      passed to both the BRecvPost and BRecvWait functions, and should not
611      be manipulated between the two calls.
612      2) request should have 4 entries, and should be passed in both calls also. */
613
614   static void BRecvWait(MPI_Request request[],
615                         int isubx, int isuby,
616                         long int dsizex, realtype uext[],
617                         realtype buffer[])
618   {
619     int i, ly;
620     long int dsizex2, offsetue, offsetbuf;
621     realtype *bufleft = buffer, *bufright = buffer+NVARS*MYSUB;
622     MPI_Status status;
623
624     dsizex2 = dsizex + 2*NVARS;
625
626     /* If isuby > 0, receive data for bottom x-line of uext */
627     if (isuby != 0)
628       MPI_Wait(&request[0],&status);
629
630     /* If isuby < NPEY-1, receive data for top x-line of uext */
631     if (isuby != NPEY-1)
632       MPI_Wait(&request[1],&status);
633
634     /* If isubx > 0, receive data for left y-line of uext (via bufleft) */
635     if (isubx != 0) {
636       MPI_Wait(&request[2],&status);
637
638       /* Copy the buffer to uext */
639       for (ly = 0; ly < MYSUB; ly++) {
640         offsetbuf = ly*NVARS;
641         offsetue = (ly+1)*dsizex2;
642         for (i = 0; i < NVARS; i++)
643           uext[offsetue+i] = bufleft[offsetbuf+i];
644       }
645     }
646
```

```
647     /* If isubx < NPEX-1, receive data for right y-line of uext (via bufright) */
648     if (isubx != NPEX-1) {
649       MPI_Wait(&request[3],&status);
650 
651       /* Copy the buffer to uext */
652       for (ly = 0; ly < MYSUB; ly++) {
653         offsetbuf = ly*NVARS;
654         offsetue = (ly+2)*dsizex2 - NVARS;
655         for (i = 0; i < NVARS; i++)
656           uext[offsetue+i] = bufright[offsetbuf+i];
657       }
658     }
659   }
660 
661   /* fucomm routine.  This routine performs all inter-processor
662      communication of data in u needed to calculate f.         */
663 
664   static void fucomm(realtype t, N_Vector u, void *f_data)
665   {
666     UserData data;
667     realtype *uarray, *uext, buffer[2*NVARS*MYSUB];
668     MPI_Comm comm;
669     int my_pe, isubx, isuby;
670     long int nvmxsub, nvmysub;
671     MPI_Request request[4];
672 
673     data = (UserData) f_data;
674     uarray = NV_DATA_P(u);
675 
676     /* Get comm, my_pe, subgrid indices, data sizes, extended array uext */
677 
678     comm = data->comm;  my_pe = data->my_pe;
679     isubx = data->isubx;   isuby = data->isuby;
680     nvmxsub = data->nvmxsub;
681     nvmysub = NVARS*MYSUB;
682     uext = data->uext;
683 
684     /* Start receiving boundary data from neighboring PEs */
685 
686     BRecvPost(comm, request, my_pe, isubx, isuby, nvmxsub, nvmysub, uext, buffer);
687 
688     /* Send data from boundary of local grid to neighboring PEs */
689 
690     BSend(comm, my_pe, isubx, isuby, nvmxsub, nvmysub, uarray);
691 
692     /* Finish receiving boundary data from neighboring PEs */
693 
694     BRecvWait(request, isubx, isuby, nvmxsub, uext, buffer);
695   }
696 
697   /***************** Function called by the solver *************************/
698 
699   /* f routine.  Evaluate f(t,y).  First call fucomm to do communication of
700      subgrid boundary data into uext.  Then calculate f by a call to flocal. */
701 
702   static int f(realtype t, N_Vector u, N_Vector udot, void *f_data)
703   {
704     UserData data;
705 
```

```
706   data = (UserData) f_data;
707
708   /* Call fucomm to do inter-processor communication */
709
710   fucomm (t, u, f_data);
711
712   /* Call flocal to calculate all right-hand sides */
713
714   flocal (data->Nlocal, t, u, udot, f_data);
715
716   return(0);
717 }
718
719 /***************** Functions called by the CVBBDPRE module ***************/
720
721 /* flocal routine.  Compute f(t,y).  This routine assumes that all
722    inter-processor communication of data needed to calculate f has already
723    been done, and this data is in the work array uext.                    */
724
725 static int flocal(long int Nlocal, realtype t, N_Vector u,
726                   N_Vector udot, void *f_data)
727 {
728   realtype *uext;
729   realtype q3, c1, c2, c1dn, c2dn, c1up, c2up, c1lt, c2lt;
730   realtype c1rt, c2rt, cydn, cyup, hord1, hord2, horad1, horad2;
731   realtype qq1, qq2, qq3, qq4, rkin1, rkin2, s, vertd1, vertd2, ydn, yup;
732   realtype q4coef, dely, verdco, hordco, horaco;
733   int i, lx, ly, jx, jy;
734   int isubx, isuby;
735   long int nvmxsub, nvmxsub2, offsetu, offsetue;
736   UserData data;
737   realtype *uarray, *duarray;
738
739   uarray = NV_DATA_P(u);
740   duarray = NV_DATA_P(udot);
741
742   /* Get subgrid indices, array sizes, extended work array uext */
743
744   data = (UserData) f_data;
745   isubx = data->isubx;   isuby = data->isuby;
746   nvmxsub = data->nvmxsub; nvmxsub2 = data->nvmxsub2;
747   uext = data->uext;
748
749   /* Copy local segment of u vector into the working extended array uext */
750
751   offsetu = 0;
752   offsetue = nvmxsub2 + NVARS;
753   for (ly = 0; ly < MYSUB; ly++) {
754     for (i = 0; i < nvmxsub; i++) uext[offsetue+i] = uarray[offsetu+i];
755     offsetu = offsetu + nvmxsub;
756     offsetue = offsetue + nvmxsub2;
757   }
758
759   /* To facilitate homogeneous Neumann boundary conditions, when this is
760   a boundary PE, copy data from the first interior mesh line of u to uext */
761
762   /* If isuby = 0, copy x-line 2 of u to uext */
763   if (isuby == 0) {
764     for (i = 0; i < nvmxsub; i++) uext[NVARS+i] = uarray[nvmxsub+i];
```

```
765     }
766
767     /* If isuby = NPEY-1, copy x-line MYSUB-1 of u to uext */
768     if (isuby == NPEY-1) {
769       offsetu = (MYSUB-2)*nvmxsub;
770       offsetue = (MYSUB+1)*nvmxsub2 + NVARS;
771       for (i = 0; i < nvmxsub; i++) uext[offsetue+i] = uarray[offsetu+i];
772     }
773
774     /* If isubx = 0, copy y-line 2 of u to uext */
775     if (isubx == 0) {
776       for (ly = 0; ly < MYSUB; ly++) {
777         offsetu = ly*nvmxsub + NVARS;
778         offsetue = (ly+1)*nvmxsub2;
779         for (i = 0; i < NVARS; i++) uext[offsetue+i] = uarray[offsetu+i];
780       }
781     }
782
783     /* If isubx = NPEX-1, copy y-line MXSUB-1 of u to uext */
784     if (isubx == NPEX-1) {
785       for (ly = 0; ly < MYSUB; ly++) {
786         offsetu = (ly+1)*nvmxsub - 2*NVARS;
787         offsetue = (ly+2)*nvmxsub2 - NVARS;
788         for (i = 0; i < NVARS; i++) uext[offsetue+i] = uarray[offsetu+i];
789       }
790     }
791
792     /* Make local copies of problem variables, for efficiency */
793
794     dely = data->dy;
795     verdco = data->vdco;
796     hordco = data->hdco;
797     horaco = data->haco;
798
799     /* Set diurnal rate coefficients as functions of t, and save q4 in
800     data block for use by preconditioner evaluation routine            */
801
802     s = sin((data->om)*t);
803     if (s > ZERO) {
804       q3 = EXP(-A3/s);
805       q4coef = EXP(-A4/s);
806     } else {
807       q3 = ZERO;
808       q4coef = ZERO;
809     }
810     data->q4 = q4coef;
811
812
813     /* Loop over all grid points in local subgrid */
814
815     for (ly = 0; ly < MYSUB; ly++) {
816
817       jy = ly + isuby*MYSUB;
818
819       /* Set vertical diffusion coefficients at jy +- 1/2 */
820
821       ydn = YMIN + (jy - RCONST(0.5))*dely;
822       yup = ydn + dely;
823       cydn = verdco*EXP(RCONST(0.2)*ydn);
```

```
824       cyup = verdco*EXP(RCONST(0.2)*yup);
825       for (lx = 0; lx < MXSUB; lx++) {
826
827         jx = lx + isubx*MXSUB;
828
829         /* Extract c1 and c2, and set kinetic rate terms */
830
831         offsetue = (lx+1)*NVARS + (ly+1)*nvmxsub2;
832         c1 = uext[offsetue];
833         c2 = uext[offsetue+1];
834         qq1 = Q1*c1*C3;
835         qq2 = Q2*c1*c2;
836         qq3 = q3*C3;
837         qq4 = q4coef*c2;
838         rkin1 = -qq1 - qq2 + 2.0*qq3 + qq4;
839         rkin2 = qq1 - qq2 - qq4;
840
841         /* Set vertical diffusion terms */
842
843         c1dn = uext[offsetue-nvmxsub2];
844         c2dn = uext[offsetue-nvmxsub2+1];
845         c1up = uext[offsetue+nvmxsub2];
846         c2up = uext[offsetue+nvmxsub2+1];
847         vertd1 = cyup*(c1up - c1) - cydn*(c1 - c1dn);
848         vertd2 = cyup*(c2up - c2) - cydn*(c2 - c2dn);
849
850         /* Set horizontal diffusion and advection terms */
851
852         c1lt = uext[offsetue-2];
853         c2lt = uext[offsetue-1];
854         c1rt = uext[offsetue+2];
855         c2rt = uext[offsetue+3];
856         hord1 = hordco*(c1rt - RCONST(2.0)*c1 + c1lt);
857         hord2 = hordco*(c2rt - RCONST(2.0)*c2 + c2lt);
858         horad1 = horaco*(c1rt - c1lt);
859         horad2 = horaco*(c2rt - c2lt);
860
861         /* Load all terms into duarray */
862
863         offsetu = lx*NVARS + ly*nvmxsub;
864         duarray[offsetu]   = vertd1 + hord1 + horad1 + rkin1;
865         duarray[offsetu+1] = vertd2 + hord2 + horad2 + rkin2;
866       }
867     }
868
869     return(0);
870   }
871
872   /* Check function return value...
873        opt == 0 means SUNDIALS function allocates memory so check if
874                 returned NULL pointer
875        opt == 1 means SUNDIALS function returns a flag so check if
876                 flag >= 0
877        opt == 2 means function allocates memory so check if returned
878                 NULL pointer */
879
880   static int check_flag(void *flagvalue, char *funcname, int opt, int id)
881   {
882     int *errflag;
```

```
883
884   /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
885   if (opt == 0 && flagvalue == NULL) {
886     fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n",
887             id, funcname);
888     return(1); }
889
890   /* Check if flag < 0 */
891   else if (opt == 1) {
892     errflag = (int *) flagvalue;
893     if (*errflag < 0) {
894       fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with flag = %d\n\n",
895               id, funcname, *errflag);
896       return(1); }}
897
898   /* Check if function returned NULL pointer - no memory allocated */
899   else if (opt == 2 && flagvalue == NULL) {
900     fprintf(stderr, "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n",
901             id, funcname);
902     return(1); }
903
904   return(0);
905 }
```

G Listing of fcvkryx.f

```
C     ----------------------------------------------------------------
C     $Revision: 1.1 $
C     $Date: 2006/07/05 15:50:04 $
C     ----------------------------------------------------------------
C     FCVODE Example Problem: 2D kinetics-transport, precond. Krylov
C     solver.
C
C     An ODE system is generated from the following 2-species diurnal
C     kinetics advection-diffusion PDE system in 2 space dimensions:
C
C     dc(i)/dt = Kh*(d/dx)**2 c(i) + V*dc(i)/dx + (d/dy)(Kv(y)*dc(i)/dy)
C                           + Ri(c1,c2,t)      for i = 1,2,   where
C     R1(c1,c2,t) = -q1*c1*c3 - q2*c1*c2 + 2*q3(t)*c3 + q4(t)*c2 ,
C     R2(c1,c2,t) =  q1*c1*c3 - q2*c1*c2 - q4(t)*c2 ,
C     Kv(y) = Kv0*exp(y/5) ,
C     Kh, V, Kv0, q1, q2, and c3 are constants, and q3(t) and q4(t)
C     vary diurnally.
C
C     The problem is posed on the square
C     0 .le. x .le. 20,    30 .le. y .le. 50   (all in km),
C     with homogeneous Neumann boundary conditions, and for time t
C     in 0 .le. t .le. 86400 sec (1 day).
C     The PDE system is treated by central differences on a uniform
C     10 x 10 mesh, with simple polynomial initial profiles.
C     The problem is solved with CVODE, with the BDF/GMRES method and
C     the block-diagonal part of the Jacobian as a left
C     preconditioner.
C
C     Note: this program requires the dense linear solver routines
C     DGEFA and DGESL from LINPACK, and BLAS routines DCOPY and DSCAL.
C
C     The second and third dimensions of U here must match the values
C     of MX and MY, for consistency with the output statements
C     below.
C     ----------------------------------------------------------------
C
      IMPLICIT NONE
C
      INTEGER*4 MX, MY, NEQ
      PARAMETER (MX=10, MY=10)
      PARAMETER (NEQ=2*MX*MY)
      INTEGER*4 LENIPAR, LENRPAR
      PARAMETER (LENIPAR=6+2*MX*MY, LENRPAR=12+8*MX*MY)
C
      INTEGER METH,ITMETH,IATOL,ITASK,IER,LNCFL,LNPS
      INTEGER LNST,LNFE,LNSETUP,LNNI,LNCF,LQ,LH,LNPE,LNLI,LNETF
      INTEGER JOUT,JPRETYPE,IGSTYPE,MAXL
      INTEGER*4 IOUT(25),IPAR(LENIPAR)
      INTEGER*4 NST,NFE,NPSET,NPE,NPS,NNI,NETF
      INTEGER*4 NLI,NCFN,NCFL
      DOUBLE PRECISION ATOL,AVDIM,T,TOUT,TWOHR,RTOL,FLOOR,DELT
      DOUBLE PRECISION U(2,MX,MY),ROUT(10),RPAR(LENRPAR)
C
      DATA TWOHR/7200.0D0/, RTOL/1.0D-5/, FLOOR/100.0D0/,
     &     JPRETYPE/1/, IGSTYPE/1/, MAXL/0/, DELT/0.0D0/
      DATA LNST/3/, LNFE/4/, LNETF/5/,  LNCF/6/, LNNI/7/, LNSETUP/8/,
     &     LQ/9/, LNPE/18/, LNLI/20/, LNPS/19/, LNCFL/21/
```

```
      DATA LH/2/
C
C     Load problem constants into IPAR, RPAR, and set initial values
      CALL INITKX(MX, MY, U, IPAR, RPAR)
C
C     Set other input arguments.
      T = 0.0D0
      METH = 2
      ITMETH = 2
      IATOL = 1
      ATOL = RTOL * FLOOR
      ITASK = 1
C
      WRITE(6,10) NEQ
 10   FORMAT('Krylov example problem:'//
     &       ' Kinetics-transport, NEQ = ', I4/)
C
      CALL FNVINITS(1, NEQ, IER)
      IF (IER .NE. 0) THEN
        WRITE(6,20) IER
 20     FORMAT(///' SUNDIALS_ERROR: FNVINITS returned IER = ', I5)
        STOP
      ENDIF
C
C     Initialize CVODE
      CALL FCVMALLOC(T, U, METH, ITMETH, IATOL, RTOL, ATOL,
     &     IOUT, ROUT, IPAR, RPAR, IER)
      IF (IER .NE. 0) THEN
        WRITE(6,30) IER
 30     FORMAT(///' SUNDIALS_ERROR: FCVMALLOC returned IER = ', I5)
        STOP
        ENDIF
C
      CALL FCVSPGMR(JPRETYPE, IGSTYPE, MAXL, DELT, IER)
      IF (IER .NE. 0) THEN
        WRITE(6,40) IER
 40     FORMAT(///' SUNDIALS_ERROR: FCVSPGMR returned IER = ', I5)
        CALL FCVFREE
        STOP
      ENDIF
C
      CALL FCVSPILSSETPREC(1, IER)
C
C Loop over output points, call FCVODE, print sample solution values.
      TOUT = TWOHR
      DO JOUT = 1, 12
C
         CALL FCVODE(TOUT, T, U, ITASK, IER)
C
         WRITE(6,50) T, IOUT(LNST), IOUT(LQ), ROUT(LH)
 50      FORMAT(/' t = ', E11.3, 3X, 'nst = ', I5,
     &          '  q = ', I2, '  h = ', E14.6)
         WRITE(6,55) U(1,1,1), U(1,5,5), U(1,10,10),
     &               U(2,1,1), U(2,5,5), U(2,10,10)
 55      FORMAT('  c1 (bot.left/middle/top rt.) = ', 3E14.6/
     &          '  c2 (bot.left/middle/top rt.) = ', 3E14.6)
C
         IF (IER .NE. 0) THEN
            WRITE(6,60) IER, IOUT(15)
```

```
 60         FORMAT(///' SUNDIALS_ERROR: FCVODE returned IER = ', I5, /,
     &           '                 Linear Solver returned IER = ', I5)
            CALL FCVFREE
            STOP
         ENDIF
C
         TOUT = TOUT + TWOHR
C
       ENDDO

C      Print final statistics.
       NST = IOUT(LNST)
       NFE = IOUT(LNFE)
       NPSET = IOUT(LNSETUP)
       NPE = IOUT(LNPE)
       NPS = IOUT(LNPS)
       NNI = IOUT(LNNI)
       NLI = IOUT(LNLI)
       AVDIM = DBLE(NLI) / DBLE(NNI)
       NCFN = IOUT(LNCF)
       NCFL = IOUT(LNCFL)
       NETF = IOUT(LNETF)
       WRITE(6,80) NST, NFE, NPSET, NPE, NPS, NNI, NLI, AVDIM, NCFN,
     &     NCFL, NETF
  80   FORMAT(//'Final statistics:'//
     &     ' number of steps        = ', I5, 5X,
     &     ' number of f evals.     =', I5/
     &     ' number of prec. setups = ', I5/
     &     ' number of prec. evals. = ', I5, 5X,
     &     ' number of prec. solves = ', I5/
     &     ' number of nonl. iters. = ', I5, 5X,
     &     ' number of lin. iters.  = ', I5/
     &     ' average Krylov subspace dimension (NLI/NNI)  = ', E14.6/
     &     ' number of conv. failures.. nonlinear = ', I3,
     &     ' linear = ', I3/
     &     ' number of error test failures = ', I3)
C
       CALL FCVFREE
C
       STOP
       END

C      ----------------------------------------------------------------

       SUBROUTINE INITKX(MX, MY, U0, IPAR, RPAR)
C      Routine to set problem constants and initial values
C
       IMPLICIT NONE
C
       INTEGER*4 MX, MY, IPAR(*)
       DOUBLE PRECISION RPAR(*)
C
       INTEGER*4 MM, JY, JX, P_IPP, P_BD, P_P
       DOUBLE PRECISION U0
       DIMENSION U0(2,MX,MY)
       DOUBLE PRECISION Q1, Q2, Q3, Q4, A3, A4, OM, C3, DY, HDCO
       DOUBLE PRECISION VDCO, HACO, X, Y
       DOUBLE PRECISION CX, CY, DKH, DKV0, DX, HALFDA, PI, VEL
C
```

```
      DATA DKH/4.0D-6/, VEL/0.001D0/, DKV0/1.0D-8/, HALFDA/4.32D4/,
     1     PI/3.1415926535898D0/
C
C     Problem constants
      MM = MX * MY
      Q1 = 1.63D-16
      Q2 = 4.66D-16
      A3 = 22.62D0
      A4 = 7.601D0
      OM = PI / HALFDA
      C3 = 3.7D16
      DX = 20.0D0 / (MX - 1.0D0)
      DY = 20.0D0 / (MY - 1.0D0)
      HDCO = DKH / DX**2
      HACO = VEL / (2.0D0 * DX)
      VDCO = (1.0D0 / DY**2) * DKV0
C
C     Load constants in IPAR and RPAR
      IPAR(1) = MX
      IPAR(2) = MY
      IPAR(3) = MM
C
      RPAR(1)  = Q1
      RPAR(2)  = Q2
      RPAR(3)  = Q3
      RPAR(4)  = Q4
      RPAR(5)  = A3
      RPAR(6)  = A4
      RPAR(7)  = OM
      RPAR(8)  = C3
      RPAR(9)  = DY
      RPAR(10) = HDCO
      RPAR(11) = VDCO
      RPAR(12) = HACO
C
C     Pointers into IPAR and RPAR
      P_IPP = 7
      P_BD  = 13
      P_P   = P_BD + 4*MM
C
      IPAR(4) = P_IPP
      IPAR(5) = P_BD
      IPAR(6) = P_P
C
C     Set initial profiles.
      DO JY = 1, MY
         Y = 30.0D0 + (JY - 1.0D0) * DY
         CY = (0.1D0 * (Y - 40.0D0))**2
         CY = 1.0D0 - CY + 0.5D0 * CY**2
         DO JX = 1, MX
            X = (JX - 1.0D0) * DX
            CX = (0.1D0 * (X - 10.0D0))**2
            CX = 1.0D0 - CX + 0.5D0 * CX**2
            U0(1,JX,JY) = 1.0D6 * CX * CY
            U0(2,JX,JY) = 1.0D12 * CX * CY
         ENDDO
      ENDDO
C
      RETURN
```

```
      END

C     ----------------------------------------------------------------

      SUBROUTINE FCVFUN(T, U, UDOT, IPAR, RPAR, IER)
C     Routine for right-hand side function f
C
      IMPLICIT NONE
C
      DOUBLE PRECISION T, U(2,*), UDOT(2,*), RPAR(*)
      INTEGER*4 IPAR(*), IER
C
      INTEGER ILEFT, IRIGHT
      INTEGER*4 JX, JY, MX, MY, MM, IBLOK0, IBLOK, IDN, IUP
      DOUBLE PRECISION Q1, Q2, Q3, Q4, A3, A4, OM, C3, DY, HDCO
      DOUBLE PRECISION VDCO, HACO
      DOUBLE PRECISION C1, C2, C1DN, C2DN, C1UP, C2UP, C1LT, C2LT
      DOUBLE PRECISION C1RT, C2RT, CYDN, CYUP, HORD1, HORD2, HORAD1
      DOUBLE PRECISION HORAD2, QQ1, QQ2, QQ3, QQ4, RKIN1, RKIN2, S
      DOUBLE PRECISION VERTD1, VERTD2, YDN, YUP
C
C     Extract constants from IPAR and RPAR
      MX = IPAR(1)
      MY = IPAR(2)
      MM = IPAR(3)
C
      Q1 = RPAR(1)
      Q2 = RPAR(2)
      Q3 = RPAR(3)
      Q4 = RPAR(4)
      A3 = RPAR(5)
      A4 = RPAR(6)
      OM = RPAR(7)
      C3 = RPAR(8)
      DY = RPAR(9)
      HDCO = RPAR(10)
      VDCO = RPAR(11)
      HACO = RPAR(12)
C
C     Set diurnal rate coefficients.
      S = SIN(OM * T)
      IF (S .GT. 0.0D0) THEN
         Q3 = EXP(-A3 / S)
         Q4 = EXP(-A4 / S)
      ELSE
         Q3 = 0.0D0
         Q4 = 0.0D0
      ENDIF
      RPAR(3) = Q3
      RPAR(4) = Q4
C
C     Loop over all grid points.
      DO JY = 1, MY
         YDN = 30.0D0 + (JY - 1.5D0) * DY
         YUP = YDN + DY
         CYDN = VDCO * EXP(0.2D0 * YDN)
         CYUP = VDCO * EXP(0.2D0 * YUP)
         IBLOK0 = (JY - 1) * MX
         IDN = -MX
```

```
294            IF (JY .EQ. 1) IDN = MX
295            IUP = MX
296            IF (JY .EQ. MY) IUP = -MX
297            DO JX = 1, MX
298               IBLOK = IBLOK0 + JX
299               C1 = U(1,IBLOK)
300               C2 = U(2,IBLOK)
301     C      Set kinetic rate terms.
302               QQ1 = Q1 * C1 * C3
303               QQ2 = Q2 * C1 * C2
304               QQ3 = Q3 * C3
305               QQ4 = Q4 * C2
306               RKIN1 = -QQ1 - QQ2 + 2.0D0 * QQ3 + QQ4
307               RKIN2 = QQ1 - QQ2 - QQ4
308     C      Set vertical diffusion terms.
309               C1DN = U(1,IBLOK + IDN)
310               C2DN = U(2,IBLOK + IDN)
311               C1UP = U(1,IBLOK + IUP)
312               C2UP = U(2,IBLOK + IUP)
313               VERTD1 = CYUP * (C1UP - C1) - CYDN * (C1 - C1DN)
314               VERTD2 = CYUP * (C2UP - C2) - CYDN * (C2 - C2DN)
315     C      Set horizontal diffusion and advection terms.
316               ILEFT = -1
317               IF (JX .EQ. 1) ILEFT = 1
318               IRIGHT = 1
319               IF (JX .EQ. MX) IRIGHT = -1
320               C1LT = U(1,IBLOK + ILEFT)
321               C2LT = U(2,IBLOK + ILEFT)
322               C1RT = U(1,IBLOK + IRIGHT)
323               C2RT = U(2,IBLOK + IRIGHT)
324               HORD1 = HDCO * (C1RT - 2.0D0 * C1 + C1LT)
325               HORD2 = HDCO * (C2RT - 2.0D0 * C2 + C2LT)
326               HORAD1 = HACO * (C1RT - C1LT)
327               HORAD2 = HACO * (C2RT - C2LT)
328     C      Load all terms into UDOT.
329               UDOT(1,IBLOK) = VERTD1 + HORD1 + HORAD1 + RKIN1
330               UDOT(2,IBLOK) = VERTD2 + HORD2 + HORAD2 + RKIN2
331            ENDDO
332         ENDDO
333     C
334         IER = 0
335     C
336         RETURN
337         END
338
339     C   ----------------------------------------------------------------------
340
341         SUBROUTINE FCVPSET(T, U, FU, JOK, JCUR, GAMMA, H,
342        &                   IPAR, RPAR, V1, V2, V3, IER)
343     C   Routine to set and preprocess block-diagonal preconditioner.
344     C   Note: The dimensions in /BDJ/ below assume at most 100 mesh points.
345     C
346         IMPLICIT NONE
347     C
348         INTEGER IER, JOK, JCUR
349         DOUBLE PRECISION T, U(2,*), FU(*), GAMMA, H
350         INTEGER*4 IPAR(*)
351         DOUBLE PRECISION RPAR(*), V1(*), V2(*), V3(*)
352     C
```

```
      INTEGER*4 MX, MY, MM, P_IPP, P_BD, P_P
      DOUBLE PRECISION Q1, Q2, Q3, Q4, C3, DY, HDCO, VDCO
C
      IER = 0
C
C     Extract constants from IPAR and RPAR
      MX = IPAR(1)
      MY = IPAR(2)
      MM = IPAR(3)
C
      Q1 = RPAR(1)
      Q2 = RPAR(2)
      Q3 = RPAR(3)
      Q4 = RPAR(4)
      C3 = RPAR(8)
      DY = RPAR(9)
      HDCO = RPAR(10)
      VDCO = RPAR(11)
C
C     Extract pointers into IPAR and RPAR
      P_IPP = IPAR(4)
      P_BD  = IPAR(5)
      P_P   = IPAR(6)
C
C     If needed, recompute BD
C
      IF (JOK .EQ. 1) THEN
C     JOK = 1. Use saved BD
        JCUR = 0
      ELSE
C     JOK = 0. Compute diagonal Jacobian blocks.
C     (using q4 value computed on last FCVFUN call).
         CALL PREC_JAC(MX, MY, MM, U, RPAR(P_BD),
     &        Q1, Q2, Q3, Q4, C3, DY, HDCO, VDCO)
         JCUR = 1
      ENDIF
C
C     Copy BD to P
      CALL DCOPY(4*MM, RPAR(P_BD), 1, RPAR(P_P), 1)
C
C     Scale P by -GAMMA
      CALL DSCAL(4*MM, -GAMMA, RPAR(P_P), 1)
C
C     Perform LU decomposition
      CALL PREC_LU(MM, RPAR(P_P), IPAR(P_IPP), IER)
C
      RETURN
      END

C     ----------------------------------------------------------------

      SUBROUTINE FCVPSOL(T, U, FU, R, Z, GAMMA, DELTA, LR,
     &                   IPAR, RPAR, VTEMP, IER)
C     Routine to solve preconditioner linear system.
C
      IMPLICIT NONE
C
      INTEGER IER, LR
      INTEGER*4 IPAR(*)
```

```
412         DOUBLE PRECISION T, U(*), FU(*), R(*), Z(2,*)
413         DOUBLE PRECISION GAMMA, DELTA, RPAR(*)
414         DOUBLE PRECISION VTEMP(*)
415   C
416         INTEGER*4 MM, P_IPP, P_P
417   C
418         IER = 0
419   C
420   C     Extract constants from IPAR and RPAR
421         MM  = IPAR(3)
422   C
423   C     Extract pointers into IPAR and RPAR
424         P_IPP = IPAR(4)
425         P_P   = IPAR(6)
426   C
427   C     Copy RHS into Z
428         CALL DCOPY(2*MM, R, 1, Z, 1)
429   C
430   C     Solve the block-diagonal system Px = r using LU factors stored in P
431   C     and pivot data in IPP, and return the solution in Z.
432         CALL PREC_SOL(MM, RPAR(P_P), IPAR(P_IPP), Z)
433
434         RETURN
435         END
436
437   C     ------------------------------------------------------------------
438
439         SUBROUTINE PREC_JAC(MX, MY, MM, U, BD,
440        &     Q1, Q2, Q3, Q4, C3, DY, HDCO, VDCO)
441   C     Routine to compute diagonal Jacobian blocks
442   C
443         IMPLICIT NONE
444   C
445         INTEGER*4 MX, MY, MM
446         DOUBLE PRECISION U(2,*), BD(2,2,MM)
447         DOUBLE PRECISION Q1, Q2, Q3, Q4, C3, DY, HDCO, VDCO
448   C
449         INTEGER*4 JY, JX, IBLOK, IBLOK0
450         DOUBLE PRECISION C1, C2, CYDN, CYUP, DIAG, YDN, YUP
451   C
452         DO JY = 1, MY
453            YDN = 30.0D0 + (JY - 1.5D0) * DY
454            YUP = YDN + DY
455            CYDN = VDCO * EXP(0.2D0 * YDN)
456            CYUP = VDCO * EXP(0.2D0 * YUP)
457            DIAG = -(CYDN + CYUP + 2.0D0 * HDCO)
458            IBLOK0 = (JY - 1) * MX
459            DO JX = 1, MX
460               IBLOK = IBLOK0 + JX
461               C1 = U(1,IBLOK)
462               C2 = U(2,IBLOK)
463               BD(1,1,IBLOK) = (-Q1 * C3 - Q2 * C2) + DIAG
464               BD(1,2,IBLOK) = -Q2 * C1 + Q4
465               BD(2,1,IBLOK) =  Q1 * C3 - Q2 * C2
466               BD(2,2,IBLOK) = (-Q2 * C1 - Q4) + DIAG
467            ENDDO
468         ENDDO
469
470         RETURN
```

```
471         END
472
473   C     ------------------------------------------------------------------
474
475         SUBROUTINE PREC_LU(MM, P, IPP, IER)
476   C     Routine to perform LU decomposition on (P+I)
477   C
478         IMPLICIT NONE
479   C
480         INTEGER IER
481         INTEGER*4 MM, IPP(2,MM)
482         DOUBLE PRECISION P(2,2,MM)
483   C
484         INTEGER*4 I
485   C
486   C     Add identity matrix and do LU decompositions on blocks, in place.
487         DO I = 1, MM
488            P(1,1,I) = P(1,1,I) + 1.0D0
489            P(2,2,I) = P(2,2,I) + 1.0D0
490            CALL DGEFA(P(1,1,I), 2, 2, IPP(1,I), IER)
491            IF (IER .NE. 0) RETURN
492         ENDDO
493   C
494         RETURN
495         END
496
497   C     ------------------------------------------------------------------
498
499         SUBROUTINE PREC_SOL(MM, P, IPP, Z)
500   C     Routine for backsolve
501   C
502         IMPLICIT NONE
503   C
504         INTEGER*4 MM, IPP(2,MM)
505         DOUBLE PRECISION P(2,2,MM), Z(2,MM)
506   C
507         INTEGER*4 I
508   C
509         DO I = 1, MM
510            CALL DGESL(P(1,1,I), 2, 2, IPP(1,I), Z(1,I), 0)
511         ENDDO
512
513         RETURN
514         END
515
516   C     ------------------------------------------------------------------
517
518         subroutine dgefa(a, lda, n, ipvt, info)
519   c
520         implicit none
521   c
522         integer info, idamax, j, k, kp1, l, nm1, n
523         integer*4 lda, ipvt(1)
524         double precision a(lda,1), t
525   c
526   c     dgefa factors a double precision matrix by gaussian elimination.
527   c
528   c     dgefa is usually called by dgeco, but it can be called
529   c     directly with a saving in time if  rcond  is not needed.
```

```
530   c     (time for dgeco) = (1 + 9/n)*(time for dgefa) .
531   c
532   c     on entry
533   c
534   c        a        double precision(lda, n)
535   c                 the matrix to be factored.
536   c
537   c        lda      integer
538   c                 the leading dimension of the array  a .
539   c
540   c        n        integer
541   c                 the order of the matrix  a .
542   c
543   c     on return
544   c
545   c        a        an upper triangular matrix and the multipliers
546   c                 which were used to obtain it.
547   c                 the factorization can be written  a = l*u  where
548   c                 l  is a product of permutation and unit lower
549   c                 triangular matrices and  u  is upper triangular.
550   c
551   c        ipvt     integer(n)
552   c                 an integer vector of pivot indices.
553   c
554   c        info     integer
555   c                 = 0  normal value.
556   c                 = k  if  u(k,k) .eq. 0.0 .  this is not an error
557   c                      condition for this subroutine, but it does
558   c                      indicate that dgesl or dgedi will divide by zero
559   c                      if called.  use  rcond  in dgeco for a reliable
560   c                      indication of singularity.
561   c
562   c     linpack. this version dated 08/14/78 .
563   c     cleve moler, university of new mexico, argonne national lab.
564   c
565   c     subroutines and functions
566   c
567   c     blas daxpy,dscal,idamax
568   c
569   c     internal variables
570   c
571   c     gaussian elimination with partial pivoting
572   c
573         info = 0
574         nm1 = n - 1
575         if (nm1 .lt. 1) go to 70
576         do 60 k = 1, nm1
577            kp1 = k + 1
578   c
579   c        find l = pivot index
580   c
581            l = idamax(n - k + 1, a(k,k), 1) + k - 1
582            ipvt(k) = l
583   c
584   c        zero pivot implies this column already triangularized
585   c
586            if (a(l,k) .eq. 0.0d0) go to 40
587   c
588   c           interchange if necessary
```

```
c
               if (l .eq. k) go to 10
                  t = a(l,k)
                  a(l,k) = a(k,k)
                  a(k,k) = t
   10          continue
c
c              compute multipliers
c
               t = -1.0d0 / a(k,k)
               call dscal(n - k, t, a(k + 1,k), 1)
c
c              row elimination with column indexing
c
               do 30 j = kp1, n
                  t = a(l,j)
                  if (l .eq. k) go to 20
                     a(l,j) = a(k,j)
                     a(k,j) = t
   20             continue
                  call daxpy(n - k, t, a(k + 1,k), 1, a(k + 1,j), 1)
   30          continue
            go to 50
   40       continue
               info = k
   50       continue
   60    continue
   70    continue
         ipvt(n) = n
         if (a(n,n) .eq. 0.0d0) info = n
         return
         end

C        ------------------------------------------------------------------

         subroutine dgesl(a, lda, n, ipvt, b, job)
c
         implicit none
c
         integer lda, n, job, k, kb, l, nm1
         integer*4 ipvt(1)
         double precision a(lda,1), b(1), ddot, t
c
c        dgesl solves the double precision system
c        a * x = b  or  trans(a) * x = b
c        using the factors computed by dgeco or dgefa.
c
c        on entry
c
c           a       double precision(lda, n)
c                   the output from dgeco or dgefa.
c
c           lda     integer
c                   the leading dimension of the array  a .
c
c           n       integer
c                   the order of the matrix  a .
c
c           ipvt    integer(n)
```

```
c                the pivot vector from dgeco or dgefa.
c
c        b       double precision(n)
c                the right hand side vector.
c
c        job     integer
c                = 0         to solve  a*x = b ,
c                = nonzero   to solve  trans(a)*x = b  where
c                            trans(a)  is the transpose.
c
c     on return
c
c        b       the solution vector  x .
c
c     error condition
c
c        a division by zero will occur if the input factor contains a
c        zero on the diagonal.  technically this indicates singularity
c        but it is often caused by improper arguments or improper
c        setting of lda .  it will not occur if the subroutines are
c        called correctly and if dgeco has set rcond .gt. 0.0
c        or dgefa has set info .eq. 0 .
c
c     to compute  inverse(a) * c  where  c  is a matrix
c     with  p  columns
c           call dgeco(a,lda,n,ipvt,rcond,z)
c           if (rcond is too small) go to ...
c           do 10 j = 1, p
c              call dgesl(a,lda,n,ipvt,c(1,j),0)
c        10 continue
c
c     linpack. this version dated 08/14/78 .
c     cleve moler, university of new mexico, argonne national lab.
c
c     subroutines and functions
c
c     blas daxpy,ddot
c
c     internal variables
c
      nm1 = n - 1
      if (job .ne. 0) go to 50
c
c        job = 0 , solve  a * x = b
c        first solve  l*y = b
c
         if (nm1 .lt. 1) go to 30
         do 20 k = 1, nm1
            l = ipvt(k)
            t = b(l)
            if (l .eq. k) go to 10
               b(l) = b(k)
               b(k) = t
   10       continue
            call daxpy(n - k, t, a(k + 1,k), 1, b(k + 1), 1)
   20    continue
   30    continue
c
c        now solve  u*x = y
```

```
c
            do 40 kb = 1, n
               k = n + 1 - kb
               b(k) = b(k) / a(k,k)
               t = -b(k)
               call daxpy(k - 1, t, a(1,k), 1, b(1), 1)
   40       continue
         go to 100
   50    continue
c
c           job = nonzero, solve  trans(a) * x = b
c           first solve  trans(u)*y = b
c
            do 60 k = 1, n
               t = ddot(k - 1, a(1,k), 1, b(1), 1)
               b(k) = (b(k) - t) / a(k,k)
   60       continue
c
c           now solve trans(l)*x = y
c
            if (nm1 .lt. 1) go to 90
            do 80 kb = 1, nm1
               k = n - kb
               b(k) = b(k) + ddot(n - k, a(k + 1,k), 1, b(k + 1), 1)
               l = ipvt(k)
               if (l .eq. k) go to 70
                  t = b(l)
                  b(l) = b(k)
                  b(k) = t
   70          continue
   80       continue
   90       continue
  100    continue
         return
         end

C        ----------------------------------------------------------------------

         subroutine daxpy(n, da, dx, incx, dy, incy)
c
c        constant times a vector plus a vector.
c        uses unrolled loops for increments equal to one.
c        jack dongarra, linpack, 3/11/78.
c
         implicit none
c
         integer i, incx, incy, ix, iy, m, mp1
         integer*4 n
         double precision dx(1), dy(1), da
c
         if (n .le. 0) return
         if (da .eq. 0.0d0) return
         if (incx .eq. 1 .and. incy .eq. 1) go to 20
c
c           code for unequal increments or equal increments
c           not equal to 1
c
         ix = 1
         iy = 1
```

```
766         if (incx .lt. 0) ix = (-n + 1) * incx + 1
767         if (incy .lt. 0) iy = (-n + 1) * incy + 1
768         do 10 i = 1, n
769           dy(iy) = dy(iy) + da * dx(ix)
770           ix = ix + incx
771           iy = iy + incy
772      10 continue
773         return
774   c
775   c        code for both increments equal to 1
776   c
777   c
778   c        clean-up loop
779   c
780      20 m = mod(n, 4)
781         if ( m .eq. 0 ) go to 40
782         do 30 i = 1, m
783           dy(i) = dy(i) + da * dx(i)
784      30 continue
785         if ( n .lt. 4 ) return
786      40 mp1 = m + 1
787         do 50 i = mp1, n, 4
788           dy(i) = dy(i) + da * dx(i)
789           dy(i + 1) = dy(i + 1) + da * dx(i + 1)
790           dy(i + 2) = dy(i + 2) + da * dx(i + 2)
791           dy(i + 3) = dy(i + 3) + da * dx(i + 3)
792      50 continue
793         return
794         end
795   C     ------------------------------------------------------------------
796
797         subroutine dscal(n, da, dx, incx)
798   c
799   c     scales a vector by a constant.
800   c     uses unrolled loops for increment equal to one.
801   c     jack dongarra, linpack, 3/11/78.
802   c
803         implicit none
804   c
805         integer i, incx, m, mp1, nincx
806         integer*4 n
807         double precision da, dx(1)
808   c
809         if (n.le.0) return
810         if (incx .eq. 1) go to 20
811   c
812   c        code for increment not equal to 1
813   c
814         nincx = n * incx
815         do 10 i = 1, nincx, incx
816           dx(i) = da * dx(i)
817      10 continue
818         return
819   c
820   c        code for increment equal to 1
821   c
822   c
823   c        clean-up loop
824   c
```

```
825      20 m = mod(n, 5)
826         if ( m .eq. 0 ) go to 40
827         do 30 i = 1, m
828           dx(i) = da * dx(i)
829      30 continue
830         if ( n .lt. 5 ) return
831      40 mp1 = m + 1
832         do 50 i = mp1, n, 5
833           dx(i) = da * dx(i)
834           dx(i + 1) = da * dx(i + 1)
835           dx(i + 2) = da * dx(i + 2)
836           dx(i + 3) = da * dx(i + 3)
837           dx(i + 4) = da * dx(i + 4)
838      50 continue
839         return
840         end
841
842   C     ------------------------------------------------------------------
843
844         double precision function ddot(n, dx, incx, dy, incy)
845   c
846   c     forms the dot product of two vectors.
847   c     uses unrolled loops for increments equal to one.
848   c     jack dongarra, linpack, 3/11/78.
849   c
850         implicit none
851   c
852         integer i, incx, incy, ix, iy, m, mp1
853         integer*4 n
854         double precision dx(1), dy(1), dtemp
855   c
856         ddot = 0.0d0
857         dtemp = 0.0d0
858         if (n .le. 0) return
859         if (incx .eq. 1 .and. incy .eq. 1) go to 20
860   c
861   c        code for unequal increments or equal increments
862   c          not equal to 1
863   c
864         ix = 1
865         iy = 1
866         if (incx .lt. 0) ix = (-n + 1) * incx + 1
867         if (incy .lt. 0) iy = (-n + 1) * incy + 1
868         do 10 i = 1, n
869           dtemp = dtemp + dx(ix) * dy(iy)
870           ix = ix + incx
871           iy = iy + incy
872      10 continue
873         ddot = dtemp
874         return
875   c
876   c        code for both increments equal to 1
877   c
878   c
879   c        clean-up loop
880   c
881      20 m = mod(n, 5)
882         if ( m .eq. 0 ) go to 40
883         do 30 i = 1,m
```

```
884           dtemp = dtemp + dx(i) * dy(i)
885       30  continue
886           if ( n .lt. 5 ) go to 60
887       40  mp1 = m + 1
888           do 50 i = mp1, n, 5
889             dtemp = dtemp + dx(i) * dy(i) + dx(i + 1) * dy(i + 1) +
890      *                dx(i + 2) * dy(i + 2) + dx(i + 3) * dy(i + 3) +
891      *                dx(i + 4) * dy(i + 4)
892       50  continue
893       60  ddot = dtemp
894           return
895           end
896
897   C       ------------------------------------------------------------------
898
899           integer function idamax(n, dx, incx)
900   c
901   c       finds the index of element having max. absolute value.
902   c       jack dongarra, linpack, 3/11/78.
903   c
904           implicit none
905   c
906           integer i, incx, ix
907           integer*4 n
908           double precision dx(1), dmax
909   c
910           idamax = 0
911           if (n .lt. 1) return
912           idamax = 1
913           if (n .eq. 1) return
914           if (incx .eq. 1) go to 20
915   c
916   c          code for increment not equal to 1
917   c
918           ix = 1
919           dmax = abs(dx(1))
920           ix = ix + incx
921           do 10 i = 2, n
922              if (abs(dx(ix)) .le. dmax) go to 5
923              idamax = i
924              dmax = abs(dx(ix))
925        5     ix = ix + incx
926       10  continue
927           return
928   c
929   c          code for increment equal to 1
930   c
931       20  dmax = abs(dx(1))
932           do 30 i = 2, n
933              if (abs(dx(i)) .le. dmax) go to 30
934              idamax = i
935              dmax = abs(dx(i))
936       30  continue
937           return
938           end
939
940   C       ------------------------------------------------------------------
941
942           subroutine  dcopy(n, dx, incx, dy, incy)
```

```
c
c     copies a vector, x, to a vector, y.
c     uses unrolled loops for increments equal to one.
c     jack dongarra, linpack, 3/11/78.
c
      implicit none
c
      integer i, incx, incy, ix, iy, m, mp1
      integer*4 n
      double precision dx(1), dy(1)
c
      if (n .le. 0) return
      if (incx .eq. 1 .and. incy .eq. 1) go to 20
c
c        code for unequal increments or equal increments
c          not equal to 1
c
      ix = 1
      iy = 1
      if (incx .lt. 0) ix = (-n + 1) * incx + 1
      if (incy .lt. 0) iy = (-n + 1) * incy + 1
      do 10 i = 1, n
        dy(iy) = dx(ix)
        ix = ix + incx
        iy = iy + incy
   10 continue
      return
c
c        code for both increments equal to 1
c
c
c        clean-up loop
c
   20 m = mod(n, 7)
      if ( m .eq. 0 ) go to 40
      do 30 i = 1, m
        dy(i) = dx(i)
   30 continue
      if ( n .lt. 7 ) return
   40 mp1 = m + 1
      do 50 i = mp1, n, 7
        dy(i) = dx(i)
        dy(i + 1) = dx(i + 1)
        dy(i + 2) = dx(i + 2)
        dy(i + 3) = dx(i + 3)
        dy(i + 4) = dx(i + 4)
        dy(i + 5) = dx(i + 5)
        dy(i + 6) = dx(i + 6)
   50 continue
      return
      end
```

H Listing of fcvkryx_bbd_p.f

```
C     ------------------------------------------------------------------
C     $Revision: 1.1 $
C     $Date: 2006/07/05 15:50:04 $
C     ------------------------------------------------------------------
C     Diagonal ODE example.  Stiff case, with diagonal preconditioner.
C     Uses FCVODE interfaces and FCVBBD interfaces.
C     Solves problem twice -- with left and right preconditioning.
C     ------------------------------------------------------------------
C
C     Include MPI-Fortran header file for MPI_COMM_WORLD, MPI types.

      IMPLICIT NONE
C
      INCLUDE "mpif.h"
C
      INTEGER*4 NLOCAL
      PARAMETER (NLOCAL=10)
C
      INTEGER NOUT, LNST, LNFE, LNSETUP, LNNI, LNCF, LNETF, LNPE
      INTEGER LNLI, LNPS, LNCFL, MYPE, IER, NPES, METH, ITMETH
      INTEGER LLENRW, LLENIW, LLENRWLS, LLENIWLS
      INTEGER IATOL, ITASK, IPRE, IGS, JOUT
      INTEGER*4 IOUT(25), IPAR(2)
      INTEGER*4 NEQ, I, MUDQ, MLDQ, MU, ML, NETF
      INTEGER*4 NST, NFE, NPSET, NPE, NPS, NNI, NLI, NCFN, NCFL, NGEBBD
      INTEGER*4 LENRW, LENIW, LENRWLS, LENIWLS, LENRWBBD, LENIWBBD
      DOUBLE PRECISION Y(1024), ROUT(10), RPAR(1)
      DOUBLE PRECISION ALPHA, TOUT, ERMAX, AVDIM
      DOUBLE PRECISION ATOL, ERRI, RTOL, GERMAX, DTOUT, T
C
      DATA ATOL/1.0D-10/, RTOL/1.0D-5/, DTOUT/0.1D0/, NOUT/10/
      DATA LLENRW/1/, LLENIW/2/, LNST/3/, LNFE/4/, LNETF/5/,  LNCF/6/,
     1     LNNI/7/, LNSETUP/8/, LLENRWLS/13/, LLENIWLS/14/,
     1     LNPE/18/, LNLI/20/, LNPS/19/, LNCFL/21/
C
C     Get NPES and MYPE.  Requires initialization of MPI.
      CALL MPI_INIT(IER)
      IF (IER .NE. 0) THEN
         WRITE(6,5) IER
 5       FORMAT(///' MPI_ERROR: MPI_INIT returned IER = ', I5)
         STOP
      ENDIF
      CALL MPI_COMM_SIZE(MPI_COMM_WORLD, NPES, IER)
      IF (IER .NE. 0) THEN
         WRITE(6,6) IER
 6       FORMAT(///' MPI_ERROR: MPI_COMM_SIZE returned IER = ', I5)
         CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
         STOP
      ENDIF
      CALL MPI_COMM_RANK(MPI_COMM_WORLD, MYPE, IER)
      IF (IER .NE. 0) THEN
         WRITE(6,7) IER
 7       FORMAT(///' MPI_ERROR: MPI_COMM_RANK returned IER = ', I5)
         CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
         STOP
      ENDIF
C
```

```
C     Set input arguments.
      NEQ = NPES * NLOCAL
      T = 0.0D0
      METH = 2
      ITMETH = 2
      IATOL = 1
      ITASK = 1
      IPRE = 1
      IGS = 1
C     Set parameter alpha
      ALPHA  = 10.0D0
C
C     Load IPAR and RPAR
      IPAR(1) = NLOCAL
      IPAR(2) = MYPE
      RPAR(1) = ALPHA
C
      DO I = 1, NLOCAL
         Y(I) = 1.0D0
      ENDDO
C
      IF (MYPE .EQ. 0) THEN
         WRITE(6,15) NEQ, ALPHA, RTOL, ATOL, NPES
 15      FORMAT('Diagonal test problem:'//' NEQ = ', I3, /
     &          ' parameter alpha = ', F8.3/
     &          ' ydot_i = -alpha*i * y_i (i = 1,...,NEQ)'/
     &          ' RTOL, ATOL = ', 2E10.1/
     &          ' Method is BDF/NEWTON/SPGMR'/
     &          ' Preconditioner is band-block-diagonal, using CVBBDPRE'
     &         /' Number of processors = ', I3/)
      ENDIF
C
      CALL FNVINITP(MPI_COMM_WORLD, 1, NLOCAL, NEQ, IER)
C
      IF (IER .NE. 0) THEN
         WRITE(6,20) IER
 20      FORMAT(///' SUNDIALS_ERROR: FNVINITP returned IER = ', I5)
         CALL MPI_FINALIZE(IER)
         STOP
      ENDIF
C
      CALL FCVMALLOC(T, Y, METH, ITMETH, IATOL, RTOL, ATOL,
     &               IOUT, ROUT, IPAR, RPAR, IER)
C
      IF (IER .NE. 0) THEN
         WRITE(6,30) IER
 30      FORMAT(///' SUNDIALS_ERROR: FCVMALLOC returned IER = ', I5)
         CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
         STOP
      ENDIF
C
      MUDQ = 0
      MLDQ = 0
      MU = 0
      ML = 0
      CALL FCVBBDINIT(NLOCAL, MUDQ, MLDQ, MU, ML, 0.0D0, IER)
      IF (IER .NE. 0) THEN
         WRITE(6,35) IER
 35      FORMAT(///' SUNDIALS_ERROR: FCVBBDINIT returned IER = ', I5)
```

```
117           CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
118           STOP
119        ENDIF
120  C
121        CALL FCVBBDSPGMR(IPRE, IGS, 0, 0.0D0, IER)
122        IF (IER .NE. 0) THEN
123           WRITE(6,36) IER
124   36      FORMAT(///' SUNDIALS_ERROR: FCVBBDSPGMR returned IER = ', I5)
125           CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
126           STOP
127        ENDIF
128  C
129        IF (MYPE .EQ. 0) WRITE(6,38)
130   38   FORMAT(/'Preconditioning on left'/)
131  C
132  C     Looping point for cases IPRE = 1 and 2.
133  C
134   40   CONTINUE
135  C
136  C     Loop through tout values, call solver, print output, test for failure.
137        TOUT = DTOUT
138        DO 60 JOUT = 1, NOUT
139  C
140           CALL FCVODE(TOUT, T, Y, ITASK, IER)
141  C
142           IF (MYPE .EQ. 0) WRITE(6,45) T, IOUT(LNST), IOUT(LNFE)
143   45      FORMAT(' t = ', E10.2, 5X, 'no. steps = ', I5,
144       &          '   no. f-s = ', I5)
145  C
146           IF (IER .NE. 0) THEN
147              WRITE(6,50) IER, IOUT(15)
148   50         FORMAT(///' SUNDIALS_ERROR: FCVODE returned IER = ', I5, /,
149       &              '                 Linear Solver returned IER = ', I5)
150              CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
151              STOP
152           ENDIF
153  C
154           TOUT = TOUT + DTOUT
155   60   CONTINUE
156  C
157  C     Get max. absolute error in the local vector.
158        ERMAX = 0.0D0
159        DO 65 I = 1, NLOCAL
160           ERRI  = Y(I) - EXP(-ALPHA * (MYPE * NLOCAL + I) * T)
161           ERMAX = MAX(ERMAX, ABS(ERRI))
162   65   CONTINUE
163  C     Get global max. error from MPI_REDUCE call.
164        CALL MPI_REDUCE(ERMAX, GERMAX, 1, MPI_DOUBLE_PRECISION, MPI_MAX,
165       &                0, MPI_COMM_WORLD, IER)
166        IF (IER .NE. 0) THEN
167           WRITE(6,70) IER
168   70      FORMAT(///' MPI_ERROR: MPI_REDUCE returned IER = ', I5)
169           CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
170           STOP
171        ENDIF
172        IF (MYPE .EQ. 0) WRITE(6,75) GERMAX
173   75   FORMAT(/'Max. absolute error is', E10.2/)
174  C
175  C     Print final statistics.
```

```
      IF (MYPE .EQ. 0) THEN
         NST = IOUT(LNST)
         NFE = IOUT(LNFE)
         NPSET = IOUT(LNSETUP)
         NPE = IOUT(LNPE)
         NPS = IOUT(LNPS)
         NNI = IOUT(LNNI)
         NLI = IOUT(LNLI)
         AVDIM = DBLE(NLI) / DBLE(NNI)
         NCFN = IOUT(LNCF)
         NCFL = IOUT(LNCFL)
         NETF = IOUT(LNETF)
         LENRW = IOUT(LLENRW)
         LENIW = IOUT(LLENIW)
         LENRWLS = IOUT(LLENRWLS)
         LENIWLS = IOUT(LLENIWLS)
         WRITE(6,80) NST, NFE, NPSET, NPE, NPS, NNI, NLI, AVDIM, NCFN,
     &               NCFL, NETF, LENRW, LENIW, LENRWLS, LENIWLS
 80      FORMAT(/'Final statistics:'//
     &          ' number of steps        = ', I5, 4X,
     &          ' number of f evals.     = ', I5/
     &          ' number of prec. setups = ', I5/
     &          ' number of prec. evals. = ', I5, 4X,
     &          ' number of prec. solves = ', I5/
     &          ' number of nonl. iters. = ', I5, 4X,
     &          ' number of lin. iters.  = ', I5/
     &          ' average Krylov subspace dimension (NLI/NNI) = ',F8.4/
     &          ' number of conv. failures.. nonlinear = ', I3,
     &          '  linear = ', I3/
     &          ' number of error test failures = ', I3/
     &          ' main solver real/int workspace sizes   = ',2I5/
     &          ' linear solver real/int workspace sizes = ',2I5)
         CALL FCVBBDOPT(LENRWBBD, LENIWBBD, NGEBBD)
         WRITE(6,82) LENRWBBD, LENIWBBD, NGEBBD
 82      FORMAT('In CVBBDPRE:'/
     &          ' real/int local workspace = ', 2I5/
     &          ' number of g evals. = ', I5)
      ENDIF
C
C     If IPRE = 1, re-initialize T, Y, and the solver, and loop for
C     case IPRE = 2.  Otherwise jump to final block.
      IF (IPRE .EQ. 2) GO TO 99
C
      T = 0.0D0
      DO I = 1, NLOCAL
         Y(I) = 1.0D0
      ENDDO
C
      CALL FCVREINIT(T, Y, IATOL, RTOL, ATOL, IER)
      IF (IER .NE. 0) THEN
         WRITE(6,91) IER
 91      FORMAT(///' SUNDIALS_ERROR: FCVREINIT returned IER = ', I5)
         CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
         STOP
      ENDIF
C
      IPRE = 2
C
      CALL FCVBBDREINIT(NLOCAL, MUDQ, MLDQ, 0.0D0, IER)
```

```
      IF (IER .NE. 0) THEN
         WRITE(6,92) IER
 92      FORMAT(///' SUNDIALS_ERROR: FCVBBDREINIT returned IER = ', I5)
         CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
         STOP
      ENDIF
C
      CALL FCVSPGMRREINIT(IPRE, IGS, 0.0D0, IER)
      IF (IER .NE. 0) THEN
         WRITE(6,93) IER
 93      FORMAT(///' SUNDIALS_ERROR: FCVSPGMRREINIT returned IER = ',I5)
         CALL MPI_ABORT(MPI_COMM_WORLD, 1, IER)
         STOP
      ENDIF
C
      IF (MYPE .EQ. 0) WRITE(6,95)
 95   FORMAT(//60('-')///'Preconditioning on right'/)
      GO TO 40
C
C     Free the memory and finalize MPI.
 99   CALL FCVBBDFREE
      CALL FCVFREE
      CALL MPI_FINALIZE(IER)
C
      STOP
      END
C
C     ------------------------------------------------------------------------
C
      SUBROUTINE FCVFUN(T, Y, YDOT, IPAR, RPAR, IER)
C     Routine for right-hand side function f
      IMPLICIT NONE
C
      INTEGER*4 IPAR(*), IER
      DOUBLE PRECISION T, Y(*), YDOT(*), RPAR(*)
C
      INTEGER MYPE
      INTEGER*4 I, NLOCAL
      DOUBLE PRECISION ALPHA
C
      NLOCAL = IPAR(1)
      MYPE = IPAR(2)
      ALPHA = RPAR(1)
C
      DO I = 1, NLOCAL
         YDOT(I) = -ALPHA * (MYPE * NLOCAL + I) * Y(I)
      ENDDO
C
      IER = 0
C
      RETURN
      END
C
C     ------------------------------------------------------------------------
C
      SUBROUTINE FCVGLOCFN(NLOC, T, YLOC, GLOC, IPAR, RPAR, IER)
C     Routine to define local approximate function g, here the same as f.
      IMPLICIT NONE
C
```

```
      INTEGER*4 NLOC, IPAR(*), IER
      DOUBLE PRECISION T, YLOC(*), GLOC(*), RPAR(*)
C
      CALL FCVFUN(T, YLOC, GLOC, IPAR, RPAR, IER)
C
      RETURN
      END
C
C     ----------------------------------------------------------------------
C
      SUBROUTINE FCVCOMMFN(NLOC, T, YLOC, IPAR, RPAR, IER)
C     Routine to perform communication required for evaluation of g.
      IER = 0
      RETURN
      END
```