EMSO
Manual

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Contents

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I would like to thank the authors of the following softwares libraries for permitting the use of their code in EMSO:

DASSLC : a solver for differential-algebraic equation systems www.enq.ufrgs.br/enqlib/numeric/;

FOX-Toolkit : a C++ based Toolkit for developing Graphical User Interfaces easily and effectively www.fox-toolkit.org;

FXScintilla : an implementation of Scintilla[1] for the FOX-Toolkit www.nongnu.org/fxscintilla;

RCOMPLEX : a solver for constrained nonlinear optimization. www.enq.ufrgs.br/enqlib/numeric/;

SUNDIALS : suite of codes consisting of the solvers CVODE, KINSOL, and IDA, and variants of these www.llnl.gov/CASC/sundials/;

UMFPACK : a set of routines for solving unsymetric sparse linear systems www.cise.ufl.edu/research/sparse/umfpack;

Ipopt : a software package for large-scale nonlinear optimization. https://projects.coin-or.org/Ipopt;

In the development process the author proposed several improvements and bug-fixes sent to the original authors to be shared with the community. The source code of all the above cited softwares can be obtained in the respective URL. Any further explanation about how such softwares are used in EMSO can be obtained with the author - www.rps.eng.br.

[1] Scintilla is a free source code editing component, see www.scintilla.org.

Symbols and Conventions

In this document the following notations are used:

Piece of code: piece of code written in the EMSO modeling language or console outputs:

```
Model tank
	# body of the model
end
```

Code Identifier: emphasize identifiers that are `commands`, `file names` and related entities.

Note: a note, for instance: EMSO is an equation based description system, therefore the order of the equations does not matter.

Warning: a warning advertise, for instance: a `.mso` file free of syntax errors still can have consistency errors.

Tip: a tip for the user, for instance: always check EML for a model before develop a new one.

Linux note: note specific for POSIX systems (Linux and Unix), for instance: EMSO can be available for any POSIX compliant system upon request.

Windows note: note specific for win32 systems (Windows 95 and above and Windows NT 4 and above), for instance: the windows file system is not case sensitive.

Under construction: marks a section as not yet implemented or documented.

I. User's Guide

1 Introduction

Go any further in reading this manual or using EMSO without read, understand and accept the EMSO license, found on page vi.

In this chapter we will learn what is EMSO and why use it.

Contents

1.1 What is EMSO and EML?

EMSO stands for **E**nvironment for **M**odeling, **S**imulation and **O**ptimization. It is a complete graphical environment where the user can model complex dynamic or steady-state processes by simply selecting and connecting model blocks. In addition, the user can develop new models using the EMSO modeling language or using those already made from the EMSO **M**odel **L**ibrary (EML).

EML is an open source library of models written in the EMSO modeling language. The EMSO modeling language is an object-oriented language for modeling general dynamic or steady-state processes.

1.2 Why use EMSO?

In this section we show the key concepts of EMSO and its advantages.

1.2.1 Easy FlowSheet building

EMSO provides the facility of building complex process models, called `FlowSheet`s, by simply composing it with preexisting blocks, called `Model`s, and connecting them.

1.2.2 Integrated Graphical Interface

EMSO provides an integrated graphical interface where the user can manage their `.mso` files. Multiple files can be opened simultaneously and each file can contain an unlimited number of `Model`s, `FlowSheet`s or `Script`s. In the same interface the user can run simulations and visualize the results besides a lot of development facilities.

1.2.3 Open-Source Model Library

The `.mso` files coming with EMSO are distributed under the terms of the EMSO model license.

The EMSO distribution comes with a set of ready to use models written in the EMSO modeling language – the EMSO Model Library (EML). Therefore, complex `FlowSheet`s can be built by simply selecting EML models as `Device`s and connecting them. EML is an open-source library and can be extended or modified by the user.

1.2.4 Object-Oriented Modeling Language

EMSO provides a modeling language that allows the user to write mathematical models almost as they would appear on paper. In addition, the language is fully object-oriented, allowing the user to develop complex models by composing them with existent small models or develop specific models by deriving standard ones.

All EML models are written in the EMSO modeling language and are stored in plain text `.mso` files which can be edited or extended by the user.

1.2.5 Multi-Platform system

EMSO is available for win32, POSIX (Linux and Unix) platforms. Models developed in one platform can be freely interchanged between others.

1.2.6 Fast and Transparent Setup

Process simulators in which models are not black-boxes pieces of software obligatory have to translate the human readable description to some *solvable* form. This translation step is called setup phase.

In EMSO, the setup phase does not relies in the creation of intermediary files, compilation, linkage or translation to another language, the models are directly converted (in memory) to systems of equations. This mechanism reduces the setup time by orders of magnitude.

1.2.7 Solution Power

EMSO provides solvers for dynamic and steady-state systems which are efficient in solving both small and large scale systems. The solvers can make use of the dense or sparse linear algebra. Actually there is no limit regarding problem size other than the machine memory. In addition, new solvers can be interfaced to EMSO and used in a seamless manner.

State of art techniques as automatic and symbolic differentiation algorithms are built-in in EMSO. Furthermore, it has proved to be one of the most time efficient tools when solving large scale dynamic problems.

1.2.8 Modeling of discontinuous process

There are several processes which are in nature discontiuous, with EMSO it is easy to model continuous-discrete (hybrid) systems using conditional equations.

1.2.9 Operational procedures scripts

Under construction: To be implemented and documented.

1.2.10 Optimization

Besides dynamic and steady simulation EMSO can be used to find optimal solutions with respect to given criteria. The user just need to formulate the optimization objective (lower cost, maximum production, etc) and choose the optimization variables (manipulated variables) in the `Optimization` environment and let the system to find the best solution. See examples in the `ammonia_opt.mso` and `flash_opt.mso` in the folder `<EMSO>/mso/sample/optimization`.

1.2.11 Parameter Estimation

EMSO can perform parameter estimation of dynamic and steady-state models using the `Estimation` environment. See examples in the `BatchReactor.mso` and `sample_est.mso` files in the `<EMSO>/mso/sample/estim` folder.

1.2.12 Open Interfaces

EMSO has a set of open interfaces that allow the user to load at run-time third-party software encapsulated in dynamic link libraries. (See Part II).

In addition, there are standard interfaces for implementing new differential-algebraic equations (DAE), nonlinear algebraic equations (NLA), and nonlinear optimization problem (NLP) solvers.

1.2.13 Open Engine API

EMSO is composed by two major softwares: the graphical interface and the *engine*. The EMSO power in solving complex large-scale dynamic problems is available to be embedded in third party software through the EMSO *engine* open Application Program Interface (API). Using this technology, EMSO installation already provides an engine to build bifurcation diagrams using `AUTO2000` adapted to work with differential-algebraic equations (DAE), and also `SFunctions` for simulating dynamic models built with EMSO modeling language inside `Matlab/Simulink`® with continuous and discrete-time simulation. See the installation procedure.

AUTO2000 DAE can be donwloaded at `www.enq.ufrgs.br/enqlib/numeric`. See `www.peq.coppe.ufrj.br/auto_dae` for details.

1.3 Installation

EMSO is available for two main platform *groups*: win32 and POSIX. Installation instructions for these platforms can be found in subsection 1.3.1 and subsection 1.3.2 respectively.

1.3.1 Installing EMSO in win32 platforms

EMSO is compatible with a variety of win32 operational systems (Windows 95, Windows NT 4, Windows XP and above). In order to install EMSO in such systems one can just run the installation package `emso-win32-<VERSION>.exe` available at `www.enq.ufrgs.br/alsoc` and follow the on screen instructions.

In order to use the EMSO-AUTO interface it is also necessary to install the `AUTO2000 DAE` package, that can be downloaded at `www.enq.ufrgs.br/enqlib/numeric`, using a Linux-like environment for Windows, such as `MINGW` or `CYGWIN` in the location /usr/local/auto/2000_dae. After the installation, just run the script `auto2000_dae` provided in the root directory of the `AUTO2000 DAE`, using the command `source auto2000_dae`. There are some examples to test the installation in the directory `/usr/local/auto/2000_dae/demos/DAE`. Copy the file `auto_emso.exe` from `<EMSO>/bin` in the same location of the examples and execute the command `@r-emso ab_dae`, where `ab_dae` is the name of the example to run, or put the directory `<EMSO>/bin` in the `PATH` environment variable.

`MINGW` may be download at `www.mingw.org` and `CYGWIN` at `www.cygwin.com`.

In order to use the EMSO-Matlab/Simulink interface, just copy the files `emso_sf.dll` and `emsod_sf.dll` from the location `<EMSO>/interface/matlab` to the working directory. In the original location there are some MDL files to run some examples in the Simulink.

1.3.2 Installing EMSO in POSIX platforms

EMSO is compatible with a variety of POSIX platforms (Linux, Unix).

POSIX is the name for a series of standards being developed by the IEEE that specify a Portable Operating System interface. The "IX" denotes the Unix heritage of these standards.

In order to install EMSO in such systems you have to download the archive `emso-<PLATFORM>-<ARCH>-<VERSION>.tar.gz` available at `www.enq.ufrgs.br/alsoc`.

For instance, `emso-linux2-i386-0.9.53.tar.gz` is the installation archive for Linux version 2 or above platforms running in an `i386` compatible machine.

The installation procedure for the EMSO-AUTO interface is the same as for win32 platform, described above, just skip the part for the Linux-like environment for Windows.

In order to use the EMSO-Matlab/Simulink interface, just copy the files `emso_sf.mexlx` and `emsod_sf.mexlx` from the location `<EMSO>/interface/matlab` to the working directory. In the original location there are some MDL files to run some examples in the Simulink, if you can make Simulink work in Linux.

Note: Installation packages for any POSIX compliant platform can be produced upon request.

Once an archive compatible with your system was downloaded, EMSO can be installed with the following commands:

```
$ tar -xzvf emso-<PLATFORM>-<ARCH>-<VERSION>.tar.gz
# sudo mv emso /usr/local
# sudo ln -sf /usr/local/emso/bin/emso /usr/bin/emso
```

Note: The EMSO executable is found at the `bin` directory, the installation at `/usr/local` is not mandatory.

2 Overview

This chapter provides an overview about EMSO. First some basics are presented followed by some tutorials. These tutorials teaches how to:

- build a `FlowSheet` composed by a set of predefine `Models`;
- check the consistency of a `FlowSheet`
- run a dynamic simulations and plot results;
- customize `FlowSheet` options.

Further, the EMSO modeling language for development of new models is introduced.

Contents

2.1 EMSO Basics

EMSO is a software tool for modeling, simulation and optimization of dynamic or steady-state general processes. The referred processes are called FlowSheets.

A FlowSheet is composed by a set of components, named Devices. Each Device has a mathematical description, called Model. These are the three main EMSO entities and all of them are described in plain text files which are usually stored in .mso files. Each .mso file can have any number of any of these entities and the EMSO graphical user interface can open an unlimited number of .mso files simultaneously.

2.2 Running EMSO

EMSO is available in a variety of platforms:

- win32 platforms;
- POSIX platforms: Linux and Unix.

Windows 95 or above and Windows NT 4 or above.

Distribution for any POSIX compliant platform can be built upon request.

2.2.1 Starting EMSO in win32 platforms

If EMSO was successfully installed as described in subsection 1.3.1, it can be started by left clicking in one of the installed shortcuts: at the desktop or at the start menu.

2.2.2 Starting EMSO in POSIX platforms

If EMSO was successfully installed as described in subsection 1.3.2, it can be started with the command emso. Another option is to double-click in file <EMSO>/bin/emso, where <EMSO> is the directory where EMSO was installed, for instance /usr/local.

2.3 EMSO graphical interface

After EMSO is started a graphical user interface, as showed in Figure 2.1, raises.

Note: The EMSO graphic interface layout and behavior is identical in all platforms.

In this section a brief overview about this interface is given.

This interface is inspired on the most successfully interfaces for software development. It is divided in some panels which are treated in the following sections.

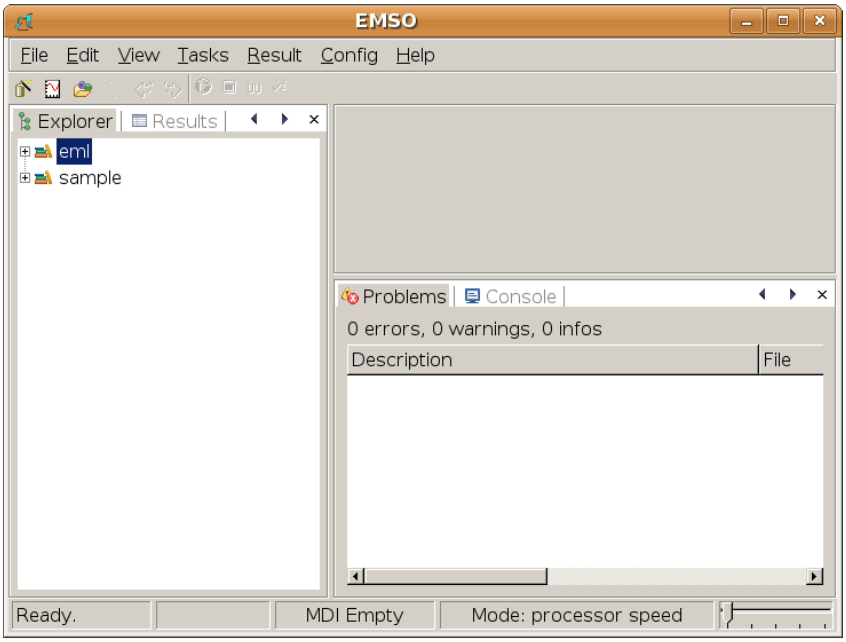


Figure 2.1: EMSO graphical user interface.

Explorer and Results Windows

The `Explorer` and `Results` windows are in the left most vertical frame of the interface in Figure 2.1.

Explorer : displays the available libraries of models and the current loaded files and its contents (`Models` and `FlowSheets`). The Figure 2.2 (a) shows a typical view of the file explorer.

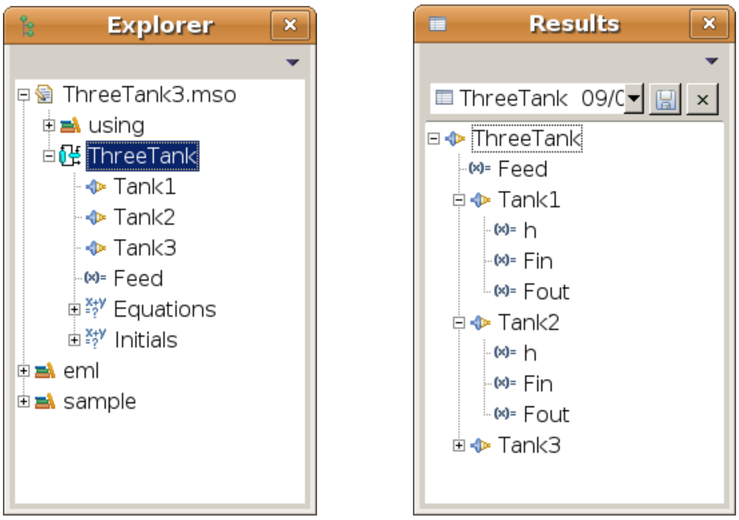
Results : for each task ride (e.g. a dynamic simulation) a new item is added to this window. A typical view of the results explorer can be seen in Figure 2.2 (b).

Tip: The position of the frames in Figure 2.1 can be freely interchanged, right click on the tab button of the window to change its position.

Each of these windows can be turned the current one by clicking in the respective tab. At any time the user can close one or more tabs. Closed tabs can be shown again with the `View` menu.

Problems Window

As in any programming or description language files can have problems. Each time that a file is opened the `Problems` window automaticaly list all errors and warnings found, as exemplified by the Figure 2.3.



(a) Explorer (b) Results explorer

Figure 2.2: EMSO Explorer and Results windows.

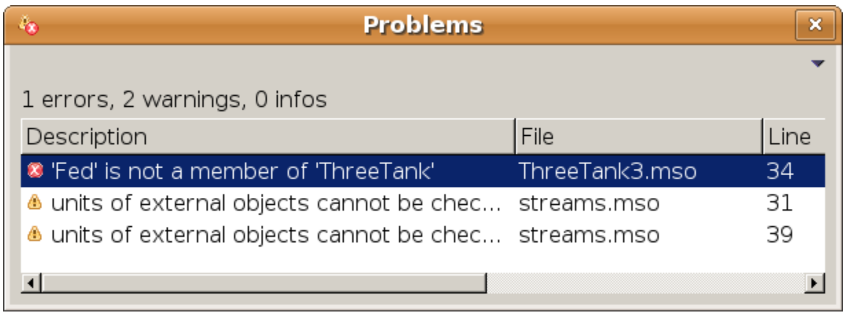


Figure 2.3: EMSO Problems Window.

Console Window

When running tasks all messages are sent to the `Console`. As can be seen in Figure 2.4, the user can select the detailing level of the messages sent to the console.

The Multiple Document Interface panel

In the center of the interface is implemented a Multiple Document Interface (MDI) panel. This panel is responsible to show the opened files and edit it, the result plots, etc.

2.4 Tutorials

In the last section we have presented how to start EMSO and its graphical interface. Now we give some tutorials introducing the key concepts of EMSO and its modeling language. The directory

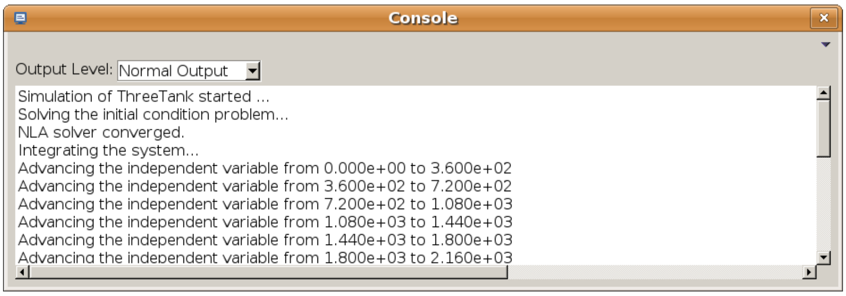


Figure 2.4: EMSO Console Window.

`<EMSO>/mso/tutorial/` contains all code samples found in this section, where `<EMSO>` is the directory where EMSO was installed.

2.4.1 Three Tank `FlowSheet`

In this section we describe how to create and simulate the dynamic model of a process composed by some tanks. The example consists of three tanks connected in series. In EMSO this process can be modeled as a `FlowSheet` containing three `Devices` each one based on a tank `Model`.

Creating a new file

In order to simulate this example, the first step is to create a new `.mso` file containing a `FlowSheet`. This is achieved by left clicking in the new file button . This will bring up the new file dialog as shown in Figure 2.5. In this window the user can select one of the available *templates*:

- FlowSheet;
- Equation FlowSheet;
- Model;
- Empty.

In this example we are interested in create a new `FlowSheet`. This is the default template item, therefore the user should left it as is. The fields `Name` and `Location` should be filled with the desired file name and directory location, respectively. The user can fill this dialog as exemplified in Figure 2.5 then left click in the `Accept` button in order to create the new file. After this EMSO will create and open a file with the given properties. At this point the interface will look like Figure 2.6.

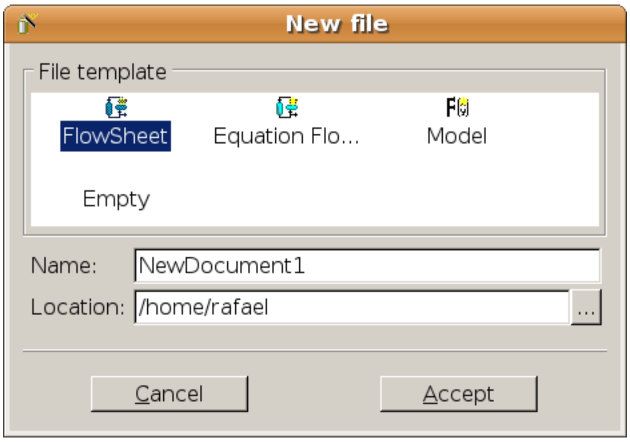


Figure 2.5: New file dialog wizard.

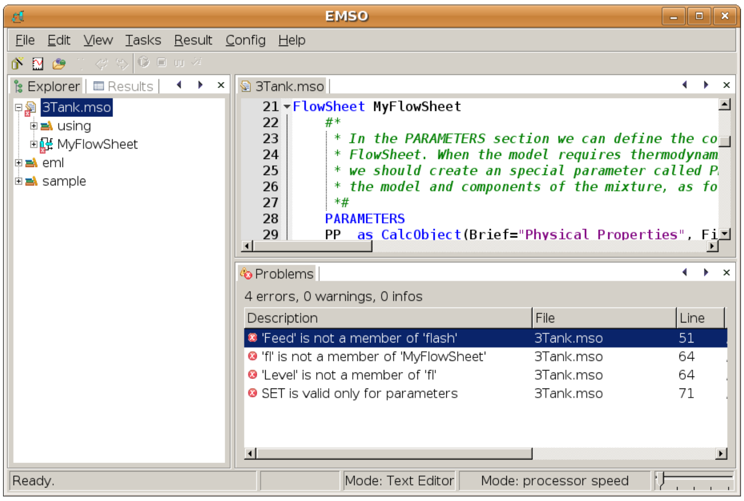


Figure 2.6: EMSO new file window.

Writing the `FlowSheet`

Before continue reading this tutorial is advisable to read the comments on the file new file created (which comes from the selected template).

The first comments are about the `using` command. This command makes available all entities contained in a given filename or directory (all files belonging to it).

In our example we will make use of one of the EML models, the `TankSimplified` model. This model is found in file `tanks.mso` in the library directory. Therefore, in order to use this model instead of *copy and paste* we will *use* this file with the `using` command as follows:

```
using "stage_separators/tanks";
```

This command turns available all entities contained in file `tank.mso` which is part of EML. For more details about `using` see subsection 3.1.5.

The file `tank.mso` (as most of the EML files) *uses* the file `types.mso` which contains the declaration of several variable types as `length`, `area`, etc.

The next step is to change the default name `NewFlowSheet` to a more meaningful name, lets say `ThreeTank`. Then we can add the `Devices` in the `DEVICES` section and connect them in the `CONNECTIONS` section. After this, the contents of the file should look like Code 2.1.

Code 2.1: File `ThreeTank1.mso`.

```
using "stage_separators/tank";

FlowSheet ThreeTank
      VARIABLES
      Feed     as flow_vol;

      DEVICES
      Tank1 as tank_simplified;
      Tank2 as tank_simplified;
      Tank3 as tank_simplified;

      CONNECTIONS
      Feed        to  Tank1.Fin;
      Tank1.Fout  to    Tank2.Fin;
      Tank2.Fout  to    Tank3.Fin;
end
```

The Code 2.1 contains no problems, once there is no item on the `Problems` window.

Warning: Even if a `.mso` file has no problems the `FlowSheets` of such file can be **not** consistent, as explained in the following section.

Checking consistency

A `FlowSheet` is consistent if it has zero degrees of freedom and zero dynamic degrees of freedom.

In order to check the `ThreeTank` consistency the user should select the corresponding `FlowSheet` item in the file explorer and then left click in the button. At this time the `Console` window will become active and will display a message like:

```
Checking the consistency for 'ThreeTank' in file '
    ThreeTank1.mso'...
Number of variables:  7
Number of equations:  6
Degrees of freedom: 1
```

```
The number of variables and equations does not match!
System is not consistent!
```

At this point the `Problems` window will also show the consistency problems. This error was expected, once we have neither specified the input flow of the first tank nor the initial level of the tanks.

Therefore, in order to get a consistent system the user should add the following commands:

```
SPECIFY
      Feed = 10 * 'm^3/h';
INITIAL
      Tank1.h = 1 * 'm';
      Tank2.h = 2 * 'm';
      Tank3.h = 1 * 'm';
```

The user can choose between to add this code into its `FlowSheet` or use the already made file `ThreeTank2.mso` found in the `tutorial` directory.

Note: EMSO is not a sequential tool, therefore the user could specify a variable other than the input flow of the first tank.

Now, if the user checks the `ThreeTank` consistency no errors will be reported and some interesting messages will be sent to the `Console`:

```
Checking the consistency for 'ThreeTank' in file 'ThreeTank2.mso'...
Number of variables:  10
Number of equations:  10
Degrees of freedom: 0
Structural differential index: 1
Dynamic degrees of freedom:  3
Number of initial Conditions: 3
System is consistent.
```

Running a Simulation

Once we have a consistent `FlowSheet` we can run a simulation. To do this the user has to select the desired `FlowSheet` in the file explorer and then left click in the button.

```
Simulation of 'ThreeTank' started ...
Simulation of 'ThreeTank' finished succesifuly in 0.02 seconds.
```

Tip: In order to get more detailed output when running a simulation just change the output level on the `Console` window and run again the simulation.

Visualizing Simulation Results

For each task ride by the user a new result is added to the results explorer. The user can see the available results by left clicking in the results explorer tab (Figure 2.2 (b)).

If a result is selected on the top list of the results, the bottom side will show the variables available for plotting. The user can plot a variable profile by double clicking in it.

If not specified the integration interval is the interval ranging from 0 to 100 seconds.

We have not configured the simulation time vector for our simulation and the default integration interval is not suitable for the dynamics of our system. We can modify the integration interval by adding, for instance, the following commands:

```
OPTIONS
      TimeStep = 0.1;
      TimeEnd = 2;
      TimeUnit = 'h';
```

Now we have an integration interval compatible with the dynamics of our system. Then if we run the simulation again, the results will be much more interesting.

Customizing the `FlowSheet`

Usually `Models` are full of parameters to be customized by the user. In our `FlowSheet` (Code 2.1) we have not changed parameter values. Hence the default values for all parameters were considered, these defaults come from the types on which the parameters are based.

In order to set values other than the defaults the user can add a `SET` section at any point after the parameter declaration. Then if we want another values for the valve constants or geometry of our tanks the following code should be added after the `DEVICES` section:

```
SET
      Tank2.k = 8*'m^2.5/h';
      Tank2.A = 4*'m^2';
```

Now we can run the simulation again and compare the results with the previous solution.

At this point our code should look like Code 2.2 found in the `tutorial` directory.

Code 2.2: File `ThreeTank3.mso`.

```
using "stage_separators/tank";

FlowSheet ThreeTank
	VARIABLES
	Feed    as flow_vol;

	DEVICES
	Tank1 as tank_simplified;
	Tank2 as tank_simplified;
	Tank3 as tank_simplified;

	CONNECTIONS
	Feed        to  Tank1.Fin;
	Tank1.Fout  to    Tank2.Fin;
	Tank2.Fout  to    Tank3.Fin;

	SPECIFY
	Feed = 10 * 'm^3/h';

	INITIAL
	Tank1.h = 1 * 'm';
	Tank2.h = 2 * 'm';
	Tank3.h = 1 * 'm';

	SET
	Tank2.k = 8 * 'm^2.5/h';
	Tank2.A = 4 * 'm^2';

	OPTIONS
	TimeStep = 0.1;
	TimeEnd = 2;
	TimeUnit = 'h';
end
```

3 EMSO Modeling Language

In this chapter, we describe in detail how one can write a `Model` or `FlowSheet` using the EMSO modeling language.

The EMSO modeling language is a case sensitive textual language. In such language the entities are written in plain text files stored, by default, in `.mso` files.

Contents

3.1 Modeling basics

As mentioned before, in EMSO a `FlowSheet` is the problem in study. But, a `FlowSheet` is composed by a set of connected `Devices`, each one having a mathematical description called `Model`.

In chapter 2 the `Model` and `FlowSheet` entities were introduced. The description of these entities share several basic concepts particular to the EMSO modeling language, which follows.

3.1.1 Object Oriented Modeling

Reuse is the key to handle complexities, this is the main idea behind the object oriented (OO) paradigm. The EMSO language can be used to create high reusable models by means of *composition* and *inheritance* OO concepts, described below.

Composition

Every process can be considered as set of sub-processes and so on, this depends only on the modeling level. *Composition* is the ability to create a new model which is composed by a set of *components*, its sub-models.

The EMSO modeling language provides unlimited modeling levels, once one model can have sub-models which can have sub-models themselves. This section aims at introducing the *composition* concept, the application of this concept in the EMSO is shown in subsection 3.2.3.

Inheritance

When modeling complex systems, set of models with a lot in common usually arises. If this is the case, an advisable modeling method is to create a *basic* model which holds all the common information and *derive* it to generate more specif models *reusing* already developed models.

In OO modeling this is achieved by *inheritance*, the ability to create a new model *based* on a preexistent one and add derivations to it. For this reason, *inheriting* is also known as *deriving*. When a model uses more than one *base* model it is said to use multiple inheritance.

The EMSO modeling language provides unlimited levels of inheritance or multiple inheritance for `Models` and `FlowSheets`. The following sections and EML are a good sources of examples of inheritances.

See the EML file `stream.mso`, for instance.

3.1.2 Writing EMSO Entities

The basic EMSO entities are `Model`s and `FlowSheet`s. The formal description of these entities always start with the entity keyword (`Model` or `FlowSheet`) and ends with the `end` keyword, as follows.

```
FlowSheet FlowSheetName
	# FlowSheet body
end

Model ModelName
	# Model body
end
```

A `.mso` file can have an unlimited number of entities declared on it. Once a entity was declared it is available to be used as a base for derivation or as a component to another Model. The detailed description of `FlowSheet`s and `Model` are found in sections 3.2 and 3.3, respectively.

3.1.3 Documenting with Comments

The EMSO modeling language is a descriptive language, a `Model` written on it contains several information about the process being modeled, as variable and parameter description, equation names, etc. But extra explanations could be useful for better understanding the model or for documenting the history of a model, the authors, the bibliography, etc. This kind of information can be inserted in EMSO entities with one of the two types of comments available:

- line comment: starting from `#` and extending until the end of line;
- block comment: starting from `#*` and extending until `*#`.

It follows below a piece of code which exemplifies both kind of comments:

```
#*
This is a block comment, it can be extended in
   multiple lines.
A block comment can give to the reader useful
   informations,
for instance the author name or a revision history:

Author: Rafael de Pelegrini Soares
  --------------------------------------------------

Revision history
```

```
$Log: streams.mso,v $
Revision 1.1.1.1  2003/06/26 16:40:37  rafael
  --------------------------------------------------

*#
# A line comment extends until the end of line.
```

3.1.4 Types

As already mentioned in chapter 2, the declaration of variables and parameters can make use of a base *type*. A type can be one of the built-in types or types derived from the built-in ones. The list of built-in types are shown in Table 3.1.

Table 3.1: List of EMSO built-in types.

Type name	Description
`Real`	Type for continuous variables or parameters, with attributes: • `Brief`: textual brief description • `Default`: default value for parameters and initial guess for variables • `Lower`: lower limit • `Upper`: upper limit • `Unit`: textual unit of measurement
`Integer`	Type for integer variables or parameters, with attributes: • `Brief`: textual brief description • `Default`: default value for parameters and initial guess for variables • `Lower`: lower limit • `Upper`: upper limit
`Switcher`	Type for textual parameters, with attributes: • `Brief` textual brief description • `Valid` the valid values for the switcher • `Default` default value for the switcher
`Boolean`	Type for logical parameters or variables, with attributes: • `Brief` textual brief description • `Default` default value for parameters and initial guess for variables
`Plugin`	Object for loading third party pieces of software providing special calculation services, see chapter 5.

As Table 3.1 shows, each built-in type has a set of attributes. These attributes can be modified when a new type is created deriving a preexistent one. For instance, consider the Code 3.1 making part of EML, in this file a set of convenient types are declared, and are used in all EML models.

Code 3.1: EML file `types.mso`.

```
# Pressure
pressure as Real (Brief = "Pressure", Default=1,
    Lower=1e-30, Upper=5e7, final Unit = 'atm');
press_delta as pressure (Brief = "Pressure
    Difference", Default=0.01, Lower=-5e6);
head_mass as Real (Brief = "Head", Default=50, Lower
    =-1e6, Upper=1e6, final Unit = 'kJ/kg');
head as Real (Brief = "Head", Default=50, Lower=-1e6
    , Upper=1e6, final Unit = 'kJ/kmol');
```

Note that type declarations can be stated only outside of any `Model` or `FlowSheet` context.

Variables can be **only** declared based on types deriving from `Real`. Note that the `Plugin` type cannot be derived to a new type, read more in chapter 5.

3.1.5 Using files

Code reuse is one of the key concepts behind EMSO. To achieve this the user can be able to use code written in another files without have to touch such files. A `.mso` file can make use of all entities declared in another files with the `using` command. This command has the following form:

```
using "file name";
```

where `"file name"` is a textual file name. Therefore, commands matching this pattern could be:

```
using "types";
using "streams";
using "tanks";
```

When EMSO find a `using` command it searches the given file name in the following order:

1. the current directory (directory of the file where the `using` was found);

2. the libraries configured on the system;

Note: As shown in the sample code, if the user suppress the file extension when `using` files EMSO will automatically add the `mso` extension.

Whenever possible the user should prefer the `using` command instead of *copy* and *paste* code.

Windows note: The EMSO language is case sensitive but the windows file system is not. Therefore, when `using` files in windows, the language became case insensitive to the file names.

3.2 Model

The basic form of a `Model` was introduced in subsection 3.1.2, here we describe how the `Model` body is written.

In Code 3.2 the syntax for writing `Model`s in the EMSO modeling language is presented.

Code 3.2: Syntax for writing `Models`.

```
Model name [as base]
   PARAMETERS
   [outer] name [as base[( (attribute = value)+ )] ];

   VARIABLES
   [in | out] name [as base[( (attribute = value)+ ) ] ];

   EQUATIONS
   ["equation name"] expression = expression;

   INITIAL
   ["equation name"] expression = expression;

   SET
   name = expression;
end
```

where the following conventions are considered:

- every command between `[ ]` is optional, if the command is used the `[ ]` must be extracted;
- the operator `( )+` means that the code inside of `( )` should be repeated **one** or more times separated by comma, but without the `( )`;

- the code a|b means a *or* b;
- name is a valid identifier chosen by the user;
- base is a valid EMSO type or already declared Model;
- expression is an mathematical expression involving any constant, variable or parameter already declared.

Therefore, using this convention, the the line 1 of Code 3.2 could be any of the following lines:

```
Model MyModel
Model MyModel as BaseModel
Model MyModel as Base1, Base2, Base3
```

As another example, consider the line 5 of Code 3.2, commands matching that pattern are:

```
MyVariable;
in MyVariable;
out MyVariable;
MyVariable as Real;
MyVariable as Real(Default=0, Upper = 100);
MyVariable as MyModel;
```

3.2.1 Parameters

Models of physical systems usually relies in a set of characteristic constants, called parameters. A parameter will never be the result of a simulation, its value needs to be known before the simulation starts.

When running an optimization or parameter estimation the value of a parameter could be the result of the calculation.

In Code 3.2, each identifier in capitals starts a new section. In line 2 the identifier PARAMETERS starts the section where the parameters are declared. A parameter declaration follows the pattern shown in line 3, this pattern is very near to that used in type declarations (see subsection 3.1.4).

In a Model any number of parameters, unique identified with different names, can be declared. Examples of parameter declarations follows:

```
PARAMETERS
	NumberOfComponents as Integer(Lower=0);
	outer OuterPar as Real;
```

Outer Parameters

As can be seen in line 3 of Code 3.2 a parameter declaration can use the `outer` prefix. When a parameter is declared with this prefix, the parameter is only a reference to a parameter with same name but declared in an outer context, for instance in a `FlowSheet`. Because of this, parameters declared with the `outer` prefix are known as outer parameters, while parameters without the prefix are known as concrete parameters.

The purpose of outer parameters is to share the value of a parameter between several `Device`s of a `FlowSheet`. Note that the value of an outer parameter comes from a parameter with same name but declared in some outer context. When the source of an `outer` parameter is a `FlowSheet` its value is specified only in the `FlowSheet` and then all models can use that value directly.

3.2.2 Variables

Every mathematical model has a set of variables once the variable values describe the behavior of the system being modeled. These values are the result of a simulation in opposition to parameters, which need to be known prior to the simulation.

In the EMSO modeling language, variables are declared in a manner very close to parameters. The `VARIABLES` identifier starts the section where the variables are declared, following the form presented in line 5 of Code 3.2. Examples of variable declarations follows:

```
VARIABLES
      T as Real(Brief="Temperature", Lower=200,
          Upper = 6000);
      in Fin as FlowRate;
      out Fout as FlowRate;
```

A `Model` can contain an unlimited number of variables, but a `Model` with no variables has no sense and is considered invalid. The user should already note that the declaration of types, variables and parameters are very similar, using a name and optionally deriving from a base. In the case of variables and parameters the base can be one of the built-in types (see Table 3.1), types deriving from the built-in ones or predeclared `Model`s.

Inputs and Outputs

When declaring variables, the prefixes `in` and `out` can be used, see line 6 of Code 3.2.

Variables declared with the `out` prefix are called output variables, while that declared with the `in` prefix are called input variables. The purpose of these kind of variables is to provide connection *ports*, enabling the user to connect output variables to input variables.

An output variable works exactly as an usual variable, but is available to be the source of a connection. However, an input variable is not a *concrete* variable, once it is only a reference to the values coming from the output variable connected to it. This connecting method is used, instead of adding new *hidden* equations for each connection, with the intent of reduce the size of the resulting system of equations. A description on how to connect variables can be found in subsection 3.3.2.

3.2.3 Composition in `Models`

In subsection 3.1.1 the composition concept was introduced. In the EMSO modeling language, to built *composed* `Models` is nothing more than declare parameters or variables but using `Models` as base instead of types.

If a `Model` is used as base for a variable such variable actually is a sub-model and the `Model` where this variable was declared is called a composed `Model`.

A variable deriving from a `Model` contains all the variables, parameters even equations of the base. In order to access the the internal entities of a sub-model, for instance in equations or for setting parameters, a *path* should be used, as exemplified in line 4 of the code below:

```
1 VARIABLES
2       controller as PID;
3 SET
4       controller.K = 10;
```

In the case of parameters deriving from a `Model`, the inheriting process has some peculiarities:

- Parameters of the base are sub-parameters;
- Variables of the base are considered as sub-parameters;
- Equations, initial conditions and all the rest of the base are unconsidered;

3.2.4 Equations

Equations are needed to describe the behavior of the variables of a `Model`. A `Model` can have any number of equations, including no equations. In EMSO an equation is an equality relation between two expressions, it is **not** an attributive relation. Therefore, the order in which the equations are declared does not matter.

Warning: A `Model` with more equations than variables is useless, once there is no way to remove equations from a model.

An equation is declared using the form presented in line 7 of Code 3.2, where `expression` is a expression involving any of preciously declared variables, parameters, operators, built-in functions and constants. A constant can be a number or the text of a unit of measurement. Details about the available operators, functions and their meaning can be found in section 3.5.

Examples of equation follows:

```
EQUATIONS
	"Total mass balance" diff(Mt) = Feed.F - (L.F
	    + V.F);
	"Vapor pressure" ln(P/'atm') = A*ln(T/'K') + B
	    /T + C + D*T^2;
```

Units of measurement

Note that `'atm'` and `'K'`, in the code above, are **not** comments, such texts are recognized as units of measurement (UOM) constants and effectively are part of the expression. In such example the UOMs are required to assure units dimension correctness, because the `ln` function expects a UOM dimensionless argument.

The UOM of a variable or parameter comes from its type or declaration, for example:

```
temperature as Real(final Unit='K', Lower = 100,
    Upper = 5000);
pressure as Real(final Unit='atm', Lower = 1e-6,
    Upper = 1000);

VARIABLES
	T1 as temperature;
	T2 as Real(Unit = 'K');

	P1 as pressure;
	P2 as pressure(Unit = 'kPa'); # error because
	    Unit was declared as final in pressure
	P2 as pressure(DisplayUnit = 'kPa');
```

An attribute of a type can be fixed with the `final` prefix. A final attribute cannot be changed when deriving from it. In the above code, the declaration of variable `P2` contains an error because the `Unit` attribute of `pressure` is final and cannot be changed.

Declaring `Unit` attributes as `final` is important because the limits (`Lower` and `Upper`) are considered to be in the same UOM as `Unit`. But making a `Unit` to be `final` still leaves to the user the option to change the UOM to be displayed in results. This can be achieved setting the `DisplayUnit` attribute accordingly.

3.2.5 Initial Conditions

EMSO can execute dynamic and steady state simulations, see subsection 3.3.4. Most dynamic systems requires a set of initial conditions in order to obtain its solution. These initial conditions are stated exactly as equations (subsection 3.2.4 but within the `INITIAL` section identifier, for instance:

```
INITIAL
	"Initial total mass" Mt = 2000 * 'kg';
```

Note that the "equations" given in the `INITIAL` section are used only in the initialization procedure of dynamic simulations.

3.2.6 Abstract `Models`

If a `Model` has less equations than variables it is known as a *rectangular* or *abstract* `Model`, because specifications, connections or extra equations are required in order to obtain its solution. If a `Model` has no equation it is known as a *pure abstract* `Model`, once it holds no information about the behavior of its variables.

Most models of a library are abstract or pure abstract where the pure abstract models are derived to generate a family of abstract models and so on. Note that is very uncommon to have a pure abstract model used directly in a `FlowSheets` as well as to use a model which is not abstract.

3.3 `FlowSheet`

In section 3.2 the `Model` body was described. When writing `FlowSheets` the user can freely make use of **all** description commands of a `Model` body, exactly as stated in section 3.2. Additionally, in the case of `FlowSheets`, the sections presented in in Code 3.3 could be used.

Code 3.3: Syntax for writing FlowSheets.

```
1  FlowSheet name [as base]
2     DEVICES
3     name [as base[( (attribute = value)+ )] ];

5     CONNECTIONS
6     name to name;

8     SPECIFY
9     name = expression;

11    OPTIONS
12    name = value;
13 end
```

Code 3.3 uses the same code conventions explained in section 3.2. It follows below the details of the sections of this code.

3.3.1 Devices

In line 2 of the Code 3.3 the DEVICES section can be seen. In this section the user can declare any number of Devices of a FlowSheet, in OO modeling these Devices are known as the *components*, see subsection 3.1.1.

The DEVICES section in a FlowSheet is a "substitute" of the VARIABLES section of a Model but no prefix is allowed.

Note: There is no sense in using the in or out prefix in FlowSheets, because these supposed inputs or outputs could not be connected once the FlowSheet is the top level model.

Exactly as variables of a Model, the base (line 3 of Code 3.3) can be any a type, or Model.

Examples of Device declarations follows:

```
DEVICES
      feed as MaterialStream;
      pump1 as Pump;
      pump2 as Pump;
```

3.3.2 Connections

In subsection 3.2.2 was described how to declare an input or output variable. However, was not specified how to connect an output variable to an input one. This can be done with the form presented in line 6 of Code 3.3, where a output variable is connected to an input.

It is stressed that the values of an input variable are only references to the values of the output connected to it avoiding extra equations representing the connections and reducing the size of the resulting system of equations.

Note that the CONNECTIONS section can be used in Models in the same way that in FlowSheets. It was omitted when the Model body was described on purpose because is more intuitive to connect variables in a FlowSheet. There is no restrictions in using connections in a Model, but, when possible, *composition* and *inheritance* should be used instead.

3.3.3 Specifications

In subsection 3.2.6 the term abstract model was defined, basically it means models with missing "equations". Most useful models are abstract, because of their flexibility. This flexibility comes from the possibility of specify or connect the models in several different fashions.

In order to simulate a FlowSheet it must have the number of variables equal number of equations. FlowSheets using abstract Models requires specifications for variables in the form presented in line 9 of Code 3.3. In a specification expression can be any expression valid for an equation (see subsection 3.2.4) and name is the name or path name of the specified variable.

3.3.4 Options

In order to adjust the simulation parameters of a FlowSheet the user can make use of the OPTIONS section. The following piece of code shows how to set simulation options of a FlowSheet:

```
OPTIONS
	TimeStart = 1;
	TimeStep = 0.1;
	TimeEnd = 10;
	TimeUnit = 'h';
	DAESolver( File = "dasslc");
```

In Table 3.2 all available options are listed.

3.4 Optimization

Optimization differ from simulation in several aspects. In simulation problems the solvers will try to find **the** solution. In optimization problems the solvers try to find the **best** solution with

Table 3.2: `FlowSheet` options, default value in **bold**.

Option name	Type	Description
TimeStart	real	The reporting integration time start: **`0`**;
TimeStep	real	The reporting integration time step: **`10`**;
TimeEnd	real	The reporting integration time end: **`100`**;
Dynamic	boolean	Execute dynamic or static simulation: **`true`** or `false`;
Integration	text	The system to be used in integration: **`"original"`**, `"index1"` or `"index0"`;
RelativeAccuracy	real	The relative accuracy: **`1e-3`**;
AbsoluteAccuracy	real	The absolute accuracy: **`1e-6`**;
EventVarAccuracy	real	The independent variable accuracy when detecting state events: **`1e-2`**;
SparseAlgebra	boolean	To use sparse linear algebra or dense: **`true`** or `false`;
InitialFile	text	Load the initial condition from result file
GuessFile	text	Load the an initial guess from result file
NLASolver	text	The NLA solver library file name to be used: **`"sundials"`**, `"nlasolver"`, or the name the file of some solver developed by the user as described in chapter 7;
DAESolver	text	The DAE solver library file name to be used: **`"dasslc"`**, `"sundials"`, `"dassl"`, `"mebdf"`, or the name the file of some solver developed by the user as described in chapter 7;

respect to some objectives and constraints. The objectives can be to minimize or maximize one or more expressions.

EMSO can be used to execute optimizations ranging from simple to large-scale. When writing optimization problems the user can freely make use of **all** description commands of a `FlowSheet` body, exactly as stated in section 3.3. Additionally, in the case of optimization problems, the sections presented in in Code 3.4 could be used.

Code 3.4: Syntax for writing `FlowSheet`s.

```
Optimization name [as base]
   MINIMIZE
   expression1;
   expression2;

   MAXIMIZE
   expression3;
   expression4;

   EQUATIONS
   expression5 < expression6;
   expression7 > expression8;

   FREE
   variable1;
   variable2;
end
```

Code 3.4 uses the same code conventions explained in section 3.2. It follows below the details of the sections of this code.

3.4.1 Simple Optimizations

An example of simple optimization problem follows:

```
Optimization hs71
      VARIABLES
      x(4) as Real(Default=1, Lower=1, Upper=5);

      MINIMIZE
      x(1)*x(4)*(x(1)+x(2)+x(3))+x(3);

      EQUATIONS
      x(1)*x(2)*x(3)*x(4) > 25;

      x(1)*x(1) + x(2)*x(2) + x(3)*x(3) + x(4)*x(4)
          = 40;

      OPTIONS
      Dynamic = false;
end
```

As can be seen in the code above, optimization problems support **inequality** constraints which are not supported in `Models` or `FlowSheets`.

In the example above, the optimization is self-contained. The variables, optimization objectives and constraints are all declared in the optimization problem body.

Tip: Optimization problems are solved exactly as `FlowSheets`, with the `run` button.

3.4.2 Large-Scale Optimization

In subsection 3.4.1 we described how to write a simple optimization problem. The same approach can be used to describe large-scale problems but this form is barely convenient.

As a convenience for the user, EMSO supports the directly optimization of already running `FlowSheets`. As an example, consider that the user has an already developed and running `FlowSheet` for a process of ammonia synthesis called `Ammonia`. Now lets consider that the user want to find the recycle fraction which yields to the minimun lost of product on the purge. For this case the following code could be used:

```
Optimization AmmoniaOptimization as Ammonia
      MINIMIZE
      productLoose;

      FREE
      Splitter102.fraction;

      OPTIONS
      Dynamic = false;
end
```

Warning: In order to optimize `FlowSheets` make sure that the `FlowSheet` can run (it should be consistent and the simulation should succed).

3.4.3 Options

In subsection 3.3.4 all options supported by `FlowSheets` were presented. Optimization problems support additional options as listed in Table 3.3.

Table 3.3: Optimization options, default value in **bold**.

Option name	Type	Description
NLPSolveNLA	boolean	Flag if the simulation solution should be used as start value for the optimization problem: **`true`** or `false`;
NLPSolver	text	The file name of the NLP solver library: **`"ipopt_emso"`**, or the name the file of some solver developed by the user as described in chapter 7;

3.4.4 Dynamic Optimization

Under construction: As of this time, EMSO only supports static optimization, dynamic optimization will be available soon.

3.5 Built-in Functions

In this section the built-in functions supported by the EMSO are listed. There are two categories of functions:

- **Element-by-element**: if the argument of the function is a vector or matrix, the function is applied in the same way to all elements of the argument. The returned value of these functions always have the same dimensions of its argument;
- **Matrix transformation**: The functions in this category make sense only for vector and matrix arguments. The return value can be a scalar, vector, or matrix depending on the function and the argument.

Examples of use of the functions are available in the folder `<EMSO>/mso/sample/miscellaneous`.

Table 3.4: Element-by-Element functions.

Function	Meaning
diff(Z)	Returns the derivative of Z with respect to time
exp(Z)	Returns the exponential function, e raised to the power Z
log(Z)	Returns the base 10 logarithm of Z
ln(Z)	Returns the natural logarithm (base e) of Z
sqrt(Z)	Returns the square root of Z
Trigonometric	
sin(Z)	Returns the sine of Z
cos(Z)	Returns the cosine of Z
tan(Z)	Returns the tangent of Z
asin(Z)	Returns the angle whose sine is Z
acos(Z)	Returns the angle whose cosine is Z
atan(Z)	Returns the angle whose tangent is Z
Hyperbolic	
sinh(Z)	Returns the hyperbolic sine of Z
cosh(Z)	Returns the hyperbolic cosine of Z
tanh(Z)	Returns the hyperbolic tangent of Z
coth(Z)	Returns the hyperbolic cotangent of Z
Discontinuous	
abs(Z)	Returns the magnitude or absolute value of Z
max(Z)	Returns the maximum value of Z
min(Z)	Returns the minimum value of Z
sign(Z)	Returns the signal of Z (-1 if Z $<$ 0 e 1 if Z$>$ 0
round(Z)	Returns the small integer value of Z

Table 3.5: Matrix Transformation Functions.

Function	Meaning
Sum	
sum(VEC)	Returns a scalar with the sum of all elements of the vector VEC
sum(MAT)	Returns a vector with the sum of each column of the matrix MAT
sumt(MAT)	Returns a vector with the sum of each row of the matrix MAT
Product	
prod(VEC)	Returns a scalar with the product of all elements of the vector VEC
prod(MAT)	Returns a vector with the product of each column of the matrix MAT
prodt(MAT)	Returns a vector with the product of each row of the matrix MAT
Transpose	
transp(MAT)	Returns the transpose of a matrix MAT

3.6 Units Of Measurement (UOM)

The units of measurement recognized by the EMSO modeling language are listed below.

3.6.1 Fundamental Units

m	length in meters
kg	mass in kilogram
s	time in seconds
K	temperature in Kelvin
A	eletric current in Ampere
mol	the amount of substance in mole
cd	the luminous intensity in Candela
rad	angle measure in radian
US$	money in dollar (USA)

3.6.2 Derived Units

Acceleration of Gravity		
ga	9.80665*m/s^2	std acceleration of gravity
Angle		
arcs	4.8481368111e-6*rad	arcsecond
arcmin	2.90888208666e-4*rad	arcminute
grad	1.57079632679e-2*rad	grad
deg	1.74532925199e-2*rad	degree

Area		
acre	4046.87260987*m^2	acre
a	100*m^2	are
ha	10000*m^2	hectare
b	1e-28*m^2	barn
Eletric		
Wb	kg*m^2/A/s^2	weber
T	kg/A/s^2	tesla
S	A^2*s^3/kg/m^2	siemens
mho	A^2*s^3/kg/m^2	mho
Fdy	96487*A*s	faraday
F	A^2*s^4/kg/m^2	farad
ohm	kg*m^2/A^2/s^3	ohm
C	A*s	relative current for batteries
V	kg*m^2/A/s^3	volt
Energy		
J	kg*m^2/s^2	joule
kJ	1e3*J	kilojoule
MJ	1e6*J	megajoule
GJ	1e9*J	gigajoule
eV	1.60217733e-19*J	electronvolt
MeV	1e6*eV	megaelectronvolt
therm	105506000*J	therm
Btu	1055.05585262*J	British thermal unit
cal	4.1868*J	calorie
kcal	1e3*cal	kilo calorie
erg	1e-7*J	erg
Force		
N	kg*m/s^2	newton
pdl	0.138254954376*N	poundal
lbf	4.44822161526*N	pounds of force
kip	4448.22161526*N	kip
gf	0.00980665*N	gram force
kgf	1e3*gf	kilogram force
dyn	0.00001*N	dyne
Length		
cm	1e-2*m	centimeter
mm	0.1*cm	millimeter
fermi	1e-15*m	fermi
$\AA$	1e-10*m	angstrom
μ	1e-6*m	micro

mil	2.54e-5*m	mil
ftUS	0.304800609601*m	international foot
fath	1.82880365761*m	fathom
rd	5.02921005842*m	rod
chain	20.1168402337*m	chain
miUS	1609.34721869*m	US statute miles
nmi	1852*m	nautical mile
mi	1609.344*m	International Mile
km	1000*m	Kilometer
au	1.495979e11*m	Astronomical Unit
lyr	9.46052840488e15*m	light year
pc	3.08567818585e16*m	parsec
Mpc	3.08567818585e22*m	megaparsec
in	0.0254*m	inch
ft	0.3048*m	foot
yd	0.9144*m	yard
Mass		
u	1.6605402e-27*kg	atomic mass unit
grain	0.00006479891*kg	grain
ct	0.0002*kg	carat
ozt	0.0311034768*kg	troy ounce
t	1000*kg	tonne
tonUK	1016.0469088*kg	ton (UK)
ton	907.18474*kg	ton
lbt	0.3732417216*kg	troy pound
slug	14.5939029372*kg	slug
oz	0.028349523125*kg	ounce
lb	0.45359237*kg	pound
g	kg/1000	gram
kmol	1e3*mol	kilomole
lbmol	453.59237*mol	pound mole
Money		
R$	US$/3.05	Brazilian money (Real)
Power		
W	$kg * m^2/s^3$	watt
kW	1e3*W	Kilowatt
MW	1e6*W	megawatt
hp	745.699871582*W	horsepower
Pressure		
Pa	kg/m/s^2 pascal	
kPa	1e3*Pa	Kilopascal

MPa	1e3*kPa	megapascal
inH2O	248.84*Pa	inch of water column
inHg	3386.38815789*Pa	inch of mercury
mmHg	133.322368421*Pa	millimeter of mercury
torr	133.322368421*Pa	torr
psi	6894.75729317*Pa	pound per square inch
bar	1e5*Pa	bar
atm	101325*Pa	atmosphere
Radiation		
R	0.000258*A*s/kg	R
Ci	3.7e10/s	curie
Bq	1/s	becquerel
Sv	m^2/s^2	sievert
rem	0.01*m^2/s^2	rem
Gy	m^2/s^2	gray
Temperature		
degR	K/1.8	degree Rankine
Time		
Hz	1/s	hertz
min	60*s	minute
rpm	1/min	revolution per minute
h	60*min	hour
d	24*h	day
yr	31556925.9744*s	year
Velocity		
c	299792458*m/s	light speed
knot	0.514444444444*m/s	knot
mph	0.44704*m/s	mile per hour
kph	0.277777777778*m/s	kilometer per hour
Viscosity		
St	0.0001*m^2/s	stoke
P	0.1*kg/m/s	poise
cP	0.001*kg/m/s	centipoise
Volume		
st	m^3	Stere
fbm	0.002359737216*m^3	board foot
pk	0.0088097675*m^3	peck
bu	0.03523907*m^3	bushel
bbl	0.158987291928*m^3	barrel
trp	4.92892159375e-6*m^3	teaspoon
tbsp	1.47867647813e-5*m^3	tablespoon

ozUK	2.8413075e-5*m^3	fluid ounce (UK)
ozfl	2.95735295625e-5*m^3	fluid ounce
cu	2.365882365e-4*m^3	US Cup
l	1e-3*m^3	liter
ml	1e-3*l	milliliter
pt	0.000473176473*m^3	pint
qt	0.000946352946*m^3	quart
gal	0.00378541178*m^3	gallon
galC	0.00454609*m^3	imperial gallon
galUK	0.004546092*m^3	gallon (UK)

3.7 Solver Options

Solver specific options can be declared in the following way, they are not case sensitive:

```
OPTIONS
        Dynamic = false;
        NLPSolveNLA = false;
        NLPSolver(File = "ipopt_emso",
            RelativeAccuracy = 1e-6, limited\_memory\
            _max\_history = 20);
```

Table 3.6: IPOPT optimization solver specific options, default value in **bold**.

Option name	Type	Description
MaxIter	integer	Maximum number of iterations: textbf`3000`
Print_level	integer	Output verbosity level. The valid range for this integer option is $0 \leq$ **printlevel** ≤ 11
Limited_memory_max_history	integer	Maximum size of the history for the limited quasi-Newton Hessian approximation. The valid range for this integer option is $0 \leq \mathbf{6} < +\infty$
Derivative_test	string	Enable derivative checker: `first-order`, `second-order`, **`none`**
Derivative_test_print_all	string	Indicates whether information for all estimated derivatives should be printed: `yes`, **`no`**
Output_file	string	File name of desired output file. **`ipopt.out`**
Mu_strategy	string	Update strategy for barrier parameter: `"adaptive"`, **`monotone`**
Print_user_options	string	Print all options set by the user: `"yes"`, **`no`**
RelativeAccuracy	real	Desired convergence tolerance (relative): $\mathbf{1 \cdot 10^{-08}}$
Acceptable_tol	real	Acceptable" convergence tolerance (relative): $\mathbf{1 \cdot 10^{-06}}$
Constr_viol_tol	real	Desired threshold for the constraint violation(Absolute): $\mathbf{1 \cdot 10^{-04}}$
Acceptable_constr_viol_tol	real	"Acceptance" threshold for the constraint violation(Absolute): $\mathbf{1 \cdot 10^{-02}}$
Dual_inf_tol	real	Desired threshold for the dual infeasibility(absolute): $\mathbf{1 \cdot 10^{-04}}$
Acceptable_dual_inf_tol	real	"Acceptance" threshold for the dual infeasibility(absolute): $\mathbf{1 \cdot 10^{-02}}$
Barrier_tol_factor	real	Factor for mu in barrier stop test.(absolute): $\mathbf{1 \cdot 10^{+01}}$
Compl_inf_tol	real	Desired threshold for the complementarity conditions: $\mathbf{1 \cdot 10^{-04}}$

Table 3.7: OPT++ optimization solver specific options, default value in **bold**.

Option name	Type	Description
MaxIterations	integer	Maximum number of iterations: **`100`**
MaxFeval	integer	Maximum number of function evaluations allowed: **`1000`**
MaxBTIter	integer	Maximum number of Back Track iterations allowed: **5**
PrintDebug	integer	Print debug information: `1`, **0**
SearchStrategy	string	Search Strategy: `BTLineSearch`, **`TrustRegion`**, `LineSearch`
MeritFun	string	Search Strategy: `ArgaezTapia`, **`NormFmu`**, `VanShanno` ;
OutputFile	string	Output file name: **`opt.out`**
RelativeAccuracy	real	set the Function tolerance: $\mathbf{1.49 \cdot 10^{-08}}$
GradTol	real	set the Function tolerance: $\mathbf{6 \cdot 10^{-06}}$
ConstrTol	real	set the Function tolerance: $\sqrt{\boldsymbol{eps}}$
StepTol	real	set the Function tolerance: $\mathbf{1.49 \cdot 10^{-08}}$
MaxStep	real	set the Function tolerance: $\mathbf{1 \cdot 10^{+03}}$
MinStep	real	set the Function tolerance: $\mathbf{1.49 \cdot 10^{-08}}$
LineSearchTol	real	set the Function tolerance: $\mathbf{1 \cdot 10^{-04}}$
TRSize	real	set the Function tolerance: $\mathbf{0.1} * \|\boldsymbol{\nabla f(x)}\|$

Table 3.8: NLASolver and Sundials specific options, default value in **bold**.

Option name	Type	Description
MaxIterations	integer	Maximum number of iterations: **`100`**
Maxatbound	integer	Maximum number of iterations at bound: **20**
MaxDumpIter	integer	Maximum dump iteration: **6**
MaxLSetupReuse	integer	Maximum Jacobian reuse in the linear solving phase: **0**
RelativeAccuracy	real	set the Function tolerance: $\mathbf{1 \cdot 10^{-03}}$
AbsoluteAccuracy	real	set the Function tolerance: $\mathbf{1 \cdot 10^{-06}}$

Table 3.9: IDASolver specific options, default value in **bold**.

Option name	Type	Description
MaxIterations	integer	Maximum number of internal steps to be taken by the solver in its attempt to reach tout. **500**
MaxOrder	integer	Maximum LMM mathod order: **5**
SuppressAlg	integer	Suppress alg. vars. from error test **0**
RelativeAccuracy	real	Set the function tolerance: $\mathbf{1 \cdot 10^{-03}}$
AbsoluteAccuracy	real	Set the function tolerance: $\mathbf{1 \cdot 10^{-06}}$
Hinit	real	Initial step size **0**
Hmax	real	Maximum absolute value of step size allowed $\mathbf{1 \cdot 10^{10}}$
Nconfac	real	Factor in nonlinear convergence test for use during integration **1.0**

Table 3.10: DASSLC specific options, default value in **bold**.

Option name	Type	Description
MaxIterations	integer	Maximum number of internal steps to be taken by the solver in its attempt to reach tout. **10**
MaxOrder	integer	Maximum LMM mathod order: **5**
Maxl	integer	max. number of iterations before restart: **5**
Kmp	integer	number of orthogonalized vectors: **5**
Istall	integer	intermediate time steps : **5**
RelativeAccuracy	real	Set the function tolerance: $\mathbf{1 \cdot 10^{-03}}$
AbsoluteAccuracy	real	Set the function tolerance: $\mathbf{1 \cdot 10^{-06}}$

4 Advanced Modeling

In chapter 3 the basic concepts of the EMSO modeling language were described. In this chapter we describe more advanced concepts.

Contents

4.1 Arrays

In EMSO we can make use of multidimensional arrays, i.e., arrays with any number dimensions.

4.1.1 Vectors

The simplest form of an array is the one dimension array – a vector. In EMSO a vector of variables is declared as follows:

```
PARAMETERS
	N as Integer(Default=10);
VARIABLES
	vector1(100) as Real(Brief="A vector with 100
	    elements");
	vector2(N)   as Real(Brief="Undefined length
	    vector");
```

In the code above two vectors were declared, `vector1` has a fixed length while `vector2` has its length equal to `N` which can be set after.

Note: In order to build more general models the user should declare the dimensions of the arrays as parameters. Remember that the dimension of an array **must** be an `Integer`.

Besides the default types, in EMSO the user can compose new models using vectors of another models as follows:

```
using "stream";

Model Mixer
	PARAMETERS
	Ninputs as Integer(Brief="Number of inputs",
	    Default=2);

	VARIABLES
	Inlet(Ninputs) as stream;
	Outlet         as stream;
```

In the piece of code above the `Inlet` is a vector of length `Ninputs` in which each element is a `stream`. The parameter `Niputs` can be set *after* in any point of a the `Model` or in the `FlowSheet`, for example:

```
FlowSheet MixProcess
	DEVICES
	mix as Mixer;
	s1 as stream;
	s2 as stream;
	s3 as stream;
```

```
        CONNECTIONS
        s1 to mix.Inlet(1);
        s2 to mix.Inlet(2);
        s3 to mix.Inlet(3);

        SET
        mix.Ninputs = 3;
end
```

Warning: Differently from some popular programming languages as C or C++ the elements of a vector or array starts from **one** and not **zero**.

4.1.2 Multidimensional Arrays

A vector is an array with only one dimension, see subsection 4.1.1

Arrays with more than one dimension are declared in an analogous way to vectors :

```
VARIABLES
        var2d(x,y)    as Real(Brief="Array with 2
            dimensions");
        var3d(x,y,z) as Real(Brief="Array with 3
            dimensions");
```

4.1.3 Equation Expansion

The loop for is treated in subsection 4.1.5

In usual programming languages, when dealing with vectors or arrays the user has to work with *loops*, like `for` or `while`. EMSO also implements a loop `for` but it has a convenient mechanism which automatically expand the equations avoiding the use of loops in most situations.

Arrays with Identical Shapes

For instance, if we wants an equation telling that the composition of an outlet stream is equal to the composition of an inlet stream:

```
EQUATIONS
        Outlet.z = Inlet.z;
```

Then EMSO automatically expands the above equation by:

$$Outlet.z_i = Inlet.z_i, i = 1 : Ncomps$$

Arrays and Scalars

If an expression involve one array and one scalar, then the scalar is expanded to match the array dimensions. For example:

```
VARIABLES
	ones(M,N)   as Real;
EQUATIONS
	ones = 1;
```

Note: The above equation `ones=1;` actually accounts as `M` times `N` equations.

4.1.4 Array Functions

EMSO implements some functions specially designed for handling arrays.

Sum

The `sum` function sums the elements of a vector or array. For example, if in a mixer model we want to calculate the resulting outlet flow rate we could use:

$$Outlet.F = \sum_i Inlet_i.F$$

The above equation can be obtained by the last line of the following model:

```
Model Mixer
	PARAMETERS
	Ninputs as Integer(Brief="Number of inputs");

	VARIABLES
	Inlet(Ninputs) as stream;
	Outlet         as stream;

	EQUATIONS
	Outlet.F = sum(Inlet.F);
```

Note: If the argument of `sum` is a vector it will return a scalar, but if the argument is an matrix (array with two dimensions) it will return a vector with length equal to the number of lines of the matrix.

In general `sum` makes the summation of the last *dimension* of the argument. For instance, if we have:

```
VARIABLES
	var3d(x,y,z) as Real(Brief="Three dimensional
	    array");
	var2d(x,y)   as Real(Brief="Two dimensional
	    array");
EQUATIONS
	var2d = sum(var3d);
```

In the equation above, each element of var2d contains the sum of all elements of var3d over z, which is the last dimension. In other words:

$$var2d_{x,y} = \sum_{z} var3d_{x,y,z}$$

Prod

The prod function returns the productory of a vector or array. The logic of prod is exactly the same presented above for the sum function.

4.1.5 Loop For

Most equations involving arrays are more convenient handled by automatic equation expansion, see subsection 4.1.3. But in some rare situations the equation expansion cannot yield the desired result and one or more for loops are needed.

The syntax of a for loop is the following:

```
EQUATIONS
	for i in [1:Ncomps]
		Outlet.z(i) = Inlet.z(i);
	end
```

Note: The index i used by the for loop above does not need to be declared and is valid only in the context of the loop.

The above equation also can be written in a more compact fashion:

```
EQUATIONS
	Outlet.z([1:Ncomps]) = Inlet.z([1:Ncomps]);
```

4.2 Conditional Modeling

Under construction: needs to be documented

5 Calculation Object Interface

In this chapter, we describe how the `Plugin` paradigm can be used to load, at run time, third party software within EMSO entities. In chapter 6 is explained how to implement a new `Plugin` service.

Contents

5.1 Introduction

In this section we describe what is a Plugin and what it is good for.

5.1.1 What is Plugin?

Plugin is an interfacing mechanism which enables the user to load calculation services provided by third party software within EMSO. Typical cases where using Plugins is advisable are when the following calculations are required:

- Property based on correlations
- Thermo-physical properties
- CFD calculations for complex geometries

CFD is the acronym for Computational Fluid Dynamics.

5.1.2 Why use a Plugin?

EMSO is an equation-based tool, therefore most type of mathematical relations can be expressed directly as equations of a Model using the EMSO modeling language. However, there are some cases in which using equations is barely convenient. Typical examples include:

- The relationship cannot be expressed in a closed algebraic form without introducing many intermediate quantities with no physical sense;
- The relationship requires lots of data parameters;
- Already exists well established software that provides the required calculation;
- It is difficult to converge the problem without decoupling the system.

5.1.3 The Plugin Basics

Before showing how to use a Plugin, let's introduce its basics:

- Any number of Plugins can be declared within an EMSO entity (Model, FlowSheet, etc.). The declaration of a Plugin is very near to a parameter declaration;
- Each Plugin provides a set of *methods* which are the calculation routines available to be used in EMSO;
- Each *method* calculates *one* quantity (the output) for given *zero or more* other quantities (the inputs).

- The output of a *method*, as each of its inputs, can be a scalar or a vector of `Real`, `Integer` or `Boolean` and have an unit of measurement (enabling EMSO to automatic handle the required unit of measurement conversions).
- Additionally, a *method* can provide partial derivatives of its output with respect to all or some of its inputs.
- Each `Plugin` service is provided by *one* library file which *must* be compatible with the `Plugin` interface specification presented in section 6.1.

5.2 Using `Plugins`

In this section we show how to use `Plugins` within some EMSO entities.

5.2.1 Using `Plugins` in `Models`

`Plugin` is one of the EMSO built-in types, as `Real`, `Integer`, etc.

As already mentioned, the declaration of a `Plugin` is very near to a parameter declaration but using as base the EMSO built-in type `Plugin`. In Code 5.1 a typical usage of the `Plugin` paradigm can be seen.

Code 5.1: EML file `streams.mso`.

```
45 Model liquid_stream as stream
46       ATTRIBUTES
47       Pallete = false;
48       Brief = "Liquid Material Stream";
49       Info =
50       "Model for liquid material streams.
51       This model should be used only when the phase of the stream
52       is known ''a priori''.";

54       PARAMETERS
55       outer PP as Plugin(Brief = "External Physical Properties", Type="PP");

57       EQUATIONS
58       "Liquid Enthalpy"
59       h = PP.LiquidEnthalpy(T, P, z);
60       "Liquid stream"
61       v = 0;
62 end
```

Outer parameters were treated in subsection 3.2.1.

The Code 5.1 makes part of EML, in line 55 of it a `Plugin` is declared. As can be seen, it is declared with the `outer` prefix, therefore it is only an reference to a entity with same name but declared in the top level model, the `FlowSheet`.

In the case of a concrete `Plugin` (declared without the `outer` prefix) the user must supply the corresponding calculation library type and optionally supply arguments to create the object. A sample declaration of a concrete `Plugin` follows:

A calculation library must be a valid DLL (dynamic link library) or a SO (shared library) file in win32 and posix platforms respectively.

```
PARAMETERS
  PP as Plugin(Brief="Physical Properties Object",
     Type="PP");
```

In this code, the object `PP` will be created using the type `PP`. The available `Plugin` *types* are configured with help of the Plugins Configuration dialog, as shown in Figure 5.1. This dialog is can be reached by the menu `Config→Plugins`.

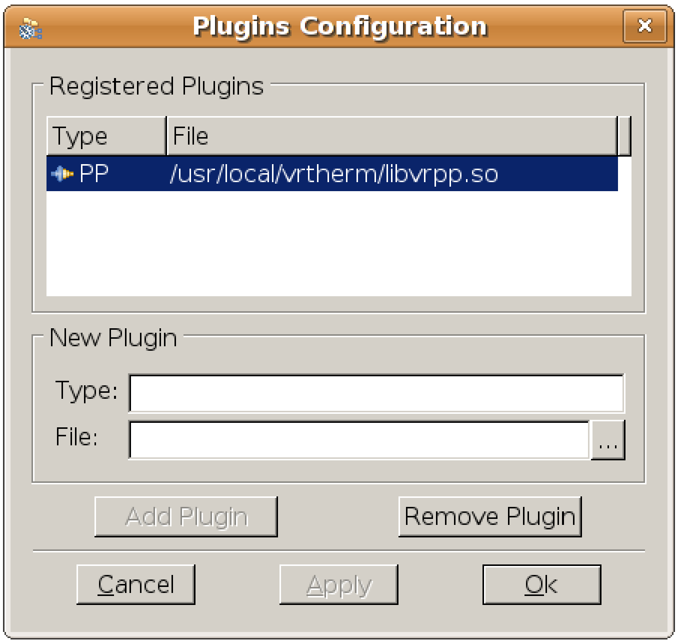


Figure 5.1: Plugins Configuration dialog.

Using the dialog shown in Figure 5.1, the user can register any number of `Plugin` types, but each type needs a unique type name. Each type is dynamic linked by EMSO with the given file.

In line 59 of Code 5.1 a `Plugin` method is called, as can be seen, this methods requires three inputs:

- `T` temperature;
- `P` pressure;
- `z` molar composition vector.

The cited method returns the molar enthalpy of the liquid phase of the mixture represented by `PP`.

Note: EMSO will check the units of measurement of all `Plugin` arguments, it also checks the units of the returned value.

II. Programming Guide

6 Developing new `Plugin` Services

In this chapter, we describe how to develop a new `Plugin` service enabling to load external software within EMSO entities. In section 5.2 the usage of the `Plugin` interface was described. Note that the information presented here is not a required to use `Plugin`s but to *develop* new services.

Contents

6.1 Interface Specification

In order to implement a `Plugin` service one can use any of the most common scientific programming languages. There are template implementations available for C, C++ and Fortran, presented in sections 6.2.1, 6.2.2 and 6.2.3 respectively. It follows bellow the concepts behind the `Plugin` interface.

Note: The information presented here is not required to *use* already made `Plugin`s but to *develop* new services.

A `Plugin` provides a set of methods, each of which receive zero or more inputs and returns one output. In order to implement a library which provides such service, one must implement the following functions:

- `create`: creates a new instance of the `Plugin` service
- `check_method`: checks if a specific method exists and returns the number of inputs and outputs
- `method_details`: provides detailed information about a specific method
- `set_parameter`: function for setting a parameter of the object
- `calc`: provides the calculation for a given method
- `destroy`: destroys an object instance created with the `create` function

In the following subsections these functions are detailed described. Note that, depending on the programming langued used to actually implement the service, a prefix in the function names can be required. For instance, when implemented in C, the `create` function should be `eo_create`. In Frotran, depending the compiler it should be `_eo_create`. For more details check subsection 6.2.1, subsection 6.2.2, or subsection 6.2.3.

6.1.1 Create Function

When a new EMSO task is started, like a dynamic simulation, for each concrete `Plugin` declared, EMSO creates a new instance of such object. In this creation procedure the `create` function is called in order to load the instance specific data.

The `create` function has the following form:

```
create(objectHandler, retVal, msg)
```

where the arguments are as described in Table 6.1.

Table 6.1: Arguments of the `Plugin create` function.

Argument name	Type	Description
`objectHandler`	[out] integer	Unique identifier of the object instance created (will be used to identify the instance in subsequent calls).
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

EMSO does not need to known what really happens in the `create` function, but the expected behavior is:

- create the memory to some data structure which holds the instance dependent data;
- if some error or warning has occurred set `retVal` accordingly and copy a message to the `msg`
- return the memory address of the data structure (or an integer which unique identifies it) in the `objectHandler`

As EMSO `Models`, a `Plugin` can have parameters. An example could be the required precision to be used when calculating a method. These parameters can be set as usuall in the `Model`, for instance:

```
PARAMETERS
    PP as Plugin(Brief="Physical Properties Object",
          Type = "PP", VapourModel = "PR",
             LiquidModel = "PR");
```

For each attribute given EMSO will make a call to the `set_parameter` function. The prototype of the `set_parameter` function is as follows:

```
set_parameter(objectHandler,
              parameterName, valueType, valueLength,
              values, valuesText,
              retVal, msg)
```

where the arguments are as described in Table 6.2.

The expected behavior of the `set_parameter` function is:

Table 6.2: Arguments of the Plugin set_parameter function.

Argument name	Type	Description
objectHandler	[in] integer	Identifier of the object instance coming from the create function.
parameterName	[in] text	The name of the parameter to be set.
valueType	[in] integer	The type of the parameter (1 for Real, 2 for Integer, 3 for Boolean and 4 for text)
valueLength	[in] integer	The length of the value (1 if is a scalar)
values	[in] real vector	The vector of values (empty if the type is text)
valuesText	[in] text vector	The vector of values (empty if the type is not text)
retVal	[out] integer	Return flag, see **??**.
msg	[out] text	A text space where error messages should be copied.

- Check if the given parameterName is a valid parameter, otherwise set retVal accordingly and copy a message to msg
- If the parameter is valid, store it to be used later

6.1.2 Destroy Function

When a Plugin instance is created the create function is called. Then, when the object is no longer used by EMSO it is destroyed. In some point of the destruction procedure the destroy function is called. This function has the following form:

```
destroy(objectHandler, retVal, msg)
```

where the arguments are as described in Table 6.3.

The expected behavior of the destroy function is to release any memory, close data banks, etc. regarding the given objectHandler.

6.1.3 Verification Functions

A priori, EMSO does not known what are the methods supplied by a particular Plugin nor the number or kind of its inputs

Table 6.3: Arguments of `destroy` function.

Argument name	Type	Description
`objectHandler`	[in] integer	Identifier of the object instance coming from the `create` function.
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

and outputs. This information is obtained with the functions `check_method` and `method_details`.

Basically, the former function is used to check the existence of a method and has the following form:

```
check_method(objectHandler, methodName, methodID,
             numOfInputs, numOfOutputs,
             retVal, msg)
```

where the arguments are as described in Table 6.4.

Table 6.4: Arguments of `check_method` function.

Argument name	Type	Description
`objectHandler`	[in] integer	Identifier of the object instance coming from the `create` function.
`methodName`	[in] text	Name of the method being checked.
`methodID`	[out] integer	Unique identifier for the given method name (will be used to identify the method in subsequent calls).
`numOfInputs`	[out] integer	The number of expected inputs of the method.
`numOfOutputs`	[out] integer	The number of outputs of the method.
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

From the `check_method` function the following behavior is expected:

- Check the existence of a given `methodName`, if the method does not exist this should be reported copying some message into `error`.

- If the required method exists, return the number of inputs and the number of outputs. Optionally, an unique identifier for the method can be returned in `methodID`. Then EMSO will use this identifier in subsequent calls, this procedure can speed up the evaluation of the functions.

Upon the ascertain of a method existence with the `check_method` function, the `method_details` function is used to obtain detailed information about the method. This function has the following form:

```
method_details(objectHandler, methodName, methodID,
                  numOfInputs, inputLengths, inputTypes
                      , inputUnits,
                  numOfOutputs, outputLengths,
                      outputTypes, outputUnits,
                  hasDerivatives,
                  retVal, msg)
```

where the arguments are as described in Table 6.5.

The purpose of the `method_details` function is to provide detailed information about the inputs and outputs of a specific method. The expected behaviour is:

- Given the `methodName` (or the `methodID` previouslly returned), set `inputLengths`, `inputTypes` and `inputUnits`.
- Given the `methodName` (or the `methodID` previouslly returned), set `outputLengths`, `outputTypes` and `outputUnits`.
- If the method will provide calculation for the derivatives set `hasDerivatives` to 1.

6.1.4 Calculation Function

Given the inputs, each `Plugin` method calculates one or more outputs. This calculation is provided by the `calc` function. This should be implemented by the service, it has the following form:

```
calc(objectHandler, methodName, methodID,
      outputLength, numOfInputs, inputLengths,
          totalInputLenth,
      methodInputs, methodOutput,
      error, warning)
```

where the arguments are as described in Table 6.6.

The expected behaviour for the `calc` function is:

Table 6.5: Arguments of `check_inputs` function.

Argument name	Type	Description
`objectHandler`	[in] integer	Identifier of the object instance coming from the `create` function.
`methodName`	[in] text	Name of the method being checked.
`methodID`	[in] integer	Identifier of the method coming from the `check_method` function.
`numOfInputs`	[in] integer	The number of inputs of the method.
`inputLengths`	[out] integer vector	The length of each input.
`inputTypes`	[out] integer vector	The type of each input (1 for `Real`, 2 for `Integer` and 3 for `Boolean`).
`inputUnits`	[out] text vector	The unit of measurement of each input.
`numOfOutputs`	[in] integer	The number of outputs of the method.
`outputLengths`	[out] integer vector	The length of each output.
`outputTypes`	[out] integer vector	The type of each output (1 for `Real`, 2 for `Integer` and 3 for `Boolean`).
`outputUnits`	[out] text vector	The unit of measurement of each output.
`hasDerivatives`	[out] integer	If the method provides analytical derivatives calculation
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

Table 6.6: Arguments of `calc` function.

Argument name	Type	Description
`objectHandler`	[in] integer	Identifier of the object instance coming from the `create` function.
`methodName`	[in] text	Name of the method being checked.
`methodID`	[in] integer	Unique identifier of the method name, coming from `check_method`.
`numOfInputs`	[in] integer	The number of inputs.
`inputLengths`	[in] integer vector	The length of each input.
`totalInputLength`	[in] integer	Total input length.
`inputValues`	[in] real vector	Vector containing the input values.
`numOfOutputs`	[in] integer	The number of outputs.
`outputLengths`	[in] integer vector	The length of each input.
`totalOutputLength`	[in] integer	Total output length.
`outputValues`	[out] real vector	Vector to put the calculated output values.
`calculeDerivatives`	[in] integer	Flag if the method should calculate the derivatives or not.
`outputDerivatives`	[out] real vector	Vector to put the calculated output derivative values.
`error`	[out] text	A text space where error messages should be copied.
`warning`	[out] text	A text space where warning messages should be copied.

- Given the `methodName` (or the `methodID` set previously) and the `inputValues`, calculate the method and store the results on `outputValues`.
- Additionally, if the method has implementation for the derivatives and `calculeDerivatives` is not false, return the value of the derivatives on `outputDerivatives`.

6.2 Writing new Plugin Services

In this section we describe how to implement a new `Plugin` service using the most common scientific programming languages.

As a base concept of the `Plugin` interface was stated that an EMSO entity can have any number of `Plugin`s (see **??**). Therefore, multiple instances of a `Plugin` service can be active simultaneously. If this is the case and the service being implemented has instance dependent data, each `Plugin` instance should allocate its own data. Unfortunately, dynamic memory allocation is not a trivial task in Fortran then if the service being implemented is intended to support multiple instances the user should consider in using C or C++ or *wrap* his Fortran implementation using such languages.

6.2.1 Writing Plugin Services in Fortran

As mentioned in section 6.1, in order to implement a new `Plugin` service some functions *must* be implemented. In file `external_object.f` found at `interfaces` directory a template implementation for a `Plugin` service in Fortran is given.

The template file has the required function calling conventions, besides several comments which helps the user in the task of implementing a new service and creating the library.

6.2.2 Writing Plugin Services in C

As mentioned in section 6.1, in order to implement a new `Plugin` service some functions *must* be implemented. In file `external_object.c` found at `interfaces` directory a template implementation for a `Plugin` service in C is given. This file makes use of the interface definitions declared at `external_object.h`. Note that the header file should not be modified by the user.

The template file has the required function calling conventions, besides several comments which helps the user in the task of implementing a new service and creating the library.

6.2.3 Writing **`Plugin`** Services in C++

As mentioned in section 6.1, in order to implement a new `Plugin` service some functions *must* be implemented. When using C++, this functions actually are *member* functions of a class. In file `external_object.cpp`, found at `interfaces` directory, a template implementation for a `Plugin` service in C++ is given. This file makes use of the interface definitions declared in file `external_object.h`. Note that the header file should not be modified by the user.

The C++ template file has a skeleton implementation that should be filled by the user, besides several comments which helps the user in the task of implementing a new service and creating the library. Actually, when implement a new `Plugin` services in C++ the user can choose between implement the interfaces exactly as described in the C template file or to implement it as class. The C++ template file uses the *class* approach.

6.3 Documenting **`Plugin`** Services

VRTherm is a software for physical properties prediction from VRTech `www.vrtech.com.br`.

The software VRTherm is a typical example of `Plugin`. Its documentation can be used as a base for developing the manual for a new service.

Basicaly, a good `Plugin` documentation should include at least:

- how to install the service;
- how to use the service
  - what is the `File` of the library;
  - specify whether the service supports multiple instances or not;
  - valid parameters and its purposes;
  - document the methods supplied by the service as well as the inputs and outputs.

7 Developing new Solvers

In this chapter, we describe how to develop new solver services enabling to solve the problems coming from the `FlowSheets` with custom solvers. These solvers are called *external solvers* because they could be freely implemented by third parties and are implemented in a very similar way to `Plugins` described in chapter 6.

Contents

7.1 NLA Solvers

Nonlinear-algebraic (NLA) systems arise naturally from steady-state mathematical models or in the initialization of dynamic simulations. In order to obtain the numerical solution, EMSO automatically converts this kind of problem into the following formulation:

$$F(y) = 0, \; y_l < y < y_u \tag{7.1}$$

where y is the vector of variables to solve, $F(y)$ is the vector of functions (the equations), y_l and y_u are the lower and upper bounds, respectivelly.

In this section we describe how to implement a new solver for systems as Equation 7.1.

When communicating to solvers EMSO acts as a server which give informations about the problem being solved. For NLA problems EMSO **provides** four functions to the solver:

- `ResFn`: returns the residuals for a given y
- `LSetup`: tells EMSO to update the Jacobian matrix $\partial F/\partial y$
- `LSolve`: solves for x the linear system $Ax = b$ for a given b, where A is the Jacobian matrix $\partial F/\partial y$
- `LProd`: makes the product $y = \alpha Ax + \beta y$, where A is the Jacobian matrix, α and β are scalars, x and y are given vectors.

This operation is also known as the GEMV BLAS operation

Using the functions provided by EMSO, a new NLA solver needs to **implement** the following routines:

- `create`: creates a new instance of the NLA external solver for a given problem structure;
- `solve`: solves the problem;
- `destroy`: destroy the external solver instance created with the `create` function;

7.1.1 Residuals Function

For any point y_c which is not the solution of Equation 7.1 we will have a residual:

$$F(y_c) = res \tag{7.2}$$

EMSO can calculate the residuals vector res with the `ResFn` function which has the following form:

```
ResFn(y, res, EMSOdata, retVal)
```

where the arguments are as in Table 7.1.

Table 7.1: Arguments of the `ResFn` function.

Argument name	Type	Description
`y`	[in] real	Vector with the current point for y
`res`	[out] real	Residuals vector, will be calculated as a function of y.
`EMSOdata`	-	EMSO problem specific data (should not be used by the solver).
`retVal`	[out] integer	Return flag, see **??**.

7.1.2 Jacobian

Newton's like methods can solve Equation 7.1 iteratively with some modification of the following equation:

$$\frac{\partial F}{\partial y}(y^n - y^{n+1}) = -F(y^n) \tag{7.3}$$

where $\partial F / \partial y$ is the Jacobian and $F(y^n)$ is the residuals vector (subsection 7.1.1).

Using Equation 7.3 to solve the problem the solver will need to solve a linear systems of equations. This can be done directly by EMSO with the `LSolve` function:

```
LSolve(x. b, EMSOdata, retVal)
```

where the arguments are as in Table 7.2.

Note: The `LSolve` function solves for x **given** a vector b, depending on the implementation of the solver, b can be $-F(y^n)$ or not.

It should be noted that the Jacobian is opaque to the solver. As a consequence, EMSO can use efficient storage structures (dense or sparse) and specific algorithms for solving the linear system which are independent from the solver implementation.

Table 7.2: Arguments of the `LSolve` function.

Argument name	Type	Description
`x`	[out] real	Vector with the solution of the linear system
`b`	[in] real	The independent vector b
`EMSOdata`	-	EMSO problem specific data (should not be used by the solver)
`retVal`	[out] integer	Return flag, see **??**.

The `LSolve` function solves the linear system using the Jacobian of the system. But aiming at efficiency EMSO does not updates the Jacobian matrix each time it solves the linear system. The solver needs to explicitly tell EMSO to update the Jacobian with the function `LSetup`:

```
LSetup(EMSOdata, retVal)
```

where the arguments are as in Table 7.3.

Table 7.3: Arguments of the `LSetup` function.

Argument name	Type	Description
`EMSOdata`	-	EMSO problem specific data (should not be used by the solver)
`retVal`	[out] integer	Return flag, see **??**.

As can be seen in Table 7.3 the `LSetup` function does not require an input argument for y. EMSO uses the y values given at the last call to `ResFn` (subsection 7.1.1), this method improve the efficiency when calculating the Jacobian using automatic differentiation.

7.1.3 Matrix Multiplication

Some modifications of the Newton method may require addition linear algebra operations using the Jacobian matrix. For these cases, EMSO provides a general product function, as follows:

$$y = \alpha A x + \beta y$$

where A is the Jacobian matrix, α and β are scalars, x and y are given vectors.

Note: The `LProd` function considers that x and y are given vectors, therefore x or y can be the current solution point or the current vector of residuals, it is up to the designed of the solver.

Some codes may need a simplified version of the product, $y = \alpha A x$. This is easily achieved passing β equal zero to the function `LProd`.

The `LProd` function has the following prototype:

```
LProd(alpha, x, beta, y, EMSOdata, retVal)
```

where the arguments are as in Table 7.4.

Table 7.4: Arguments of the `LProd` function.

Argument name	Type	Description
`alpha`	[in] real	Given scalar
`x`	[in] real	Given vector
`beta`	[in] real	Given scalar
`y`	[inout] real	Given vector, will hold the result of the operation
`EMSOdata`	-	EMSO problem specific data (should not be used by the solver).
`retVal`	[out] integer	Return flag, see **??**.

7.1.4 Create and Destroy Functions

EMSO can run concurrent simulations, and so, in order to support this feature, a new solver instance is created for each new simulation started. Each time EMSO needs a new solver it calls the `create` function of the solver. As a consequence, each instance of the solver should have its own memory space to avoid conflicts when running concurrent simulations.

The `create` function should allocate any memory needed by the solver. All allocated memory should be released by the `destroy` function.

The `create` function has the following form:

```
create(solverID, numOfEqs, resFn, y0, ylb, yub,
       EMSOdata, iopt, ropt, retVal, msg)
```

where the arguments are as described in Table 7.5.

Table 7.5: Arguments of the NLA solver `create` function.

Argument name	Type	Description
`solverID`	[out] integer	Unique identifier of the solver instance created (will be used to identify the instance in subsequent calls).
`numOfEqs`	[in] integer	The number of equations of the system.
`resFn`	[in] function	Function that calculates the residuals of the system.
`y0`	[in] real vector	Initial values of the variables.
`ylb`	[in] real vector	Lower bound for the variables.
`yub`	[in] real vector	Upper bound for the variables.
`EMSOdata`	[in] integer	EMSO problem specific data (only to pass back to `resFn`, `lsetup` and `lsolve`)
`iopt`	[in] integer vector	The vector of integer options, see **??**.
`ropt`	[in] real vector	The vector of real options, see **??**.
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

Warning: The solver should return a unique `SolverID` for each call to `create` because this integer will be used to identify the solver instance in subsequent calls to `solve` or `destroy`.

When EMSO does not need the solver anymore it calls the `destroy` function on it:

```
destroy(solverID, retVal, msg)
```

where the arguments are as described in Table 7.6.

Table 7.6: Arguments of the NLA solver `destroy` function.

Argument name	Type	Description
`solverID`	[in] integer	Unique identifier of the solver instance (returned by `create`).
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

Using the given `solverID` the solver should release any memory associated with that solver instance.

Note: When using C or C++, an easy way to implement an unique identifier for the solver is to create an structure or class for the solver and return its address as the identifier. Then the solver just needs to cast back the `SolverId` to get the address of the structure.

7.1.5 Solve Function

Once the solver instace has been created (as described in subsection 7.1.4), EMSO will generate a call to the `solve` function each time EMSO needs to solve the problem.

The `solve` function has the following form:

```
solve(solverID, numOfEqs, resFn, lsetup, lsolve,
      y, ylb, yub, EMSOdata, rtol, atol,
      iopt, ropt, retVal, msg)
```

where the arguments are as described in Table 7.10.

Table 7.7: Arguments of the NLA solver `solve` function.

Argument name	Type	Description
`solverID`	[out] integer	Unique identifier of the solver instance (returned by `create`).
`numOfEqs`	[in] integer	The number of equations of the system.
`resFn`	[in] function	Function that calculates the residuals of the system.
`y`	[inout] real vector	Initial values of the variables and the solution at the end.
`ylb`	[in] real vector	Lower bound for the variables.
`yub`	[in] real vector	Upper bound for the variables.
`EMSOdata`	[in] integer	EMSO problem specific data (only to pass back to `resFn`, `lsetup` and `lsolve`)
`rtol`	[in] real	The relative accuracy
`atol`	[in] real	The absolute accuracy (optionally a vector)
`iopt`	[in] integer vector	The vector of integer options, see **??**.
`ropt`	[in] real vector	The vector of real options, see **??**.
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

EMSO can call multiple times the `solve` function before destoying it. Each time EMSO asks the solver to solve the problem a initial guess `y` is given and the solution should be returned on the same vector.

Warning: The parameter `rtol` is always a real scalar but `atol` can be a vector depending on the options at `iopt`.

7.2 DAE Solvers

Differential-algebraic equations (DAE) arise naturally from dynamic modeling in several engineering areas.

Prior to a dynamic simulation, EMSO internally converts in memory the given `FlowSheet` description to a general DAE system in the following form:

$$F(t, y, y') = 0, \;\; y_l < y < y_u \tag{7.4}$$

where t is the independent variable (usually the time), y is the vector of variables, y' are the derivatives of y with respect to t and F are the equations of the problem being solved.

In EMSO a DAE solver is supposed only to advance one step forward in the solution of a problem. In other words, given a valid t_n, y_n, y'_n the DAE solver should only to advance **one** step to a next solution $t_{n+1}, y_{n+1}, y'_{n+1}$.

Note: The first solution t_0, y_0, y'_0 is obtained using a NLA solver in the initialization step.

Between calls to the DAE solver EMSO checks if events have happened and make proper reinitializations if needed.

In a very similar way to NLA solvers (section 7.1) EMSO **provides** a set of services which give informations about the problem being solved:

- `ResFn`: returns the residuals of Equation 7.4 for a given t, y, y'
- `LSetup`: tells EMSO to update the Jacobian matrices $\partial F/\partial y$ and $\partial F/\partial y'$
- `LFactor`: builds the *iteration* matrix $c\partial F/\partial y + d\partial F/\partial y'$
- `LSolve`: solves for x the linear system $Ax = b$ for a given b, where A is the *iteration* matrix $c\partial F/\partial y + d\partial F/\partial y'$

Using the functions provided by EMSO, a new DAE solver needs to **implement** the following routines:

- `create`: creates a new instance of the DAE external solver for a given problem structure;
- `step`: takes one step forward in the solution or makes an interpolation for a desired point;
- `destroy`: destroy the solver instance created with the `create` function;

7.2.1 Create and Destroy Functions

EMSO can run concurrent simulations, in order to do this a new solver instance is created for each new simulation started. The `create` function is responsible for creating a new instance of the solver and has the following form:

```
create(solverID, numOfEqs, resFn,
      indVar0, y0, yp0, variableIndexes,
      EMSOdata, rtol, atol, iopt, ropt,
      retVal, msg)
```

where the arguments are as described in Table 7.8.

Table 7.8: Arguments of the DAE solver `create` function.

Argument name	Type	Description
`solverID`	[out] integer	Unique identifier of the solver instance created (will be used to identify the instance in subsequent calls).
`numOfEqs`	[in] integer	The number of equations of the system.
`resFn`	[in] function	Function that calculates the residuals of the system.
`y0`	[in] real vector	Initial values of the variables y.
`y0`	[in] real vector	Initial values of the variable derivatives y'.
`variableIndexes`	[in] integer vector	The index of each variable (only for high index problems).
`EMSOdata`	[in] integer	EMSO problem specific data (only to pass back to `resFn`, `lsetup` and `lsolve`)
`rtol`	[in] real	The relative accuracy
`atol`	[in] real	The absolute accuracy (optionally a vector)
`iopt`	[in] integer vector	The vector of integer options, see **??**.
`ropt`	[in] real vector	The vector of real options, see **??**.
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

Warning: The solver should return an unique `SolverID` for each call to `create` because this integer will be used to identify the solver instance in subsequent calls to `step` or `destroy`.

When EMSO does not need the solver anymore it calls the `destroy` function on it:

```
destroy(solverID, retVal, msg)
```

where the arguments are as described in Table 7.9.

Table 7.9: Arguments of the DAE solver `destroy` function.

Argument name	Type	Description
`solverID`	[in] integer	Unique identifier of the solver instance (returned by `create`).
`retVal`	[out] integer	Return flag, see **??**.
`error`	[out] text	A text space where error messages should be copied.

Using the given `solverID` the `destroy` function should release any memory associated with that solver instance.

Note: When using C or C++ an easy way to implement an unique identifier for the solver is to create an structure or class for the solver and return its address as the identifier. Then the solver just needs to cast back the `SolverId` to get the address of the structure.

7.2.2 Step Function

After created as described in subsection 7.1.4, each time EMSO needs to solve the problem it will call the `solve` function.

The `solve` function has the following form:

```
solve(solverID, numOfEqs, resFn, lsetup, lsolve,
      y, ylb, yub, EMSOdata, rtol, atol,
      iopt, ropt, retVal, msg)
```

where the arguments are as described in Table 7.10.

EMSO can call multiple times the `solve` function before destoying it. Each time EMSO asks the solver to solve the problem a

Table 7.10: Arguments of the NLA solver `solve` function.

Argument name	Type	Description
`solverID`	[out] integer	Unique identifier of the solver instance (returned by `create`).
`numOfEqs`	[in] integer	The number of equations of the system.
`resFn`	[in] function	Function that calculates the residuals of the system.
`y`	[inout] real vector	Initial values of the variables and the solution at the end.
`ylb`	[in] real vector	Lower bound for the variables.
`yub`	[in] real vector	Upper bound for the variables.
`EMSOdata`	[in] integer	EMSO problem specific data (only to pass back to `resFn`, `lsetup` and `lsolve`)
`rtol`	[in] real	The relative accuracy
`atol`	[in] real	The absolute accuracy (optionally a vector)
`iopt`	[in] integer vector	The vector of integer options, see **??**.
`ropt`	[in] real vector	The vector of real options, see **??**.
`retVal`	[out] integer	Return flag, see **??**.
`msg`	[out] text	A text space where error messages should be copied.

initial guess `y` is given and the solution should be returned on the same vector.

Warning: The parameter `rtol` is always a real scalar but `atol` can be a vector depending on the options at `iopt`.

7.3 Writing new Solver Services

In this section we describe how to implement a new solver services for both NLA and DAE systems using the most common scientific programming languages.

As cited before EMSO is able to run concurrent simulations. Therefore, multiple instances of a external solver service can be active simultaneously. Unfortunately, dynamic memory allocation is not a trivial task in Fortran and is left as a challenge to the user. As an alternative the user should consider in using C or C++ or *wrap* his Fortran implementation using such languages.

7.3.1 Writing External Solver Services in Fortran

As mentioned in sections **??** and 7.2, in order to implement a new external solver service a set of functions *must* be implemented. In files NLASolverTemplate.f and DAESolverTemplate.f found at interfaces directory are given template implementations for an external NLA and DAE solvers services in Fortran.

The template files has the required function calling conventions, besides several comments which helps the user in the task of implementing a new service and creating the library.

7.3.2 Writing External Solver Services in C

As mentioned in section 7.2, in order to implement a new external solver service a set of functions *must* be implemented. In file ExterSolverTpl.c found at interfaces directory a template implementation for a external solver service in C is given. This file makes use of the interface definitions declared at ExternalSolver.h. Note that the header file should not be modified by the user.

The template file has the required function calling conventions, besides several comments which helps the user in the task of implementing a new service and creating the library.

7.3.3 Writing External Solver Services in C++

As mentioned in section 7.2, in order to implement a new external solver service a set of functions *must* be implemented. When using C++ this functions actually are *member* functions of a class. In file ExternalSolverTlp.cpp found at interfaces directory a template implementation for an external solver service in C++ is given. This file makes use of the interface definitions declared in file ExternlaSolver.h. Note that the header file should not be modified by the user. When included in a C++ file the ExternlaSolver.h, besides the C interfaces, declares two C++ pure abstract class called NLASolverBase and DAESolverBase.

The C++ template file has a skeleton implementation that should be filled by the user, besides several comments which helps the user in the task of implementing a new service and creating the library. Actually, when implement solver services in C++ the user can choose between implement the interfaces exactly as described in the C template files or to implement a class deriving from the given pure virtual classes as made in the C++ template file.

7.4 Documenting Solver Services

Under construction: To be documented.