PPODE SUITE
Manual

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Chapter 1

Installation

The PPODE SUITE package depends on:

MATLAB Tested on MATLAB version R2013b (8.2) 64-bit.

gfortran (GCC) Tested on version 4.8.1 64-bit.

1.1 Linux and other Unix variants

1. Meet the software requirements by installing MATLAB and the GCC package. MATLAB download and installation instructions can be found on the MathWorks website. The gfortran/GCC package can be obtained from the ⋆nix distribution repository through the distribution package manager. Using Ubuntu for example:
   ```
   $ sudo apt-get install gfortran
   ```

1.2 Windows

Currently, running the PPODE SUITE on Windows is not supported nor tested.

1. Running the PPODE SUITE on Windows would require installing a combination of GCC/Cygwin and gnumex (*http://gnumex.sourceforge.net/*) or the Intel Visual Fortran Composer. To check which versions are supported by MATLAB , check *http://www.mathworks.nl/support/compilers/R2013b/* substituting R2013b with the right version number.

1.3 General

2. Download and extract the PPODE SUITE package.
3. Open matlab and navigate to the extracted PPODE SUITE folder. Add the *PPODE* paths to the matlab path variable.
   ```
   >> PPODE_addPaths
   ```

4. Now the libraries of the different solvers can be build. In order to do so, execute the following command;

   ```
   >> PPODE_init
   ```

   The options 'Debug' can be used to build the libraries with debugging symbols.

   ```
   >> PPODE_init('Debug', 1)
   ```

   For more information, type "`help PPODE_init`" in the MATLAB command window.

Chapter 2

Usage

2.1 The ODE Function

2.1.1 Introduction

The ODE function of the problem should be written in Fortran95. Here are some main Fortranpeculiarities to consider when writing Fortrancode.

Line Formatting The maximum line width is 72 characters. The first character is used to indicate whether the line is a comment line. The second to fifth character are used to indicate labels. The 6^{th} character is used to indicate the continuation of the previous line.

Listing 2.1: Syntax Example

```
c        1         2         3         4         5         6         7
c23456789012345678901234567890123456789012345678901234567890123456789012

! Comments should be introduced by either a 'c' or a '!'.
      if (answer .gt. 42) go to 4242
 4242 ydot(s) = y(1) * (kp * y(s - 1) - gp * y(s)) + gm * y(s + 1) +
     + km * y(s)
```

For Loops For loops are written using the `do` statement. They should be written in the form `do ⟨label⟩ ⟨var⟩=⟨start⟩, ⟨stop⟩[, ⟨step⟩]`. The label should refer to a `continue` statement at the end of the loop.

Listing 2.2: Do-Loop

```
      a = 0
      do 42 i=1, 20
        a = a + 1
   42 continue
! a has the value 20 here.
```

Case Sensitivity The Fortranlanguage is not case sensitive.

2.1.2 Template

The Fortransubroutine that defines the ODE system should have the following arguments:

neq *input* Number of equations.

t *input* The current time point.

y *input* The current value of all states. The length of this vector is equal to `neq`.

ydot *output* This is a vector of length `neq` to which all derivatives of the states should be written.

The parameters are passed using a `common` block. The variable **np** represents the number of parameters. The vector **p** contains the values of all parameters.

Listing 2.3: ODE Template

```
c-----------------------------------------------------------------------
c
c PPODE ODE function - Model Name
c   Short model description.
c
c DEVELOPED BY:
c
c   Pascal Pieters <p.a.pieters@student.tue.nl>
c
c-----------------------------------------------------------------------
c
c ARGUMENTS:
c
c    neq :in    Number of states/equations.
c      t :in    Current time point.
c      y :in    Vector of the current values of the states.
c   ydot :out   Vector of the numerical derivatives of the states.
c
c PARAMETERS:
c
c   p(1) :in    s   : Parameter description.
c   p(2) :in    kp  : ...
c
c-----------------------------------------------------------------------

      subroutine func (neq, t, y, ydot)
      integer neq, i, s, np
      double precision t, y, ydot, kp
      double precision , pointer :: p(:)
      dimension y(neq), ydot(neq)
      common  /funcpar/ np, p

      s = int(p(1))
      kp = p(2)
      ...
      ydot(i) = ...
      ...
      return
      end
```

Examples can be found in the "⟨PPODE SUITE Source⟩/examples" folder.

2.1.3 Sparse Jacobian Matrix

When using the solver that uses a sparse matrix implementation for the Jacobian matrix, the number of non-zero values of the Jacobian matrix should be supplied. This is done using a Fortransubroutine called `nonzero`. The arguments of this subroutine are the following:

neq *input* Number of equations.

npar *input* Number of parameters.

par *input* The values of all parameters. Contrary to the ODE function, where the number of parameters and parameter values are supplied using a `common` block, both are given as arguments here.

nnz *output* The number of nonzero elements in the Jacobian matrix. This value can be determined using the definition of the Jacobian matrix:

$$J_{m,n} = \begin{pmatrix} \frac{\partial F_1}{\partial x_1} & \cdots & \frac{\partial F_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial x_1} & \cdots & \frac{\partial F_m}{\partial x_n} \end{pmatrix} \tag{2.1}$$

In the case of an ODE system, m and n are both equal to the number of equations. F represents the system of ODEs. The number of nonzero elements can also be determined using trial and error. By just trying some values for `nnz`, the error messages might give away the correlation between `nnz` and the parameter and number of equations.

2.2 Building the MEX Function

The MATLAB function `PPODE_build`, included in the PPODE SUITE , can be used to build the ODE Fortranfile against the right solver libraries. First of all, make sure the PPODE SUITE paths are added to the MATLAB path variable.

```
>> PPODE_addPaths
```

And the libraries are build.

```
>> PPODE_init
```

Now the function `PPODE_build` can be used. Extensive help can of course be acquired using "`help PPODE_build`". The simplest usage of the function is the following:

```
>> PPODE_build('odeproblem.F', 'odeproblem_stiffsolver')
```

This command will generate a MEX file named 'odeproblem_stiffsolver' of the problem defined by 'odeproblem.F', using the default (stiff) solver. The correct file extension is automatically added to the MEX file, so do not supply an extension for the second function argument.

The first two mandatory arguments, extra options can be specified. This is done by first giving the option name and then the value. For example, if the problem is not stiff and one would like verbose output, a non-stiff solver should be specified and the verbose mode should be enabled:

```
>> PPODE_build('odeproblem.F', 'odeproblem_stiffsolver', ...
     'Solver', 'Non-Stiff', 'Verbose', 1)
```

Note that both the option name and value are case insensitive.

2.3 Executing the MEX Function

The MEX function generated by the PPODE build function can be called as follows:

```
   >> [⟨t⟩, ⟨y⟩] = ⟨F⟩(⟨neq⟩, ⟨abstol⟩, ⟨reltol⟩, ⟨times⟩, ⟨par⟩, ⟨y0⟩)
```

Where ⟨F⟩ is the name of the MEX function, ⟨neq⟩ is the number of equations, ⟨abstol⟩ and phreltol are the absolute and relative tolerances respectively, ⟨times⟩ is a vector of time points at which output is desired, ⟨par⟩ is a vector of parameter values and ⟨y0⟩ is a vector of the initial values of the states. The function returns the vector ⟨t⟩ with the time points at which the values of the states are calculated. The matrix ⟨y⟩ contains the values of all states at the time points specified by ⟨t⟩.

Chapter 3

Solvers

3.1 Introduction

The solver for the ODE problem can be specified using the 'Solver' option of the `PPODE_build` function:

```
   >> PPODE_build(⟨source⟩, ⟨target⟩, 'Solver', ⟨solver⟩)
```

Valid options for ⟨solver⟩ are:

'Stiff' (or 'BDF') The BDF based solver of the LSODE package. *See 3.2.1.*

'Stiff2' (or 'CVODE') The BDF based solver of the CVODE package. *See* **??**.

'MEBDFSO' (or 'MEBDFSparse') The modified extended BDF based solver using a sparse Jacobian matrix. *See 3.2.2.*

'LSODES' (or 'BDFSparse') The BDF based solver using a sparse Jacobian matrix. *See* **??**.

'Non-Stiff' (or 'Adams-Moulton') The Adams-Moulton based solver of the LSODE package. *See 3.3.1.*

'Non-Stiff2' (or 'CVODEAM') The Adams-Moulton based solver of the CVODE package. *See* **??**.

'RK23', 'RK45', 'RK78' The Runge-Kutta based solvers of the RKSUITE package. *See 3.3.2.*

'Switching' (or 'LSODA') The solver that switches between the non-stiff Adams-Moulton based solver and the stiff BDF based solver of the LSODE package. *See 3.4.1.*

If you do not know which solver to choose, but you already know which MATLAB solver performs best, table 3.1 might be helpfull.

MATLAB	Equivalent	Probably Also Suitable
ode45	'RK45'	'RK78', 'Non-Stiff', 'Non-Stiff2'
ode23	'RK23'	'RK45', 'Non-Stiff', 'Non-Stiff2'
ode113	'Non-Stiff', 'Non-Stiff2'	'RK45'
ode15s	'Stiff', 'Stiff2'	'Switching' (partially stiff problems), 'MEBDFSO' (large number of states that are not very interdependent)
ode23s	-	'Stiff', 'Stiff2', 'Switching', 'MEBDFSO'
ode23t	-	'Switching', 'Stiff', 'Stiff2', 'MEBDFSO'
ode23tb	-	'Switching', 'Stiff', 'Stiff2', 'RK45', 'RK23', 'MEBDFSO'

Table 3.1: Solver selection helper.

3.2 Stiff

3.2.1 BDF

The Backward Differential Formulas based method uses the BDF implementation that ODEPACK supplies. The order of these formulae can range between 1 and 5 and can be limited by setting the 'MaxOrder' option when building the ODE system.

Credits

Credits for the ODEPACK package obtained from (*http://www.netlib.org/*).

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3.2.2 Modified Extended BDF using Sparse Jacobian

The Modified Extended Backward Differential Formulae based method uses the BDF implementation that MEBDFSO supplies. The order of these formulas can range between 1 and 5 and can be limited by setting the 'MaxOrder' option when building the ODE system.

Credits

Credits for the MEBDFSO package obtained from (*http://www.netlib.org/*).

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3.3 Non-Stiff

3.3.1 Adams-Moulton Methods

The Adams-Moulton method based solver uses the Adams-Moulton implementation that ODEPACK supplies. The order of these formulae can range between 1 and 12 and can be limited by setting the 'MaxOrder' option when building the ODE system.

Credits

Credits for the ODEPACK package obtained from (*http://www.netlib.org/*).

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3.3.2 Runge-Kutta Methods

The Runga-Kutta methods based solver uses the RKSUITE package. Three Runge-Kutta pairs are available: 2-3, 4-5 and 7-8. Use higher orders in combination with smaller tolerances.

Credits

Credits for the RKSUITE package obtained from (*http://www.netlib.org/*).

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3.4 Mixed

3.4.1 Switching between BDF and Adams-Moulton Methods

The switching method uses the LSODA subroutine that the ODEPACK package supplies. This method automatically switches between the BDF based stiff solver (order 1-5) and the Adams-Moulton methods based non-stiff solver (order 1-12).

Credits

Credits for the ODEPACK package obtained from (*http://www.netlib.org/*) and the LSODA subroutine in particular.

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