mini_ker manual

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The TEF Collaboration

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Introduction

Mini_ker is a modeling tool, built especially in order to implement models written following the TEF (Transfer Evolution Formalism) formalism, a mathematical framework for system analysis and simulation. Mini_ker allows for timewise simulation, system analysis, adjoint computation, Kalman filtering and more.

Mini_ker uses a fortran preprocessor, `mortran`, designed in the 1970's, to ease model writing. For example partial derivatives can be symbolicaly determined by `mortran`. For the selection of compile-time features another set of preprocessor directives, the *cmz directives* are used. In most cases the user don't need to know anything about that preprocessing that occurs behind the scene, he simply writes down the equations of his model and he is done.

A comprehensive description of the TEF formalism in available on http://www.lmd.jussieu.fr/ZOOM/documents.dir/tef-GB-partA5.pdf). The Mini_ker software is a reduced version of **ZOOM**, that can only handle a hundreds of variables, but is much easier to use.

Intended audience

The reader should have notions in system dynamics. Moreover a minimal knowledge of programmation and fortran is required. What is required is a basic understandic of variable types, affectation and fortran expressions.

Reading guide

The first chapter is a brief overview of the TEF. The following describes how to write, compile and run a model in mini_ker. Reading the sections of this chapter up to the section *Symbolic model description* is required to know the syntax of model description in Mini_ker.

Reading up to the section *Controlling the run* is required to be able to use mini_ker. In this section it is assumed that mini_ker is properly setup. The installation instructions are in the appendix at Appendix A [Installation], page 41.

The next chapter describes advanced features, first a general introduction to features settings and then a description of other model description related features.

The next chapter describes system analysis tools available with mini_ker. The sections are independant and each describes how to use a specific feature. If you plan on using these features, you should also read Section 3.1 [Overview of feature setting], page 13.

In the appendix the instructions for the installation are described (see Appendix A [Installation], page 41). 2 programming environment to compile the model are available, with cmz and make, you can skip the method description you are not interested in. A reference for the usefull cmz directives is also in the appendix (see Appendix B [Cmz directives reference], page 44).

1 An overview of the TEF formalism

The TEF (Transfer Evolution Formalism) is based on partitionning and recoupling of model subsystems. It allows the study of the coupling between subsystems by the mean of a linearization and a time discretization.

1.1 Cell and transfer equations

In the TEF, a model is mathematically represented by a set of equations corresponding to two kinds objects:

1. cells which are elementary models and correspond to state equations such as:

$$\partial_t \eta(t) = g(\eta(t), \varphi(t))$$

   η represent the state variables of cells and the φ represent the dependent boundary conditions, *i.e.* the variables considered as boundary conditions by a cell, but depending upon the complete model state. This dependent boundary conditions are required to make the cells correspond to well-posed problems.

2. transfers which are determined by constraint equations such as:

$$\varphi(t) = f(\eta(t), \varphi(t))$$

1.2 Linearization and discretization in the TEF

The relations between sub-systems is excessively difficult to exhibit when having to cope with non-linear system. In the TEF, the TLS (Tangent Linear System) is constructed along the trajectory. One consider the system over a small portion along the trajectory, say between t and $t + \delta t$. The variation $\delta\eta$ of η and $\delta\varphi$ of φ is obtained through Taylor expansion.

A time scheme is then applied to the TLS (a Crank-Nicholson scheme), to obtain an algebraic system describing the relationships between variations of transfers and cells variables:

$$\begin{pmatrix} A & B \\ C^+ & D \end{pmatrix} \begin{pmatrix} \delta\eta \\ \delta\varphi \end{pmatrix} = \begin{pmatrix} \Gamma \\ -\Omega \end{pmatrix}$$

The blocks appearing in the matrix are constructed with partial derivative of f and g, and with δt. From this system the elimination of $\delta\eta$ leads to another formulation giving the coupling between transfers, and allows for the $\delta\varphi$ computation. The $\delta\varphi$ value is then substitued in $\delta\eta$.

2 Mini_ker model programming

mini_ker works by combining the model specification code given by the user and other source files provided in the package. The code is generated, preprocessed, compiled, linked and the resulting program can be run to produce the model trajectory and dynamic analysis.

The code provided in the package contains a principal program, some usefull subroutines and pieces of code called *sequences* combined with the different codes. Among those sequences some hold the code describing the model, these sequences are to be written by the user (sequences are similar with include files).

2.1 General structure of the code

The sequences used to enter model description hold the vector dimensions, mathematical formulae for each cell and transfer components, time step steering. During the code generation stage, cmz directives are preprocessed, then the user pseudo-Fortran instructions are translated by `mortran` using macros designed to generate in particular all Fortran instructions computing the Jacobian matrices used in TEF modelling.

A first users' sequence to program is: '`dimetaphi`' where the model dimensions are given, for the two vector-array `eta(.)` for cells and `ff(.)` for transfers (see Section 2.2.2 [Entering model size], page 4). The sequence '`zinit`' contains the mathematical formulation of the models (see Section 2.2.3 [Model equation and parameters], page 5). Another sequence '`zsteer`') is introduced at the end of the time step advance of the simulation, where the user can monitor the time step values, printing levels, perform numerical tests and so on (see Section 2.5.1 [Executing code at the end of each time step], page 11).

2.2 Mini_ker programming illustrated

The general TEF system writes:

$$\begin{aligned} \partial_t \eta(t) &= g(\eta(t), \varphi(t)) \\ \varphi(t) &= f(\eta(t), \varphi(t)) \end{aligned}$$

To illustrate the model description in mini_ker a simple predator-prey model of Lotka-Voltera is used. This model can be written in the following TEF form:

$$\begin{cases} \partial_t \eta_{prey} = a\eta_{prey} - a\varphi_{meet} \\ \partial_t \eta_{pred} = -c\eta_{pred} + c\varphi_{meet} \end{cases}$$
$$\varphi_{meet} = \eta_{prey}\eta_{pred}$$

with two cell equations, *i.e.* state evolution of the prey and predator groups, and one transfer accounting for the meeting of individuals of different group.

2.2.1 All you need to know about mortran and cmz directives

The first stage of code generation consists in cmz directives preprocessing. Cmz directives are used for conditional selection of features, and sequence inclusion. At that point you don't need to know anything about these directives. They are only usefull if you want to

take advantage of advanced features (see Section 3.8 [Programming with cmz directives], page 22).

The code in sequences is written in mortran and the second stage of code generation consists in mortran macro expansion. The mortran language is described in its own manual, here we only explain the very basics which is all you need to use mini_ker. mortran is almost fortran, the differences are the following:

- The code is free-form, and each statement should end with a semi-colon `;`.
- Comments may be introduced by an exclamation mark `!` at the beginning of a line, or appear within double quotes `"`.
- It is possible to use blocs, for `do` or `if` for example, and they are enclosed within '`<`' and '`>`'.

The following fictious code is legal mortran:

```
real
  param;
param = 3.; ff(1) = ff(3)**eta(1);       "a comment"
! a line comment
do inode=1,n_node <eta_move(inode)=0.01; eta_speed(inode)=0.0;>;
```

Thanks to mortran the model code is very simply specified, as you'll see next.

2.2.2 Entering model size

The dimension of the model is entered in the sequence '`dimetaphi`', using the fortran `parameter` `np` for `eta(.)` and `mp` for `ff(.)`. For this model, we have two cell components and only one transfer.

```
parameter (np=2,mp=1);
```

You should not change the layout of the parameter statement as the mortran preprocessor matches the line.

You also have to provide other parameters even if you don't have any use for them. If you don't it will trigger fortran errors. It includes the `maxstep` parameter that can have any value but 0, `lp` that should be 0, and `nxp`, `nyp` and `nzp` that should also be 0. The layout is the following:

```
parameter (lp=0);
parameter (nxp=0,nyp=0,nzp=0);
parameter (maxstep=100 000);
```

You can also add your own variable definitions in this sequence. For example if you want to declare the variable `anint` as `integer` the '`dimetaphi`' sequence could look like:

```
parameter (np=2,mp=1);

parameter (lp=0);
parameter (nxp=0,nyp=0,nzp=0);
parameter (maxstep=100 000);

integer anint;
```

2.2.3 Entering model equation and parameters

The model equation and parameters and some mini_ker parameters are entered in the '`zinit`' sequence. The whole listing is outputed to give an idea of the model length, then the example is detailed.

```
!%%%%%%%%%%%%%%%%%%%%%%
! Parameters
!%%%%%%%%%%%%%%%%%%%%%%

! required parameters
     dt=.01;             "initial time-step"
     nstep=10 000;       "number of iterations along the trajectory"
     time=0.;            "time initialisation "

! model parameters
     apar = 1.5;
     cpar = 0.7;

! miscalleneous parameters
     modzprint = 1000;    "printouts frequency"

print*,'************************************';
print*,'Lotka-Volterra model with parameters as:';
z_pr: apar,bpar;
print*,'************************************';

!%%%%%%%%%%%%%%%%%%%%%%
! Transfer definition
!%%%%%%%%%%%%%%%%%%%%%%
! meeting of prey and predator
    f_set Phi_tef(1) = eta(1)*eta(2);          "transfer definition"

!%%%%%%%%%%%%%%%%%%%%%%
! Cell definition
!%%%%%%%%%%%%%%%%%%%%%%

! eta(1) : pray
! eta(2) : predator

f_set  deta_tef(1) = apar*eta(1)-apar*ff(1);     "cell time advance"
f_set  deta_tef(2) = - cpar*eta(2) + cpar*ff(1); "definition       "

!%%%%%%%%%%%%%%%%%%%%%%
! Initial states
!%%%%%%%%%%%%%%%%%%%%%%

     eta(1) = 1.;
```

```
      eta(2) = 1.;
;
    OPEN(50,FILE='title.tex',STATUS='UNKNOWN');   "title file"
    write(50,5000) apar,cpar;
5000;format('Lotka-Volterra par:',2F4.1);
```

Variables and model parameters

The following variables are required:

`dt` The time step.

`time` Model time initialisation.

`nstep` Number of iterations along the trajectory.

There are no other required variables. It is possible to add more variables, though (and likewise it is possible to write any fortran or mortran code). For example a variable called `modzprint` is traditionnaly used for the frequency of the printout of the model matrix and vectors during the model run (see Section 2.5.2 [Controlling the printout and data output], page 12).

In the predator-prey example there are also two model parameters. The fortran variables are called here `apar` for a and `cpar` for c. The predator-prey code variable initializations finally reads

```
!%%%%%%%%%%%%%%%%%%%%%
! Parameters
!%%%%%%%%%%%%%%%%%%%%%

      dt=.01;
      nstep=10 000;
      time=0.;

! model parameters
      apar = 1.5;
      cpar = 0.7;

      modzprint = 1000;
```

Model equations

The model equations for cells and transfers are entered using a mortran macro, `f_set`, setting the `eta(.)` evolution with `deta_tef(.)` and the transfer definitions `ff(.)` with `Phi_tef(.)`.

`f_set` *Phi_tef*(`i`) = *f*(*eta*(.),*ff*(.)) [Macro]

This macro defines the transfer i static equation. `f` is a fortran expression which may be function of cell state variables, '`eta(1)`'...'`eta(np)`' and transfers '`ff(1)`'...'`ff(mp)`'.

In the case of the predator prey model, the transfer definition for φ_{meet} is:

```
f_set Phi_tef(1) = eta(1)*eta(2);
```

`f_set` *deta_tef*(`i`) = *g*(*eta*(`i`),*ff*(.)) [Macro]

This macro defines the cell *i* time evolution model. `g` is a expression which may be function of cell state variables, '`eta(1)`'...'`eta(np)`' and transfers '`ff(1)`'...'`ff(mp)`'.

The two cell equations of the predator-prey model are, with index 1 for the prey (η_{prey}) and index 2 for the predator (η_{pred}):

```
f_set  deta_tef(1) = apar*eta(1)-apar*ff(1);
f_set  deta_tef(2) = - cpar*eta(2) + cpar*ff(1);
```

The whole model is:

```
!%%%%%%%%%%%%%%%%%%%%
! Transfer definition
!%%%%%%%%%%%%%%%%%%%%
! rencontres (meeting)
    f_set Phi_tef(1) = eta(1)*eta(2);

!%%%%%%%%%%%%%%%%%%%%
! Cell definition
!%%%%%%%%%%%%%%%%%%%%

! eta(1) : prey
! eta(2) : predator

    f_set  deta_tef(1) = apar*eta(1)-apar*ff(1);
    f_set  deta_tef(2) = - cpar*eta(2) + cpar*ff(1);
```

Starting points

The cells require starting points. The transfers may also have starting points although they are recomputed from the cell values.

In the predator-prey model the starting points for cells are:

```
!     initial state
!     -------------
     eta(1) = 1.;
     eta(2) = 1.;
```

When there is a non trivial implicit relationship between the transfers in the model it may be usefull or even necessary to set some transfers to non-zero values. This difficulty is only relevant for the first step. The uninitialized transfers have a zero value, so an initialization to another value may help avoiding singular functions or matrix and ensure convergence.

title file

For some graphics generation a file with name '`title.tex`' is required which sets the title. The following instructions take care of that:

```
OPEN(50,FILE='title.tex',STATUS='UNKNOWN');
write(50,5000) apar,cpar;
```

```
5000;format('Lotka-Volterra par:',2F4.1);

    close(50);
```

In that case the parameter values are written down, to differenciate between different runs.

2.3 Symbolic model description

A language for the symbolic description of a model is also available, which eventually will generate the same Fortran code as the basic language. In that case the coordinate of the states `eta(.)` and the transfers `ff(.)` are not index with numbers but are given a name. The model equations are entered in two mortran blocks, one for the transfers, the other for the cells.

`set_Phi` introduces the transfer block, `set_eta` introduces the cells block. In each block the couple variable, function are specified. For transfers the function defines the transfer itself while for cells the function describes the cell evolution. The variable is specified with `var:`, the function is defined with `fun:`.

The same above example can be equivalently entered as:

```
!%%%%%%%%%%%%%%%%%%%%%%
! Transfer definition
!%%%%%%%%%%%%%%%%%%%%%%
! rencontre (meeting)
set_Phi
< var: ff_interact, fun: f_interact = eta_prey*eta_pred;
>;

!%%%%%%%%%%%%%%%%%%%%%%
! Cell definition
!%%%%%%%%%%%%%%%%%%%%%%

set_eta
< var: eta_prey, fun: deta_prey =   apar*eta_prey - apar*ff_interact;
  var: eta_pred, fun: deta_pred = - cpar*eta_pred + cpar*ff_interact;
>;
```

Whenever the user is not concerned by giving a specific name to a component function, it is possible to specify the equation only with `eqn:`. Therefore the user may replace an instruction as:

```
  var: ff_dump,
  fun: f_dump  = - rd*(eta_speed - eta_speed_limiting);
```

by:

```
  eqn: ff_dump = - rd*(eta_speed - eta_speed_limiting);
```

In that case, the unnamed function will take the name of the defined variable preceded by the '$' sign: `$ff_dump`.

It is also possible to use the basic instructions `f_set` in the same program, but one has to be careful and do not overwrite the same vector components as the one entered using the `set_` instructions.

The correspondence with basic components are printed out at execution time as explained in Section 2.4.3 [Running a simulation and using the output], page 10.

2.4 Setting and running a model

In this section it is assumed that a programming environment has been properly setup. This environment may use either cmz or make to drive the preprocessing and compilation. You can skip the part related with the environment you don't use.

For instructions regarding the installation, see Appendix A [Installation], page 41.

2.4.1 Setup a model and compile with cmz

The user defined sequences are '`KEEP`' in the cmz world. The most common organization is to have a cmz file in a subdirectory of the directory containing the mini_ker cmz file. In this cmz file there should be a '`PATCH`' called '`zinproc`' with the KEEPs within the patch. The KEEPs must be called '`$zinit`' and '`$dimetaphi`'.

From within cmz in the directory of your model the source extraction, compilation and linking should be triggered by `mod`. This macro uses the '`selseq.kumac`' information to find the mini_ker cmz file. `mod` should create a directory with the same name than the cmz file, '`mymodel/`' in our example. In this directory there is another directory '`cfs/`' containing the sources extracted from the cmz file.

The file '`mymodel_o.tmp`' contains all the mortran code generated by cmz with the sequences substituted, including the '`$zinit`' and '`$dimetaphi`' sequences. The fortran produced by the preprocessing and splitting of this file is in files with the traditional '`.f`' suffix. The principal program is in '`principal.f`'.

`mod` also triggers compilation and linking. The object files are in the same '`cfs/`' directory and the executable is in the '`mymodel/`' directory, with name '`mymodel.exe`'.

2.4.2 Setup a model and compile with make

With make, the sequences are files ending with '`.mti`' (for mortran include files), called '`zinit.mti`' and '`dimetaphi.mti`'. They are included by `mortran` in other source files. You also need a '`Makefile`' to drive the compilation of the model.

If you don't need additional code or libraries to be linked with your model you have two alternatives.

1. The simplest alternative is to run the `start_miniker` script with argument the model file name. It should copy a '`zinit.mti`' and '`dimetaphi.mti`' files ready to be edited and a Makefile ready to compile the model. For the predator prey model, for example, you could run

   ```
   $ start_miniker predator
   ```

2. Otherwise you can copy the Makefile from '`template/Makefile`' in the directory containing the sequences. You should then change the compiled model file name, by changing the value of the `model_file_name` variable to the model file name of your choice in the Makefile. It is set to '`mymodel`' in template. For the predator-prey model it could be set like

   ```
   model_file_name = predator
   ```

   If you want to put the executable model file in another directory, you could set

```
model_file_name = some_dir/predator
```

The other items set in the default Makefile should be right.

The preprocessing and the compilation are launched with

```
make all
```

The mortran files are generated by the cmz directive preprocessor from files found in the package source directories. The mortran files end with '`.mtn`' for the main files and '`.mti`' for include files. They are output in the current directory. The mortran preprocessor then preprocess these mortran files and includes the sequences. The resulting fortran is also in the current directory, in files with a '`.f`' suffix. Some fortran files ending with '`.F`' may also be created by the cmz directive preprocessor. The object files resulting from the compilation of all the fortran files (generated from mortran or directly from fortran files) are there too.

In case you want to override the default sequences or a subroutine file you just have to create it in your working directory along with the '`zinit.mti`' and '`dimetaphi.mti`'. For example you could want to create a '`zsteer.mti`' file (see Section 2.5.1 [Executing code at the end of each time step], page 11), a '`zcmd_law.mti`' file (see Section 4.2.2 [Control laws], page 28), a '`monitor.f`' file (see Section 3.2.1 [Turning the model into a subroutine], page 13) to take advantage of features presented later in this manual.

More in-depth discussion of make and mini_ker is covered in Section 3.7 [Advanced use of mini_ker with make], page 20. For example it is also possible to create files that are to be preprocessed by the cmz directive preprocessor, this advanced use is more precisely covered in Section 3.8 [Programming with cmz directives], page 22.

2.4.3 Running a simulation and using the output

Once compiled the model is ready to run, it only has to be executed. On standard output informations about the states, transfers, tangent linear system and other jacobian matrices are printed. For example the predator-prey model could be executed with:

```
./predator > result.lis
```

In case of a model entered symbolically (see Section 2.3 [Symbolic model description], page 8) the correspondance between the symbolic variables and the basic vectors and functions are printed at run time:

```
---------------- Informing on Phi definition -----------------
  Var-name,           Function-name,       index in ff vector
          ff_interact              f_interact  1
--------------------------------------------------

--------------- Informing on Eta definition ------------------
 Var-name,           Function-name,       index in eta vector
             eta_prey               deta_prey  1
             eta_pred               deta_pred  2
```

Outputs are in also in '`.data`' files. Each data file has the `time` variable values as first column[1]. Following columns give the values of `eta(.)` in '`res.data`', `dEta(.)` in '`dres.data`' – the step by step variation of `eta(.)` – and `ff(.)` in '`tr.data`'.

Along the simulation the TEF jacobian matrices are computed. A transfer variables elimination process also leads to the definition of the classical state advance matrix of the system (the corresponding array is `aspha(.,.)` in the code). This matrix is output in the file '`aspha.data`' that is used to post-run dynamics analyses. The matrix columns are written on each line, column by column. See Section 4.5 [Stability analysis of fastest modes], page 34. See Section 4.6 [Generalized tangent linear system analysis], page 35. It is not used in the solving process.

Other '`.data`' files will be described later.

2.4.4 Doing graphics

The format of the '`.data`' files are coherent with GNU graphics, that is the data are simply separated with spaces. The files can be vizualised with `gnuplot`, for example. To plot `eta(`*n*`)`, the `gnuplot` statement is:

```
plot "res.data" using 1:(n+1)
```

The similar one for `ff(`*n*`)`:

```
plot "tr.data" using 1:(n+1)
```

For people using `PAW`, the CERN graphical computer code, mini_ker prepares kumacs that allow to read process the '`.data`' files in the form of *n-tuples* (see the *PAW manual* for more information). These n-tuples are ready to use only for vector dimension of at most 10 (including the variable `time`). These kumacs are overwritten each time the model is run.

2.5 Controlling the run

It is possible to add code that will be executed at the end of each time step. It is also possible to specify which time step leads to a printout on standard output. For maximal control, the code running te model may be turned into a subroutine to be called from another fortran program, this possibility is covered in Section 3.2 [Calling the model code], page 13.

2.5.1 Executing code at the end of each time step

The code in the sequence '`zsteer`' is executed at the end of each time step. It is possible to change the time step length (variable `dt`) verify that the non linearity are not too big, or perform discontinuous modifications of the states.

Many variables are available, including

`istep` The step number.

`couplage(.)`
The coupling matrix between transfers.

[1] '`dres.data`' has another time related variable as second column: `dt`, the time step that can vary in the course of a simulation.

2.5.2 Controlling the printout and data output

The printout on standard output is performed if the variable `zprint` of type `logical` is true. Therefore it is possible to control this printout by setting `zprint` false or true. For example the following code, in sequence '`zsteer`', triggers printing for every `modzprint` time step and the two following time steps:

```
ZPRINT = mod(istep+1,modzprint).eq.0;
Zprint = zprint .or. mod(istep+1,modzprint).eq.1;
Zprint = zprint .or. mod(istep+1,modzprint).eq.2;
```

The data output to '`.data`' files described in Section 2.4.3 [Running a simulation and using the output], page 10 is performed if the `logical` variable `zout` is true. For example the following code, in '`zsteer`', triggers output to '`.data`' files every `modzout` step.

```
Zout = mod(istep,modzout).eq.0;
```

3 Advanced mini_ker programming

3.1 Overview of additional features setting

It is possible to enable some features by selecting which code should be part of the principal program. Each of these optionnal features are associated with a *select flag*. For example double precision is used instead of simple precision with the '`double`' select flag, the model is a subroutine with the select flag '`monitor`', the Kalman filter code is set with '`kalman`' and the 1D gridded model capabilities are associated with '`grid1d`'. To select a given feature the cmz statement `sel` *`select_flag`* should be written down in the '`selseq.kumac`' found in the model directory. With make either the corresponding variable should be set to 1 or it should be added to the `SEL` make variable, depending on the feature.

Other features don't need different or additional code to be used. Most of the features are enabled by setting specific logical variables to '`.true.`'. This is the case for `zsensib` for sensitivities, `zback` for the adjoint model, `zcommand` if the command is in a file and `zlaw` if it is a function and `zkalman` for the Kalman filter. These select and logical flags are described in the corresponding sections.

In cmz an alternative of writing select flags to '`selseq.kumac`' is to drive the compilation with `smod` *`sel_flag`*. In that case the *sel_flag* is selected and the files and executable goes to a directory named '`sel_flag`'.

The select flags are taken into account during cmz directives preprocessing. Therefore you have the possibility to use these flags to conditionnaly include code. In most cases you don't need to include code conditionally yourself though, but if you want to, this is covered in Section 3.8 [Programming with cmz directives], page 22.

3.2 Calling the model code

When the model code is a subroutine, it can be called from another fortran program unit (or another program), and the model will be run each time the subroutine is called. This technique could be used, for example to perform optimization (see Section 4.2 [Adjoint model and optimisation with mini_ker], page 27), or to run the model with different parameters.

3.2.1 Turning the model into a subroutine

With cmz, one has to do a

```
sel monitor
```

in the '`selseq.kumac`' file and create the KEEP that call the model code. See Section 3.1 [Selecting features], page 13.

With make '`monitor`' should be added to the `SEL` variable in the '`Makefile`', for example:

```
SEL = monitor
```

A file that call the principal subroutine should also be written, using the prefered language of the user. The additional object files should then be linked with the mini_ker objects. To that aim they may be added to the `miniker_user_objects` variable.

3.2.2 Calling the model subroutine

The model subroutine is called '`principal`' and is called with the following arguments:

`principal` (*Cost, ncall, integer_flag, file_suffix, info, idxerror*) [Subroutine]

Where *Cost* is a real number, `real` or `double precision`, and is set by the `principal` subroutine. It holds the value of the cost function if such function has been defined (the use and setting of a cost function is covered later, see Section 4.2.3 [Cost function coding], page 28). *ncall* is an integer which corresponds with the number of call to `principal` done so far, it should be initialized to 0 and its value should not be changed, as it is changed in the `principal` subroutine. *integer_flag* is an integer that can be set by the user to be accessed in the `principal` subroutine. For example its value could be used to set some flags in the '`zinit`' sequence. *file_suffix* is a character string, that is suffixed to the output files names instead of '`.data`'. If the first character is the null character '`char(0)`', the default suffix, '`.data`' is appended. *info* and *idxerror* are integer used for error reporting. *idxerror* value is 0 if there was no error. It is negative for an alert, positive for a very serious error. The precise value determines where the error occured. *info* is an integer holding more precise information about the error. It is usually the information value from lapack. The precise meaning of these error codes is in table 3.1.

Source of error or warning	`info`	`idxerror`
state matrix inversion in ker	inversion	1
time advance system resolution in ker	system	1
state matrix advance in phase space, $(I - D)$ inversion	inversion	3
transfer propagator, $(I - D)$ inversion	inversion	3
kalman analysis state matrix advance in phase space, $(I - D)$ inversion	inversion	21
kalman analysis variance covariance matrix non positive	Choleski	22
kalman analysis error matrix inversion	inversion	23
kalman error matrix advance	system	24
transfers determination linearity problem for transfers		-1
transerts determination Newton D_loop does not converge		-2

table 3.1: Meaning of error codes returned by principal.

In general more information than the provided arguments has to be passed to the `principal` subroutine, in that case a `common` block, to be written in the '`dimetaphi`' sequence can be used.

3.3 Describing 1D gridded model

Specific macros have been built that allow to generically describe 1D gridded models. Because of the necessity of defining left and right limiting conditions, the models are partitionned in three groups for cell and transfer components. In the following example, a chain of masselottes linked by springs and dumps is bounded to a wall on the left, and open at right. The TEF formulation of the problem is written in the phase space (position, velocity)

for node k, with bounding conditions:

$$\begin{cases} \partial_t \eta_k^{pos} = \eta_k^{vel} \\ \partial_t \eta_k^{vel} = \left(\varphi_k^{spr} - \varphi_{k+1}^{spr} + \varphi_k^{dmp} - \varphi_{k+1}^{dmp}\right)/m_k \end{cases}$$

$$\begin{cases} \varphi_k^{spr} = -k_k(\eta_k^{pos} - \eta_{k-1}^{pos}) \\ \varphi_k^{spr} = -d_k(\eta_k^{vel} - \eta_{k-1}^{vel}) \end{cases}$$

$$\begin{cases} \eta_0^{pos} = 0 \\ \eta_0^{vel} = 0 \\ \varphi_{N+1}^{spr} = 0 \\ \varphi_{N+1}^{dmp} = 0 \end{cases}$$

where m_k is the mass of node k, r_k and d_k the rigidity of springs and dumping coefficients. There are N nodes in the grid, from 1 to N, and two nodes outside of the grid, a limiting node 0, and a limiting node $N+1$. The limiting node corresponding with node 0 is called the *down* node, while the limiting node corresponding with node $N+1$ is called the *up* node.

To enable 1D gridded models, one should set the select flag '`grid1d`' in '`selseq.kumac`', like

```
sel grid1d
```

3.3.1 Setting dimensions for 1D gridded model

In that case the number of nodes, the number of states and tranferts per node, and the number of limiting transfers and states are required. These dimensions has to be entered in the '`DimEtaPhi`' sequence. The parameters for cells are

`n_node` Number of cell nodes in the 1D grid.

`n_dwn` Number of limiting cells with index -1, *i.e.* number of cells in the limiting down node.

`n_up` Number of limiting cells with index +1, *i.e.* number of cells in the limiting up node.

`n_mult` Number of cells in each node (multiplicity).

The parameters for transfers, are similarly `m_node`, `m_dwn`, `m_up`, `m_mult`. The layout of their declaration should be respected as the precompiler matches the line.

In our example, there are 3 grids of cell and transfer variables (`n_node=m_node=3`). There are 2 cells and 2 transfers in each node (`n_mult=2` and `m_mult=2`). There is no limiting condition for the states in the down node therefore `n_up=0`. There is no transfers for the first limiting node, and therefore `m_dwn=0`. There are 2 states in the limiting node 0, the down node, `n_dwn=2`, and 2 transfers in the limiting last node the node up, and `m_up=2`.

```
! ++++++++++++++++++++++++++++++++++++++++++++++++++++++++
! nodes parameters, and Limiting Conditions (Low and High)
! ++++++++++++++++++++++++++++++++++++++++++++++++++++++++
      parameter (n_node=3,n_dwn=2,n_up=0,n_mult=2);
```

```
         parameter (m_node=3,m_dwn=0,m_up=2,m_mult=2);
! --------------------------------------------------------
```

The dimension of the parameter arrays should also be declared in the '`dimetaphi`' sequence. Here we have 3 parameters, for m_k, r_k and d_k:

```
dimension rk(n_node),rd(n_node),rmassm1(n_node);
```

3.3.2 1D gridded Model coding

The model code and parameters go in the '`zinit`' sequence.

Parameters

A value for the mini_ker parameters and the model parameters should be given in '`zinit`', in our example we have

```
!%%%%%%%%%%%%%%%%%%%%%%
! Parameters
!%%%%%%%%%%%%%%%%%%%%%%
data rk/n_node*1./;
data rd/n_node*0.1/;
data rmassm1/n_node*1./;
     dt=.01;
     nstep=5 000;
     modzprint = 1000;
     time=0.;
```

Limiting conditions

The limiting states and transfer variables and the corresponding equations are declared using the symbolic model description (see Section 2.3 [Symbolic model description], page 8). There are 4 blocks, for node and up and down and for states and transfers:

`set_dwn_eta`
: down node cells

`set_up_eta`
: up node cells

`set_dwn_phi`
: down node transfers

`set_up_phi`
: up node transfers

The following scheme illustrates the example:

```
!%%%%%%%%%%%%%%%%%%%%%%%%%%================================================
! Maillage convention inode
!%%%%%%%%%%%%%%%%%%%%%%%%%%                                 Open ended
!(2 Down    Phi    Eta                         (n_node)
! Eta)  \|       .-----.       .-----.          .-----.        /
! wall  \|-\/\/\-|     |-\/\/\-|     |  . . .  -|     |-\/\/\- |dummy
!  pos  \|--***--|  1  |--***--|  2  |  . . .  -|  n  |--***-- |Phis
! speed \|   1   |_____|   2   |_____|      n   |_____|  n+1   \(2 Up Phi)
!
```

Two states are associated with the down node, they correspond with the position and speed of the wall. As the wall don't move these states are initialized to be 0, and the cells are stationnary cells, therefore these values remain 0.

```
! Down cells (wall)
! -----------------
eta_pos_wall = 0; eta_speed_wall = 0.;

set_dwn_eta
< var: eta_pos_wall,  fun: deta_pos_wall  = 0.;
  var: eta_speed_wall, fun: deta_speed_wall= 0.;
>;
```

There are 2 limiting transfers in the up node. They correspond with an open end and are therefore set to 0.

```
! limiting Transfers : dummy ones
! -------------------------------
set_Up_Phi
< var:ff_dummy_1, fun: f_dummy_1=0.;
  var:ff_dummy_2, fun: f_dummy_2=0.;
>;
```

Starting points

The cell node state values are initialized. They are in an array indexed by the `inode` variable. In the example the variable corresponding with position is `eta_move` and the variable corresponding with speed is `eta_speed`. Their initial values are set with the following mortran code

```
!---------------
! Initialisation
!---------------
;
do inode=1,n_node <eta_move(inode)=0.01; eta_speed(inode)=0.0;>;
```

The transfers may be similarly initialized, still with `inode` as the node index.

Grid node equations

Each node is associated with an index `inode`. It allows to refer to the preceding node, with `inode-1` and the following node `inode+1`. The node states are declared in `set_node_Eta` block and the transfers are in `set_node_Phi` blocks.

In the example, the cells are declared with

```
! node cells
! ----------
;
set_node_Eta
< var: eta_move(inode),  fun: deta_move(inode) = eta_speed(inode);
  var: eta_speed(inode),
  fun: deta_speed(inode) = rmassm1(inode)
                           *( - ff_spring(inode+1) + ff_spring(inode)
```

```
                                    - ff_dump(inode+1)  + ff_dump(inode)
                                   );
  >;
```

The transfers are (`ff_spring` corresponds with springs and `ff_dump` with dumps):

```
  !%%%%%%%%%%%%%%%%%%%%%%
  ! Transfer definition
  !%%%%%%%%%%%%%%%%%%%%%%
  ! node transfers
  ! --------------
  ! convention de signe spring : comprime:= +
  set_node_Phi
  < var: ff_spring(.),
    fun:
     f_spring(inode)= -rk(inode)*(eta_move(inode) - eta_move(inode-1));
    var: ff_dump(.),
    fun:
     f_dump(inode)  = -rd(inode)*(eta_speed(inode) - eta_speed(inode-1));
  >;
```

The limiting states and transfers are associated with the states or transfers with index `inode+1` or `inode-1` appearing in node cell and transfer equations (`inode-1` for down limiting conditions and `inode+1` for up limiting conditions) in their order of appearance. In our example, in the `eta_speed` state node equation `ff_spring(inode+1)` appears before `ff_dump(inode+1)` and is therefore associated with `ff_dummy_1` while `ff_dump(inode+1)` is associated with the `ff_dummy_2` limiting transfer, as `ff_dummy_1` appears before `ff_dummy_2` in the limiting up transfers definitions.

All variable names and functions are free but has to be different. Any particular node-attached variable k is referred to as: '`(inode:k)`', where k has to be a Fortran expression allowed in arguments. The symbol '`inode`' is reserved. As usual other Fortran instructions can be written within the Mortran block '`< >`' of each `set_` block.

3.4 Double precision

The default for real variables is the `real` Fortran type. It is possible to use double precision instead. In that case all the occurences of '`real` ' in mortran code is substituted with '`double precision` ' and the Lapack subroutine names are replaced by the double precision names.

This feature is turned on by `sel double` in '`selseq.kumac`' with cmz and `double = 1` in the '`Makefile`' with make.

In order for the model to run in double or simple precision some care should be taken to use the generic intrinsic functions, like `sin` and not `dsin`. No numerical constant should be passed directly to subroutines or functions, but instead a variable with the right type should be used to hold the constant value, taking advantage of the implicit casts to the variable type.

3.5 Parameters

It is possible to specify some Fortran variables as model parameters. Model parameters may be used in sensitivities (see Section 4.1.4 [Sensitivity to a parameter], page 26) and in the adjoint model (see Section 4.2.4 [Sensitivity of cost function to parameters], page 29). Nothing special is done with parameters with kalman filtering.

To specify parameters, first the number of such parameters has to be declared in '`dimetaphi`' with the parameter `lp`. Then, if there are two parameters, they are first declared with

```
parameter (lp=1);
```

The parameters are fortran variables that should be initialized somewhere in `zinit`. For a variable to be considered as a parameter, it should be passed as an argument to the `Free_parameters` macro. For example if `apar` and `cpar` (from the predator example) are to be considered as parameters, `Free_parameters` should be called with:

```
Free_parameter: apar, cpar;
```

Forward sensitivities are explained later (see Section 4.1.4 [Sensitivity to a parameter], page 26), the syntax only is described here. When a parameter is used for forward sensitivities, it should be marked by enclosing its name between '`[fwd:`' and '`]`' in the `Free_parameter` list. For example if `apar` is used for forward sensitivities, the `Free_parameter` call becomes

```
Free_parameter: [fwd: apar], cpar;
```

When used with grid1d models (see Section 3.3 [Describing 1D gridded model], page 14) the `inode` number may appear in parenthesis:

```
Free_parameter: rd(1), rk(2);
```

3.6 Observations and data

Some support for observations and interactions with data is available. The observations are functions of the model variables. They don't have any action on the model result, but they may (in theory) be observed and measured. The natural use of these observations is to be compared with data that correspond with the values from real measurements. They are used in the Kalman filter (see Section 4.3 [Kalman filter], page 29).

The observation vector is noted ω, the observation function is noted h:

$$\omega = h(\eta, \varphi)$$

3.6.1 Observations

The size of the observation vector is set in the '`dimetaphi`' sequence by the `nobsp` parameter. For example if there is one observation:

```
parameter (nobsp=1);
```

The observation functions are set by a `f_set` macro in the '`zinit`' sequence with `Obs_tef(.)`.

`f_set` *Obs_tef*(`i`) = *f*(*eta*(.),*ff*(.)) [Macro]

This macro defines the observation equation. `f` is a fortran expression which may be function of cell state variables, '`eta(1)`'...'`eta(np)`' and transfers '`ff(1)`'...'`ff(mp)`'.

For example, in the predator-prey model if we only have access to the total population of prey and predators, we would have:

```
f_set Obs_tef(1) = eta(1) + eta(2);
```

The corresponding code is used with `sel obs` in '`selseq.kumac`' with cmz and `obs = 1` in '`Makefile`' with make. And the feature is turned on and off at run time with the logical flag `zobs`.

The observation vector is called `etaobs(.)`, it is output in the file '`obs.data`'.

At each time step the derivative of the observation function with respect with transfers and cells variables are recomputed. The elimination of transfers is also performed to get the partial derivative of the observation function of the equivalent model, with states only, with respect to the states. The matrix are:

`obetad(.,.)`
: derivative of observation function with respect with transfers.

`obphid(.,.)`
: derivative of observation function with respect with cell variables.

`obspha(.,.)`
: derivative of observation function in state space with respect with cell variables.

3.6.2 Data

The convention for data is that whenever some data are available, the logical variable `zgetobs` should be set to '`.true.`'. And the `vobs(.)` vector should be filled with the data values. This vector has the same dimension than the observation vector and each coordinate are meant to correspond with the corresponding coordinate of the observation vector.

This feature is turned on by setting the logical variable `zdata` to '`.true.`', and the `zgetobs` flag is typically set in the '`zsteer`' sequence (see Section 2.5.1 [Executing code at the end of each time step], page 11). At each time data are available (`zgetobs` is true) the observations are written to the file '`data.data`'. With the Kalman filter more informations are outputted to the '`data.data`' file, see Section 4.3.2.2 [Kalman filter results], page 32.

3.7 Advanced use of mini_ker with make

3.7.1 Make variables

The '`Makefile.miniker`' Makefile provided in the distribution should be included as it defines a lot of important variables and rules.

The following make variables can be set by the user:

`miniker_dir`
: that variable should hold the mini_ker sources directory. If you installed mini_ker that variable should be set to '`$(includedir)/mini_ker`'. If you use

the sources right from the sources directory it should be set to the sources package directory.

`MTNDIRS` This variable can hold a '`:`' delimited list of directories that will be searched for mortran include files.

`CMFDIRS` This variable can hold a '`:`' delimited list of directories that will be searched for cmz directive include files.

`SEL` This variable holds a '`,`' delimited list of select flags, for example `monitor`, `grid1d`, `debug`.

`LDADD` This variable can be used to add libraries flags and files. It is used in the default linking command/rule.

`miniker_user_objects`
This variable should hold a space separated list of additional object files to be linked with the model and helper object files.

`CAR2TXTFLAGS`
cmz directives preprocessor flag.

`kalman` This variable should be set to 1 if you want to use the kalman filter (see Section 4.3 [Kalman filter], page 29).

`double` This variable should be set to 1 if you want to have a double precision code (see Section 3.4 [Double precision], page 18).

`obs` This variable should be set to 1 if you want to have a handling of observations as described in Section 3.6.1 [Observations], page 19.

The following variables are allready set and may be used (some are set by ./configure see Section A.4.2 [Configuration], page 42):

`miniker_principal_objects`
The list of object files needed for the model build, together with some helper object files often used but not strictly required for the linking.

`DEPDIR` The name of a hidden directory containing the dependencies computed for the main mortran files.

`F77`
`FC`
`FFLAGS`

`LDFLAGS` Compiler and linker related variables set by ./configure.

`LIBS` This variable should hold the link flags and files required to build mini_ker, set by ./configure.

`CAR2TXT`
`MORTRAN`
`MTNFLAGS`
`MTNDEPEND`
Preprocessor and preprocessor flags, set by ./configure.

3.7.2 Rules

The following rules are defined in the '`Makefile.miniker`' file.

`miniker-clean`
: remove the fortran files generated from the mortran files. Remove the object files.

`miniker-mtn-clean`
: remove the mortran files generated from the files with cmz directives.

  Various rules to preprocess files with cmz directives and mortran files and to compile fortran files.

If the user needs a mortran main file, he may take advantage of the rule used to compute the dependencies of a mortran file. If the file is called, say, '`mtnfile.mtn`' leading to '`mtnfile.f`', the following include should lead to the updating and inclusion of a file describing the dependencies of '`mtnfile.mtn`' in the '`Makefile`':

```
include $(DEPDIR)/mtnfile.Pf
```

3.7.3 Linking rule

The rule used for the linking of the model file is not in the '`Makefile.miniker`' file but should be provided in the user '`Makefile`' for more flexibility. The default rule uses the variables `miniker_user_objects` for additional object files and `LDADD` for additionnal linking flags and files, those variables are there to be changed by the user.

The object files required by the mini_ker code are in the make variable `miniker_principal_objects`, this variable is also used. The value of the variables `FC` for the Fortran compiler, `FFLAGS` for the Fortran compiler flags and `LDFLAGS` for the linker flags should be set to right values; `LIBS` should also be right and hold the link flags and link files required to compile the mini_ker model. These variables are set by by `./configure` during configuration (see Section A.4.2 [Configuration], page 42) and used in the default rule:

```
$(model_file): $(miniker_user_objects) $(miniker_principal_objects)
        $(FC) $(FFLAGS) $(LDFLAGS) $^ $(LDADD) $(LIBS) -o $@
```

In case this isn't right it may be freely changed. You should certainly refer to the section "Top" in *GNU Make Manual* manual to understand what that rule exactly means and make your own.

3.8 Programming with cmz directives

In cmz the KEEP and DECK have their cmz directives preprocessed as part of the source files extraction. And some directives are automatically set when creating the KEEP or DECK. With make files with these directives has to be created within the files that are to be preprocessed by the cmz directives preprocessor.

3.8.1 Files with cmz directives with make

A file that contains cmz directives should have a file suffix corresponding with the language of the resulting file and with the normal file suffix of that language. More precisely '`cm`' should be added before the normal file suffix and after the '`.`'. Therefore if the resulting file language is associated with a suffix '*`.suf`*', the file with cmz directives should have a

'`.cmsuf`' suffix. The tradition is to have a different suffix for main files and include files. A file containing cmz directives will be called a *cmfile* in the following.

Rules for preprocessing of the files are defined in the file '`Makefile.miniker`' for the file types described in table 3.2:

language	**file type**	**cmfile suffix**	**suffix**	**language**
fortran	main/deck	.cmf	.f	ftn
fortran preprocessed	main/deck	.cmF	.F	f77
fortran preprocessed	include/keep	.cminc	.inc	f77
mortran	main/deck	.cmmtn	.mtn	mtn
mortran	include/keep	.cmmti	.mti	mtn

table 3.2: Association between file language, file type, file suffixes and language identifier in cmz directives. A main file is called a *deck* in cmz and an include file is called a *keep*.

To add directories searched for cmfiles they should be added to the `CMFDIRS` makefile variable, separate by '`:`'.

3.8.2 Cmz directives used with mini_ker

The main feature of cmz directive is to use code conditionnaly for a given select flag. For example when the double precision is selected (see Section 3.4 [Double precision], page 18) the use of the conditionnal `double` flag may be required in case there is a different subroutine name for different types. If, for example, the user use the subroutine `smysub` for simple precision and `dmysub` for double precision the following code is an example of what could appear in the user code:

```
+IF,double
 call dmysub(eta);
+ELSE
 call smysub(eta);
+ENDIF
```

For a complete reference on cmz directives see the appendix Appendix B [Cmz directives reference], page 44.

4 Dynamic analysis of systems in mini_ker

4.1 Automatic sensitivity computation

Another direct usage of the system Jacobian matrices concerns automatic sensitivity determination, as either:

- the sensitivity of all variables to perturbation in the initial condition of one state variable;
- the same sensitivities to an initial pulse on a transfer;
- the same sensitivities for a change in a parameter;
- the sensitivity of the matrix of advance in state space to a change in a parameter.

One has to raise the flag `ZSensib` in Zinit, to enable sensitivities computation:

```
ZSensib = .true.;
```

It is noteworthy that these sensitivity analyses are not based on differences between two runs with different initial states or parameter values, but on the formal derivatives of the model, which is much more robust and rigorous[1].

4.1.1 Initial state sensitivity

Each state is associated with the element of the `sens(.)` array with the same index. For example, `eta(1)` is associated with `sens(1)`. If an element of the `sens(.)` array is set to '`1.`' the sensitivity is computed, and if it is set to '`0.`' it isn't. For example in the following code the sensitivity to `eta(3)` is computed, but not to `eta(1)` and `eta(2)`:

```
sens(1) = 0.;
sens(2) = 0.;
sens(3) = 1.;
```

If the sensitivity to a state is computed, then mini_ker propagates the derivative of all variables (cells and transfers), at every time step, with respect to the initial value of that state. This allows to carry out a sensitivity analysis to the initial state.

These sensitivity goes to the result files '`sens.data`' for cells and '`sigma.data`' for transfers. In those file the first column corresponds with time, and the other columns are derivative of the cell states (in '`sens.data`') and transfers (in '`sigma.data`') with respect with the initial value of the perturbed state.

In our example, the second column of '`sens.data`' will contain the derivative of $\eta_1(t)$ with respect to $\eta_3(t = 0)$. Drawing the second column of '`sens.data`' against the first one gives the time evolution of the sensitivity of `eta(1)` to a change in the initial value of `eta(3)`. In the same way, the jth column of '`sigma.data`' will be the derivative of $\phi_{j-1}(t)$ with respect to $\eta_3(t = 0)$.

An application of this can be to calculate the sensitivity of the model to the initial conditions and to assess the predictability of the corresponding system.

[1] For a comprehensive description of automatic sensitivity analysis, see the document http://lmd.jussieu.fr/zoom/documents.dir/sensibilite.ps .

4.1.2 Sensitivity to a pulse or a step transfer perturbation

Each transfer is associated with the element of the `dfdpi(.)` array with the same index. For example, `ff(1)` is associated with `dfdpi(1)`. If an element of the `dfdpi(.)` array is set to '`1.`' the sensitivity to a pulse (or a step) on the corresponding transfer is computed, and if it is set to '`0.`' it isn't.

For example, if `dfdpi(2)` is set to '`1.`' instead of '`0.`', mini_ker calculates the model normal trajectory and the sensitivity of all variables at every time step to an initial pulse applied to `ff(2)`. One can find in '`sens.data`' the sensitivity of all the state variables `eta(.)` to an initial pulse on `ff(2)`; and in '`sigma.data`' the sensitivity of all the transfer variables `ff(.)` to that pulse.

The choice between an impulse initial perturbation or a step is made giving a value of '`2`' (pulse) or '`3`' (step) to the variable `ko_Pert_type`.

4.1.3 Extended Sensitivity studies

The GTLS is characterized by the Jacobian matrices computed along with the system trajectory. Many different integration of extra variables can also be computed. Four standard sensitivity analyses are proposed.

A first example is the state transition matrix $\Phi(t,0)$ and its TEF complement $\Psi(t,0)$ for transfers. To obtain these matrices, one needs to set the Fortran parameter `nxp` to the value of `np` in `dimetaphi`:

```
parameter (nxp=np,nyp=0,nzp=0);
```

and to give initial values to $\Phi(0,0)$ in `ZINIT`:

```
! State transition matrix computation
! -----------------------------------
! Initial Condition Perturbation case
  ko_Pert_type = 1;

  if nxp.eq.np
  < Do ((i=1,np),j=1,nxp)< Phi_t(i,j) = 0.;>;
    <i=1,np; Phi_t(i,i) = 1. >;
  >;
```

One gets the results in two data files '`phit.data`' and '`psit.data`' where the matrices are ordered column wise, as usual. It is possible to compute a reduced number of columns `nxp < np`, in what case initial conditions corresponding to state variables to be subject to a petrurbation have to be given.

An advantage of the on line determination of the state transition matrix – compared to the use of `sltcirc` covered in Section 4.6 [Generalized linear tangent system analysis], page 35 is:

1. it can be done in double precision easily;
2. the output can be reduced using `modzout`.

For instance a determinatioin of the Lyapunov exponents needs quite a long trajectory that one does not want to output systematically.

Three matrices are available: `Phi_t(np,nxp)`, `Psi_t(mp,nxp)` and `dPsi_t(np,nxp)`, as well as `aspha(np,np)`, The logical file number from 51 to 99 are free for recording one's results.

4.1.3.1 Four different types of sensitivity

Four type of sensitivity are proposed as standard, which are selected from the value of `ko_Pert_type`. We have already seen the determination of the state transistion matrices Φ, Ψ with `ko_Pert_type=1`.

Now, the sensitivity to transfer perturbation can also be determined, corresponding to either an initial pulse or a step function, with in that case an extra option regarding the form of the response function.

- impulse perturbation : `ko_Pert_type=2;`
- step function perturbation: `ko_Pert_type=3`; $\Rightarrow$ diagonal of type $\frac{1}{1-g_{j,j}(t,0)}$;
- `ko_Pert_type=4`, same step but diagonal response of the type $\frac{g_{j,j}}{1-g_{j,j}(t,0)}$;

The mathematical explanation concerning these calculus are to be published in the future.

The results are again in the arrays `Phi_t`, `Psi_t`, with a maximum number of `nxp = mp` columns; In either of the preceding cases, one has to give the initial values for `Phi_t` in '`zinit`', give a dimension to `nxp`, and select a type of perturbation with `ko_Pert_type`.v Example:

```
! extension propagator calculus
! ------------------------------
! Transfers perturbation with initial impulsion
  ko_Pert_type = 2;

  if nxp.ge.0
  < Do ((i=1,np),j=1,nxp)< Phi_t(i,j) = 0.;>;
  >;
```

One must be aware that the option `dfdpi` also inherits of the type of perturbation selected with `ko_Pert_type`.

4.1.4 Sensitivity to a parameter

A forward sensitivity to a parameter will be computed when specified as described in Section 3.5 [Parameters], page 18. For example, suppose that the sensitivity to an initial change in the `apar` parameter of the predator model is of interest. In that case the number of parameters should be set to 1 in '`dimetaphi`':

```
parameter (lp=1);
```

The sensitivity should be turned on, but only for `apar`, as a forward parameter specified on the `Free_parameter` list:

```
Zsensib = .true.;
do i=1,np <sens(i) = 0.;>
Free_parameter: [fwd: apar];
```

The result are still in '`sens.data`' for cells and '`sigma.data`' for transfers.

4.1.5 Advance matrix sensitivity

It is possible to look at the sensitivity of the matrix of advance in states space (the matrix `aspha`) with regard with a parameter. The parameter must be counted in the parameter number and be in the parameter list flagged as the forward parameter, like in

```
Free_parameter: [fwd: apar];
```

This feature is associated with a selecting flag, '`dPi_aspha`'. One gets the result in the matrix `d_pi_aspha(.,.)` of dimension (`np`,`np`).

This matrix may be used to compute other quantities, for example it may be used to compute the sensitivity of the eigenvalues of the state-advance matrix with regard to the parameter. These additional computations have to be programmed by the user in '`zsteer`' with matrices declared and initialized in '`zinit`'. An example is given in the example '`lorhcl`'.

4.2 Adjoint model and optimisation with mini_ker

In the following a possible use of mini_ker for optimisation is discussed. More precisely the use of adjoint and control laws in mini_ker are presented. Optimisation isn't the only application of these tools, but it is the most common one. In that case the adjoint may be used to determine the gradient of a functional to perturbations in the control laws, and an optimisation process can use this information to search for the optimum. Another application of the adjoint is to compute the sensitivity of a cost function to parameters.

4.2.1 Overview of optimisation with mini_ker

In the proposed method, mini_ker is run twice, one time forward and then backward to determine the trajectory and the adjoint model. After that the control laws are modified by a program external to mini_ker. The same steps are repeated until convergence. More pecisely,

forward The command law $h(t)$ is given (by an explicit law or with a file). The trajectory is computed in a classical way, with the additionnal computation of the functional to be optimised, J, prescribed with specific `f_set` macros. The states, transfers and control laws are stored.

backward The adjoint variable is computed from the last time T backward. The time increment is reused as it could have changed during the forward simulation. The system is solved by using the same technics as in the forward simulation, but with a negative time step.

external phase
Now the command should be corrected. This step isn't covered here, but, for example, minuit the optimisation tool from the CERN could be used. In order to ease such a use of mini_ker, the principal program has to be compiled as a subroutine to be driven by an external program (see Section 3.2 [Calling the model code], page 13).

The functionnal J to be optimised is defined as

$$J = \psi[\eta(T), \varphi(T), h(T)] + \int_0^T l[\eta(\tau), \varphi(\tau), h(\tau)]\, d\tau$$

Where ψ is the final cost function, l is the integrand cost function and h represents the control laws.

The general use of the adjoint model of a system, is to determine the gradient of this functional to be optimised, J to perturbations in the system trajectory, that is, along its GTLS[2].

4.2.2 Control laws

The control laws are associated with transfers or cells, meaning that a command associated with a cell is the only command that may appear in the cell and the same is true for the command associated with a transfer. It is still possible to add a command acting anywhere by defining a transfer equal to that command.

The control laws associated with states are in the `ux_com(.)` array, control laws associated with transfers are in the `uy_com(.)` array. The control laws may be prescribed even when there is no adjoint computed, nor any optimisation, and they are used during simulation. To enable the use of command, the logical flag `Zcommand` should be `.true.`.

The command can be given either as:

1. a table of numerical values in the files '`uxcom.data`' and '`uycom.data`'.
2. a function of the problem variables. To turn that feature on the logical flag `Zlaw` should be set to `.true.` in '`zinit`'. The sequence '`zcmd_law`' should hold the code filling the `ux_com(.)` and `uy_com(.)` arrays, as the code from that sequence is used whenever the control laws are needed. In that case the files '`uxcom.data`' and '`uycom.data`' will be filled by the command values generated by the function along the trajectory.

For example in the Lotka-Volterra model, the parameter `apar` could be a control variable. In that case, `apar` would be defined as the variable `ux_com(1)`, and either entered as a law in the sequence '`zcmd_law`' , either written in the file '`uxcom.data`' step by step.

4.2.3 Cost function coding

First of all the flag `zback` should be set to `.true.` in order to allow adjoint model computation:

```
Zback=.true.;
```

The two functions `cout_Psi` corresponding with the final cost and `cout_l` corresponding with the integrand cost are set up with the `f_set` macros.

`f_set` *cout_Psi* = *f*(*eta*(.),*ff*(.),*ux_com*(.),*uy_com*(.)) [Macro]

This macro defines the final cost function. `f` is a fortran expression which may be function of cell state variables, '`eta(1)`'...'`eta(np)`', transfers '`ff(1)`'...'`ff(mp)`', state control laws '`ux_com(1)`'...'`ux_com(np)`', and transfer control laws '`uy_com(1)`'...'`uy_com(mp)`'.

`f_set` *cout_l* = *f*(*eta*(.),*ff*(.),*ux_com*(.),*uy_com*(.)) [Macro]

This macro defines the integrand cost function. `f` is a fortran expression which may be function of cell state variables, '`eta(1)`'...'`eta(np)`', transfers '`ff(1)`'...'`ff(mp)`', state control laws '`ux_com(1)`'...'`ux_com(np)`', and transfer control laws '`uy_com(1)`'...'`uy_com(mp)`'.

[2] General Tangent Linear System circulating along a trajectory.

For example, the following code sets a cost function for the masselot model:

```
! Initialisation
  F_set cout_Psi = eta_move(inode:1);
!and f_set cout_l integrand in the functionnal
  F_set cout_l = 0.;
```

In that example the functional is reduced to the final value of the first state component. Here, the adjoint vector will correspond to the final sensitivity (at $t = 0$) of that component (here the first masselot position) to a perturbation in all initial conditions[3].

The following variables are set during the backward phase, and output in the associated files:

var	**file**	**explanation**
`w_adj(.)`	'`wadj.data`'	adjoint to `eta(.)`
`v_adj(.)`	'`vadj.data`'	adjoint to `ff(.)`
`graduej(.)`	'`gradxj.data`'	adjoint to `ux_com(.)`
`gradufj(.)`	'`gradyj.data`'	adjoint to `uy_com(.)`
`hamilton`	'`hamilton.data`'	time increment, hamiltonian, cost function increment

4.2.4 Sensitivity of cost function to parameters

The sensitivity of the cost function to all the parameters given as arguments of `Free_parameters` is computed. For the predator model the sensitivity of a cost function consisting in the integral of the predator population with respect with `apar` an `cpar` is obtained with a number of parameters set to 2 in '`dimetaphi`':

```
parameter (lp=2);
```

And the cost function and `Free_parameters` list in '`zinit`':

```
f_set cout_Psi = eta(2);
f_set cout_l = eta(2);
Free_parameters: apar,cpar;
```

`apar` and `cpar` also have to be initialized. The result is outputted in '`gradpj.data`'.

4.3 Kalman filter

The Kalman filter allows for data assimilation along the model run. In that case it is assumed that there is a real model with stochastic perturbations on the states, and that noisy observations are available. The situation implemented in mini_ker corresponds with a continuous stochastic perturbation on the state and discrete noisy observations. In the TEF this leads to:

$$\begin{aligned} \partial_t \eta(t) &= g(\eta(t), \varphi(t)) + W(t)\mu \\ \varphi(t) &= f(\eta(t), \varphi(t)) \\ \omega(s) &= h(\eta(s), \varphi(s)) + \nu \end{aligned}$$

The observations ω are available at discrete time steps s. The stochastic perturbation on state, μ is characterized by a variance-covariance matrix Q and the noise on the observation,

[3] For detailed explanation of the adjoint model, see the document in pdf or .ps.gz

ν has a variance-covariance matrix R. W relates states with stochastic perturbations. At each time step the Kalman filter recomputes an estimation of the state and the variance-covariance matrix of the state.

In the following we use the example of a linear model with perturbation on state and observation of state. The model has 3 states and 3 corresponding transfers (equal to the states), but the error on the state is of dimension 2. The 3 states are observed. The corresponding equations read:

$$\begin{cases} \partial_t \eta_1 = a_{11}\eta_1 + a_{12}\varphi_2 + a_{13}\varphi_3 + W_{11}\mu_1 + W_{12}\mu_2 \\ \partial_t \eta_2 = a_{21}\varphi_1 + a_{22}\eta_2 + a_{23}\varphi_3 + W_{21}\mu_1 + W_{22}\mu_2 \\ \partial_t \eta_3 = a_{31}\varphi_1 + a_{32}\varphi_2 + a_{33}\eta_3 + W_{31}\mu_1 + W_{32}\mu_2 \end{cases}$$

$$\begin{cases} \varphi_1 = \eta_1 \\ \varphi_2 = \eta_2 \\ \varphi_3 = \eta_3 \end{cases}$$

$$\begin{cases} \omega_1 = \varphi_1 + \nu_1 \\ \omega_2 = \eta_2 + \nu_2 \\ \omega_3 = \eta_3 + \nu_3 \end{cases}$$

4.3.1 Coding the Kalman filter

First of all the Kalman filter code should be used. The observations code is also required (see Section 3.6.1 [Observations], page 19). If cmz is used the code should be selected with the select flags kalman and obs in the '`selseq.kumac`':

```
sel kalman
sel obs
```

With make the `kalman` variable should be set to 1, this will also trigger the selection of the observations:

```
kalman = 1
```

The kalman code is actually used by setting the flag `zkalman` to `.true.`, for example in the '`zinit`':

```
zkalman = .True.;
```

This will set the `zobs` and `zdata` flags to `.true.` (see Section 3.6 [Observations and data], page 19).

With the Kalman filter the dimension of estimated states, of the error on the state and of the observation, the W matrix, the observation function, the initial variance-covariance matrices on the state and the variance-covariance matrices of errors have to be given.

4.3.1.1 Kalman filter vectors dimensions

These dimensions should be set in the '`dimetaphi`' sequence. The size of the estimated states is given by the parameter `nkp`. You can set this to `np` if all the states are estimated, but in case there are some deterministic state variables, `nkp` may be less than `np`. In that case the first `nkp` elements of `eta(.)` will be estimated using the Kalman filter.

The error on state dimension is associated with the parameter `nerrp` and the size of the observations vector is `nobsp` (see Section 3.6.1 [Observations], page 19). In our example the dimensions are set with:

```
parameter (nkp=np);
parameter (nobsp=3);
parameter (nerrp=2);
```

All the states are estimated, there are 3 observation functions and the error on the state vector is of dimension 2.

4.3.1.2 Error and observation matrices

Initial variance-covariance matrix on the state

The variance-covariance on the state matrix is `covfor(.,.)`. The initial values have to be given for this matrix, as in our example:

```
covfor(1,1) = 1000.; covfor(1,2) = 10.; covfor(1,3) = 10.;
covfor(2,1) = 10.; covfor(2,2) = 5000.; covfor(2,3) = 5.;
covfor(3,1) = 10.; covfor(3,2) = 5.; covfor(3,3) = 2000.;
```

This matrix is updated by the filter at each time step because the states are pertubated by some noise, and when assimilation takes place as new information reduce the error.

Observations and error on state matrix

The matrix that relates errors on states vector components to states, corresponding with W is `mereta(.,.)`. In our example it is set by:

```
mereta(1,1) = 1.;  mereta(1,2) = 0.;
mereta(2,1) = 0.;  mereta(2,2) = 1.;
mereta(3,1) = 0.5;  mereta(3,2) = 0.5;
```

The observation functions are set by a `f_set` macro with `Obs_tef(.)` as described in Section 3.6.1 [Observations], page 19. In our example the observation functions are set by:

```
f_set Obs_tef(1) = ff(1) ;
f_set Obs_tef(2) = eta(2);
f_set Obs_tef(3) = eta(3);
```

Error variance-covariance matrices

The variance-covariance matrix on observation noise is `covobs(.,.)` set, in our example, by:

```
covobs(1,1) = 0.3; covobs(1,2) = 0.; covobs(1,3) = 0.;
covobs(2,1) = 0.; covobs(2,2) = 0.1; covobs(2,3) = 0.;
covobs(3,1) = 0.; covobs(3,2) = 0.; covobs(3,3) = 0.2;
```

The variance-covariance matrix on state noise is `coveta(.,.)` set, in our example, by:

```
coveta(1,1) = 0.2; coveta(1,2) = 0.001;
coveta(2,1) = 0.001; coveta(2,2) = 0.1;
```

These matrices are not changed during the run of the model as part of the filtering process. They may be changed by the user in '`zsteer`'.

4.3.2 Kalman filter run and output

4.3.2.1 Feeding the observations to the model

The observations must be made available to the model during the run. These observations are set in the `vobs(.)` array, and the assimilation (also called the analysis step of the filter) takes place if the logical variable `zgetobs` is `.true.` (see Section 3.6.2 [Data], page 20).

These steps are typically performed in the '`zsteer`' sequence. In this sequence there should be some code such that when there are data ready to be assimilated, `zgetobs` is set to `.true.` and the data is stored in `vobs(.)`.

4.3.2.2 Kalman filter results

The estimated states and transfers are still in the same '`.data`' files, '`res.data`' and '`tr.data`' and there is the additional file with observations, called '`obs.data`' (see Section 3.6.1 [Observations], page 19). Each time `zgetobs` is `.true.` the data, and the optimally weighted innovations are output in the file associated with data, '`data.data`' (see Section 3.6.2 [Data], page 20).

4.3.3 Executing code after the analysis

The analysis takes place before the time step advance when `zgetobs` is `.true.`. It may be usefull to add some code after the analysis and before the time step advance. For example the analysis may lead to absurd values for some states or parameters, it could be usefull to correct them in that case. The sequence included after the analysis is called '`kalsteer`'. At this point, in addition to the usual variables the following variables could be usefull:

`etafor(.)`
: The state before the analysis.

`kgain(.)` The Kalman gain.

`innobs(.)`
: The innovation vector (observations coherent with the states minus data values).

`covana(.,.)`
: The variance-covariance error matrix after the analysis.

4.4 Feedback gain

The feedback dynamic gain associated with a feedback loop can be expressed as the inverse Borel transform of the coefficient of the reduced scalar coupling matrix, $g(\tau)$, associated with a transfer. A Borel sweep provides this $g(\tau)$. Therefore it is an interesting tool for the characterization of the feedback loop[4].

As explained in the ZOOM web page document http://www.lmd.jussieu.fr/ZOOM/documents.dir/ClimSIre3.ps.gz, this allows for the calculation of the dynamic gain and factor of any feedback that goes through a unique transfer variable. An example of the conclusions that can be drawn from such an analysis is provided in the same document.

[4] More generally, the Borel sweep allows the numerical study of the dependency in τ of the Borel transform of various coefficients in the system coupling matrix.

For linear systems – whose GTLS are autonomous along the whole trajectory – the τ function of the feedback gain is independent of the position on the system trajectory. But in general it is dependant, and one can analyse the function $g(\tau; t)$ defined on a segment t of the trajectory.

The document introducing the TEF-ZOOM technique explains how a Crank-Nicolson scheme for the time discretisation symbolically gives the solution of the Borel transform of the system. One can identify the `dt` variable with the Borel τ within a factor 2. Hence, to numerically study the τ dependency of the transform of various coefficients in the system coupling matrix at one point in time, one can calculate the Borel transform of the TLS solutions by making a time-step sweep.

The function $g(\tau; t)$ is simply output for the feedback gain attached to a unique `ff(k)` transfer variable. All the relevant informations should be entered in the '`zinit`' sequence.

4.4.1 Specifying the Borel sweep

First of all the logical flag `ZBorel` should be raised:

```
ZBorel=.true.;
```

The index of the studied transfer is given in the `index_ff_gain` variable

```
index_ff_gain=7;
```

At each time step a Borel sweep may be performed. The time steps of interest are specified with three variables, one for the first step, one for the last step and one for the number of steps between two Borel sweeps:

`istep_B_deb`
: First time step for the Borel sweep.

`istep_B_fin`
: Last time step for the Borel sweep.

`istep_B_inc`
: Number of time steps between Borel sweeps.

In the following examples Borel sweeps are performed from the time step 1000 up to the time step 1200, with a sweep at each time step:

```
istep_B_deb=1000;
istep_B_fin=1200;
istep_B_inc=1;
```

For each Borel sweep, the range of the τ variable should be set. As this is a multiplicative variable the initial value, a multiplicative factor and the number of values are to be given.

`tau_B_ini`
: Initial value for τ.

`tau_B_mult`
: Multiplicative factor for sweep in *tau*.

`itau_max` Number of τ values.

For example, in the following, at each time step, the Borel transform will be computed for τ values starting at 0.2 and then multiplied a hundred times by $\sqrt{\sqrt{2}}$

```
tau_B_ini=0.2;
tau_B_mult=sqrt(sqrt(2.));
itau_max=100;
```

When the initial value of τ is set to a negative value (*i.e.* `tau_B_ini=-0.2;`), the Borel sweep will first be applied with `itau_max` negative values for `-0.2`, `tau_B_mult*(-0.2)`,..., then for the zero value, and finally for the symetric positive values, resulting in `2*itau_max+1` values for τ.

The whole example reads

```
! -------------------
! Feedback gain
! Borel
! -------------------
ZBorel=.true.;
if ZBorel
<  istep_B_deb=1000;
   istep_B_fin=1200;
   istep_B_inc=1;
;
   index_ff_gain=7;
   tau_B_ini=0.2;
   tau_B_mult=sqrt(sqrt(2.));
   itau_max=100;
   z_pr/Borel/:tau_B_mult,tau_B_ini*(tau_B_mult)**itau_max;
>;
```

Instead of using the index of the transfer in `index_ff_gain` it is possible to specify the symbolic name of the transfer, whenever the symbolic model description is used (see Section 2.3 [Symbolic model description], page 8). In that case the transfer is specified by the `zborel for` macro. For example if the transfer selected for the feedback gain computation is *b_transfer*, it can be selected with:

```
zborel for: b_transfer;
```

4.4.2 Borel sweep results

The file '`tau_Borel.data`' gives the τ values of the *tau* sweep, and the file '`gains.data`' records the feedback gain function values of $g(\tau)$, with one line for each sweep along the trajectory. In the 1.01 version, a new feature is also provided giving the poles and residuals of the Borel transform in the file '`vpgains.data`'. Consult the subroutine `Boreleig` for (not definitive) output description.

One can easily obtain the surface contours of $g(t, \tau)$ using the Fortran program provided as '`gains.f`' and its compilation shell '`gains.xqt`', that builds 2D histograms for PAW, in which one uses the '`borels.kumac`' provided kumac.

4.5 Stability analysis of fastest modes

The preceding analyses are done along with a simulation. One has also the possibility of using in a more classical fashion the state advance matrix A_{st}, after the end of the simulation. Code to perform the SVD (Singular Value Decomposition) of the state matrix

A_{st} and also of $A_{st} + A_{st}^{\dagger}$ is provided with mini_ker. The singular elements of these two matrices correspond to the most rapid modes of instability of the perturbed system.

The Singular value decomposition of a matrix is noted

$$UwV^{\dagger}$$

An executable file, '`sltc.exe`' is generated and running this file will produce the corresponding results.

4.5.1 Singular Value Decomposition with cmz

The cmz macro `smod SLTC` prepares a main program ('`circul`' of +PATCH SLTC), provided as a base for user's own analysis, in the directory '`sltc/`'.

4.5.2 Singular Value Decomposition with make

To compile the singular value decomposition executable with `make` you can do

```
make sltc.exe
```

If you want to have a separate directory for the SVD, you should copy the sequence '`dimetaphi.inc`' (or make a link to that file) to the directory. You should also copy the file '`Makefile.sltc`' from the '`template/`' directory in this directory, rename it '`Makefile`' and set the mini_ker directory path in the `miniker_dir` variable. For example, if the mini_ker directory is in '`/u/src/mini_ker`':

```
miniker_dir = /u/src/mini_ker
```

4.5.3 Singular Value Decomposition run and output

As it is, the '`sltc.exe`' executable generated by the compilation determines the SVD. This program requires '`title.tex`' (see [Title file], page 7) to transmit a title for output and graphics, and '`aspha.data`' (see Section 2.4.3 [Running a simulation and using the output], page 10) to access the state matrix. To get access to these files (in case they are not in the current directory) it is possible to make a link to the corresponding files in the model directory. Once it is done the program may be run:

```
./sltc.exe
```

The files '`u.data`', '`w.data`', and '`v.data`' holds the singular elements for A_{st} (U, w and V), and '`us.data`', '`ws.data`', and '`vs.data`' holds the singular elements of $A_{st} + A_{st}^{\dagger}$. The corresponding macros '`.kumac`' for PAW[5] are also generated.

4.6 Generalized linear tangent system analysis

The state matrix A_{st} may also be used to compute the GTLS propagator (or state transition matrix applied to perturbation), after the simulation. The algorithm is a finite product of 5th order development of $\Phi(t + \delta t, t) = \exp A_{st}\delta t$. Numerous element of analysis are given, in particular the determination of the Lyapunov exponents of the system.

An executable file, '`sltcirc.exe`' is generated and running this file will produce the corresponding results.

[5] Explanation in the research paper about SLTC (Al1 2003)

4.6.1 Generalized tangent linear system with cmz

The cmz macro `smod SLTCIRC` prepares a main program ('`circule`' of +PATCH SLTCIRC), in the directory '`sltcirc/`'.

4.6.2 Generalized tangent linear system with make

To compile the GTLS analysis executable with `make` you can do

```
make sltcirc.exe
```

If you want to have a separate directory for the GTLS analysis, you should copy the sequence '`dimetaphi.inc`' (or make a link to that file) to the directory. You should also copy the file '`Makefile.sltcirc`' from the '`template/`' directory in this directory and rename it '`Makefile`' and set the mini_ker directory path in the `miniker_dir` variable.

4.6.3 Generalized tangent linear system analysis run and output

The '`sltcirc.exe`' executable generated by the compilation computes the elements of analysis of the system. This program requires '`title.tex`' to transmit a title for output and graphics (see [Title file], page 7), '`aspha.data`' to access the state matrix and '`dres.data`', because time-step can be changed along the simulation (see Section 2.4.3 [Running a simulation and using the output], page 10)[6]. To get access to these files (in case they are not in the current directory) it is possible to make a link to the corresponding files in the model directory. Once it is done the program may be run:

```
./sltcirc.exe
```

The following table gives the correspondence between variable name, result file and ntuple number, with a short explanation:

var	**file**	**tuple**	**explanation**
`p(.,.)`	'`phit.data`'	55	propagator from 0 to t, $\Phi(t,0)$
`up(.,.)`	'`uphit.data`'	50	U in the SVD of Φ
`wp(.)`	'`wphit.data`'	51	eigen values of w in the SVD of Φ
`vp(.,.)`	'`vphit.data`'	52	V in the SVD of Φ
`wr(.)`	'`wr.data`'	53	real part of eigen values of V
`wi(.)`	'`wi.data`'	54	imaginary part of eigen values of V
`lwp(.)`	'`lwphit.data`'	67	Lyapunov exponents

[6] cf our research texts about propagator analyses in SLTC, and "les Gains sur champs (Al1 2003-2004)"

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Appendix A Installation

A.1 Programming environments

Mini_ker is not a traditionnal software in that it isn't a library or an interpreter but rather a set of source and macro file that combines with the user model code and enable to build a binary program corresponding with the model. It requires a build environment with a preprocessor, a compiler and facilities that automate these steps.

Two different environment are proposed. One use `cmz` (http://wwwcmz.web.cern.ch/wwwcmz/index.html), while the other is based on `make`. Other libraries are needed, the CERN Program Library (cernlib) and lapack.

A.2 Common requisites

Whatever method is used a fortran 77 compiler is required. The compilers that have been used so far are g77, gfortran and the sun solaris compiler.

The CERN Program Library, available at http://wwwasd.web.cern.ch/wwwasd/cernlib/, has to be installed. On windows, in case you want to use the compiler from the GNU compiler collection with cygwin or MINGW/MSYS you can use the binaries provided at http://zyao.home.cern.ch/zyao/cernlib.html. On Mac OS X, the cernlib provided by fink (package `cernlib-devel`) can be used.

You should also have LAPACK, available at http://www.netlib.org/lapack/. LAPACK can also be installed as part of the CERN Library or as part of the http://math-atlas.sourceforge.net/ implementation. On most linux distributions a lapack package is available. On Mac OS X, the ATLAS implementation provided by fink or the frameworks from Xcode can be used.

A.3 Mini_ker with cmz

First of all you have to get the cmz file '`mini_ker.cmz`' and put it in a directory. In that same directory you should create a directory for each of your models. In the model directory you should copy the file '`selseq.kumac`' available with mini_ker, and create your own cmz file for your model, called for example '`mymodel.cmz`'. You should also have installed the kumac macro files handling mortan compilation, the associated shell scripts and the mortran preprocessor.

A.4 Mini_ker with make

A.4.1 Additional requirements for Mini_ker with make

The package has been tested with GNU `make` and solaris `make`.

Suitable preprocessors should also be installed. Two preprocessors are required, one that preprocess the cmz directives, and a mortran preprocessor. A cmz directives processor written in `perl`, is distributed in the `car2txt` package available at http://www.lmd.jussieu.fr/car2txt. A `mortran` package with a command able to preprocess a mortran file given on the command line with a syntax similar with the `cpp` syntax is also required. Such a mortran is available at http://www.lmd.jussieu.fr/mortran.

A.4.2 Configuration

The package is available at http://www.lmd.jussieu.fr/ZOOM/. It is available as a compresssed tar archive. On UNIX, with GNU `tar` it may be unpacked using

```
$ tar xzvf mini_ker-1.01.00.1.tar.gz
```

The detection of the compiler, the preprocessors (car2txt and mortran), and the libraries are performed by the configure script. This script sets the apropriate variables in makefiles. It can be run with:

```
$ cd mini_ker-1.01.00.1
$ ./configure
```

If the output of `./configure` doesn't show any error it means that all the components are here. It is possible to give `./configure` switches and also specify environment variables (see also `./configure --help`):

`--with-static-cernlib`
: This command line switch forces a static linking with the cernlib (or a dynamic linking if set to no).

`--with-cernlib`
: This command line switch can be used to specify the cernlib location (if not detected or you want to use a specific cernlib).

`--with-blas`
`--with-lapack`
: With this command switch, you can specify the location of the blas and lapack libraries.

  For example, on mac OS X this can be used to specify the blas and lapack from the Apple frameworks:

```
./configure \
--with-blas=/System/Library/Frameworks/vecLib.framework/versions/A/vecLib \
--with-lapack=/System/Library/Frameworks/vecLib.framework/versions/A/vecLib
```

`F77`
`FC`
`FFLAGS`
`LDFLAGS`
: Classical compiler, compiler flags and linker flags.

`MORTRAN`
: This environment variable holds the mortran preprocessor command (default is `mortran`).

`MTNFLAGS`
: This environment variable holds command line arguments for the mortran preprocessor. It is empty in the default case.

`MTN`
: This environment variable may be used to specify the mortran executable name and/or path, it should be used by the `mortran` commmand. (default is empty, which leads to a mortran executable called `mtn`).

`MTNDEPEND`
: This environment variable may be used to specify the mortran dependencies checker executable. It should be used by the `mortran` commmand. (default is empty, which leads to a mortran dependencies checker called `mtndepend`).

After a proper configuration, if `make` is run then the example models should be build. You have to perform the configuration only once.

A.4.3 Installation with make

Mini_ker can be installed by running

```
make install
```

It should copy the sources and the '`Makefile.miniker`' file in a '`mini_ker`' directory in the `$(includedir)` directory, and copy the templates in '`$(datadir)/mini_ker`'. The default for `$(includedir)` is '`/usr/local/include`' and the default for `$(datadir)` is '`/usr/local/share`', these defaults may be changed by `./configure` switches '`--prefix`', '`--includedir`' and '`--datadir`'. See `./configure --help` and the '`INSTALL`' file for more informations. The helper script '`start_miniker`' should also be installed.

The installation is not required to use comfortably mini_ker. Indeed the only thing that changes with the sources and the '`Makefile.miniker`' directory location is the `miniker_dir` variable in a project `Makefile`.

Appendix B Cmz directives reference

The cmz directives are described together with the other features of cmz in the cmz manual at http://wwwcmz.web.cern.ch/wwwcmz/, the important ones are nevertheless recalled here, especially for those that use make and don't need the whole features of cmz.

After the description of the generic features, we turn to the cmz directive of interest. There are three kinds of cmz directives that are of use within mini_ker: one kind that introduce files, the other for conditionnal compilation and the third for sequence inclusion.

B.1 Cmz directives general syntax

The cmz directives always begin with a '`+`' in the first column, optionnaly followed by any number of '`_`' that may be used for indentation, then the directive label, case insensitive, followed by the directive arguments separated by '`,`'. The arguments are also case insensitive. Optional spaces may be around directive arguments. An optionnal '`.`' ends the directive arguments and begin a comment, everything that follows that '`.`' is ignored.

B.2 Conditional expressions

A directive argument common to all the directives is the conditionnal expression. A conditionnal expression may be true or false, it is a combination of select flags. the select flags are combined with logical operators. A select flag itself is true if it was selected. A select flag *selflag* is selected by using the `sel` *`selflag`* instruction in cmz. It is selected by passing the `-D` *`selflag`* command line switch to the call of the cmz directives preprocessor when using make.

A '`-`' negates the expression that follows. Parenthesis '`(`' and '`)`' are used for the grouping of subexpressions. '`|`' and '`,`' are for the boolean or: an expression with a or is true if the expression on the left or the expression on the right of the or is true. '`&`' is for the boolean and: an expression with an and is true if the expression on the left and the expression on the right are true.

The grouping is left to right when there is no parenthesis, with or and '`&`' having the same precedence. Therefore

```
a&b|c     ≡     (a&b)|c
a|b&c     ≡     (a|b)&c
a|b&c  is not   a|(b&c)
a&b|c  is not   a&(b|c)
```

B.3 File introduction directives

A file (or sequence) introduction directive appears at the beginning of the file. There are two different directives, one is `DECK` for normal files, the other is `KEEP` for include files (sequences). The first argument is the name of the file. The file name may not be larger than 32 characters and is converted to lower case in the general case. The optionnal following arguments may be of 2 type (and may be mixed, separated by '`,`'):

conditional
: A conditionnal is introduced by `IF=` followed by a conditionnal expression described in Section B.2 [Conditional expressions], page 44. The file is preprocessed if the conditionnal expression is true.

language specification

A language specification is introduced by a `T=`. The most common languages are '`mtn`' for the mortran, '`ftn`' for fortran not preprocessed, '`f77`' for preprocessed fortran, '`c`' for the c language and '`txt`' for text files. In general the language of the file determines the name of files the preprocessed file is extracted to, the comment style and the command for inclusions.

It is a common practice to have wrong language type in `KEEP` as the language may be determined from the `DECK` that include them with cmz, or from their file name with make. This is not recommended and considered a bad practice.

Such a directive will always appear in cmz, as it is built-in. It is recommended to have one when using make too, even though it is not required in most cases. Indeed make uses the file name directly and finds the language and file type by looking at the file extension. make should then pass the language type with a `--lang` *lang* command line switch when calling the cmz directives preprocessor. With make, the convention is to have '`cm`' added before the normal file suffix and after the '.'. The table table 3.2 shows the matching between suffixes, file type and file language.

For example, a file beginning with

```
+Deck, subroutine_foo, If=monitor&-simple, T=f77.
```

is a main preprocessed fortran file that will only be generated if '`monitor`' is selected and '`simple`' is not selected. The file to be preprocessed by make should have the '`.cmF`' suffix, and be called '`subroutine_foo.cmF`'.

A file beginning with

```
+KEEP,inc_common,If=monitor|interface,T=mtn
```

is an mortran include file that should be processed only if '`monitor`' or '`interface`' is selected. The file to be preprocessed by make should have the '`cmmti`' suffix and be called '`inc_common.cmmti`'. The resulting file when make is used will be called '`inc_common.mti`'.

B.4 Conditional directives

Conditional directives may be used to conditionnaly skip blocks of code. There are 4 conditional directives: `if`, `elseif`, `else` and `endif`. `+if` begins a conditional directives sequence, with argument a conditional expression. If the expression is true the block of code following the `+if` is outputted in the resulting file, up to another conditional directive, if it is false the code block is skipped. If the expression is false and the following conditional directive is `+elseif`, the same procedure is followed with the argument of `+elseif` which is also a conditionnal expression. More than one `+elseif` may follow a `+if`. If a `+if` or `+elseif` expression is true the following code block is outputted and all the following `+elseif` code blocks are skipped. If all the `+if` and `+elseif` expressions are false and the following coditionnal directive is `+else` then the block following the `+else` is outputted. If a previous expression was true the code block following the `+else` is skipped. The last code block is closed by `+endif`.

Conditionnal directives may be nested, a `+if` begins a deeper conditionnal sequences directives that is ended by the corresponding `+endif`.

The simplest example is:

```
     some code;
+IF,monitor
     code outputted only if monitor is true;
+ENDIF
```

If '`monitor`' is selected, the `+if` block is outputted, it leads to

```
     some code;
     code outputted only if monitor is true;
```

If '`monitor`' isn't selected the `+if` block is skipped, it leads to

```
     some code;
```

An example with `+else` may be:

```
+IF,double
 call dmysub(eta);
+ELSE
 call smysub(eta);
+ENDIF
```

If '`double`' is selected the code outputted is `call dmysub(eta);`, if '`double`' isn't selected the code outputted is `call dmysub(eta);`.

Here is a self explanatory example of use of `+elseif`:

```
+IF,monitor
  code used if monitor is selected;
+ELSEIF,kalman
  code used if kalman is selected and monitor is not;
+ELSE
  code used if kalman and monitor are not selected;
+ENDIF
```

And last an example of nested conditional directives:

```
+IF,monitor
  code used if monitor is selected;
+_IF,kalman. deep if
    code used if monitor and kalman are selected;
+_ELSE. deep else
    code used if monitor is selected and kalman is not;
+_ENDIF. end the deep conditionnals sequence
+ELSE
  code used if monitor is not selected;
+_IF,kalman
    code used if monitor is not selected but kalman is;
+_ELSE
    code used if monitor and kalman are not selected;
+_ENDIF
  other code used if monitor is not selected;
+ENDIF
```

B.5 File inclusion directive

The file (sequence) inclusion directive is `seq`. The argument of `seq` is an include files '`,`' separated list. The include files are `Keep` in cmz. The following optional arguments may be mixed:

conditional
: A conditionnal is introduced by `IF=` followed by a conditionnal expression described in Section B.2 [Conditional expressions], page 44. The directive is ignored if the conditionnal expression is false.

T=noinclude
: When this argument is present the text of the sequence will always be included in the file where the `+seq` appears.

When there is no `T=noinclude` argument, the `+seq` directive may be replaced with an inclusion command suitable for the language of the file being processed, if such command has been specified.

For example if we have the following sequence

```
+KEEP,inc,lang=C
typedef struct incstr {char* msg};
```

And the following code in the file being processed:

```
+DECK,mainf,lang=C
+SEQ,inc
int main (int argc, char* argv) { exit(0); }
```

the processing of '`mainf`' should lead to the file '`mainf.c`', containing an include command for '`inc`':

```
#include "inc.h"
int main (int argc, char* argv) { exit(0); }
```

In case the `+seq` has the `T=noinclude`:

```
+DECK,mainf,lang=C
+SEQ,inc,T=noinclude
int main (int argc, char* argv) { exit(0); }
```

The processing of '`mainf`' should lead to the file '`mainf.c`' containing the text of '`inc`':

```
typedef struct incstr {char* msg};
int main (int argc, char* argv) { exit(0); }
```

B.6 The '`self`' directive

The `self` directive is an obsolete directive that may be used for conditionnal skipping of code. For a better approach see Section B.4 [Conditional directives], page 45. The optionnal argument of `+SELF` is `If=` followed by a conditionnal expression. If the conditionnal expression is true the code following the directive is outputted, if it is false the code is skipped up to any directive (including another `+SELF`) except `+seq`.

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Version 1.2, November 2002

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